RUHR-UNIVERSITÄT BOCHUM

RUB

An introduction to numerical homogenization beyond scale separation

Patrick Henning

Ruhr-University Bochum and KTH Stockholm

6-8 October

2021 Woudschoten Conference

Outline

1. Galerkin approximations and multiscale problems.

   (what is the issue? how can we explain it [mathematically]?)

Outline

1. Galerkin approximations and multiscale problems.

   (what is the issue? how can we explain it [mathematically]?)

2. Idealized numerical homogenization and localization.

   (approaching the state of the art)

Outline

1. Galerkin approximations and multiscale problems.
   (what is the issue? how can we explain it [mathematically]?)
2. Idealized numerical homogenization and localization.
   (approaching the state of the art)
3. Survey and more advanced applications.

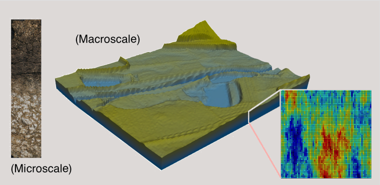
1. Galerkin approximations and multiscale problems

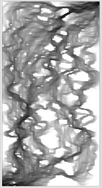
An introduction to the topic

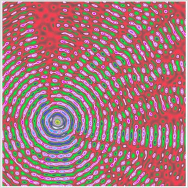
What are multiscale problems?

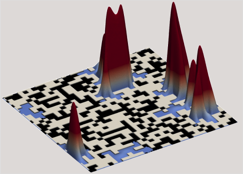
Motivation

Multiscale problems









- Hydrological simulations (groundwater).
- Two-phase flow in porous media.
- Wave propagation in heterogeneous materials.
- Anderson localization of superfluids in disorder potentials.
- ...

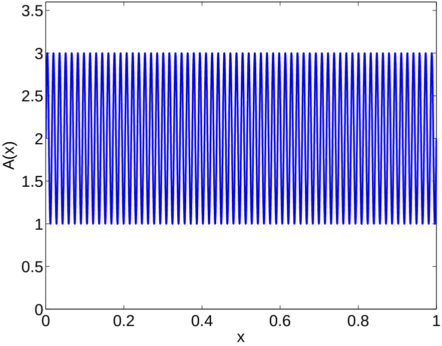
Characteristic features on multiple non-separable scales
$\Rightarrow$ standard numerical methods fail in under-resolved regimes.

Motivation: simple numerical example

Find: u with $u(0) = u(1) = 0$ and

$$-\left(A(x)\, u'(x)\right)' = 1 \quad \text{in} \quad (0,1),$$

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



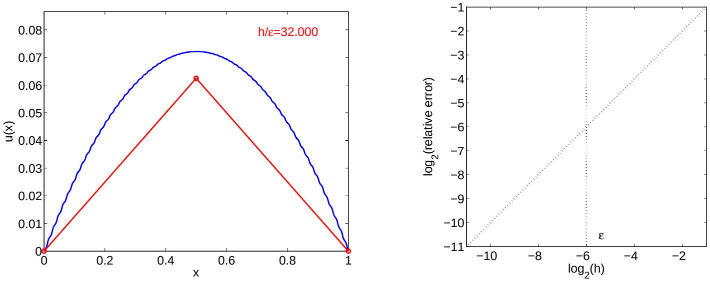
Motivation: simple numerical example

Find: u with $u(0) = u(1) = 0$ and

$$-\left(A(x)\, u'(x)\right)' = 1 \quad \text{in} \quad (0,1),$$

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

Standard $P1$-FEM estimate: $||u - u_h||_{H^1(0,1)} \lesssim h\|u\|_{H^2(0,1)}$



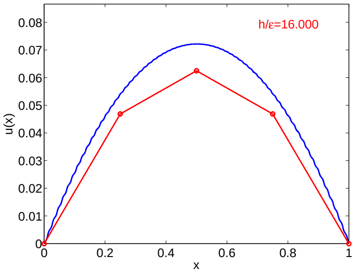
Motivation: simple numerical example

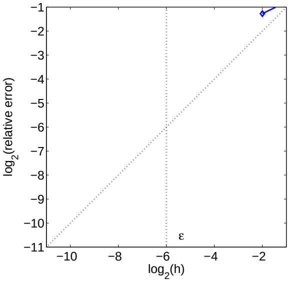
Find: u with $u(0) = u(1) = 0$ and

$$-\left(A(x)\, u'(x)\right)' = 1 \quad \text{in} \quad (0,1),$$

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

Standard $P1$-FEM estimate: $||u - u_h||_{H^1(0,1)} \lesssim h\|u\|_{H^2(0,1)}$





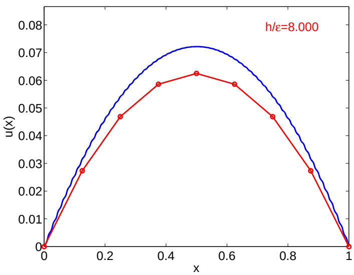
Motivation: simple numerical example

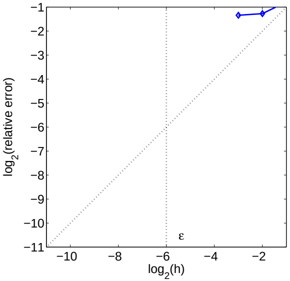
Find: u with $u(0) = u(1) = 0$ and

$$-\left(A(x)\,u'(x)\right)' = 1 \quad \text{in} \quad (0,1),$$

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

Standard $P1$-FEM estimate: $||u - u_h||_{H^1(0,1)} \lesssim h\|u\|_{H^2(0,1)}$





Motivation: simple numerical example

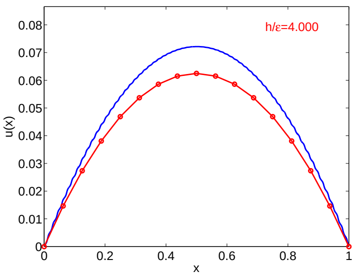
RUB

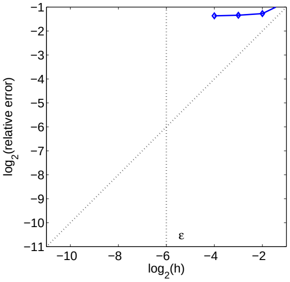
Find: u with $u(0) = u(1) = 0$ and

$$-\left(A(x)\, u'(x)\right)' = 1 \quad \text{in} \quad (0,1),$$

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

Standard $P1$-FEM estimate: $||u - u_h||_{H^1(0,1)} \lesssim h\|u\|_{H^2(0,1)}$





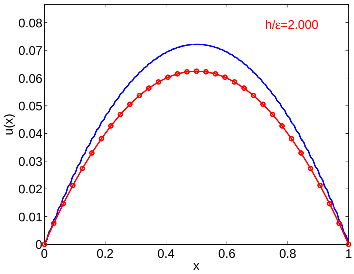
Motivation: simple numerical example

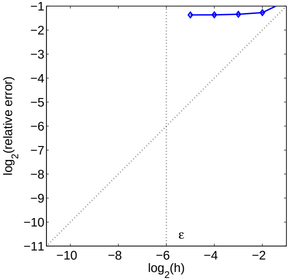
Find: u with $u(0) = u(1) = 0$ and

$$-\big(A(x)\, u'(x)\big)' = 1 \quad \text{in} \quad (0,1),$$

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

Standard $P1$-FEM estimate: $||u - u_h||_{H^1(0,1)} \lesssim h\|u\|_{H^2(0,1)}$





Motivation: simple numerical example

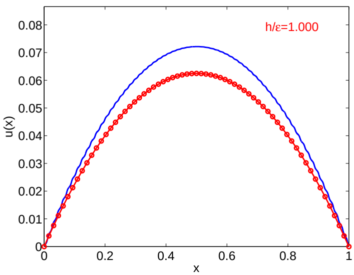
RUB

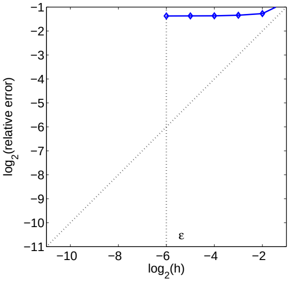
Find: u with $u(0) = u(1) = 0$ and

$$-\big(A(x)\, u'(x)\big)' = 1 \quad \text{in} \quad (0,1),$$

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

Standard $P1$-FEM estimate: $||u - u_h||_{H^1(0,1)} \lesssim h\|u\|_{H^2(0,1)}$





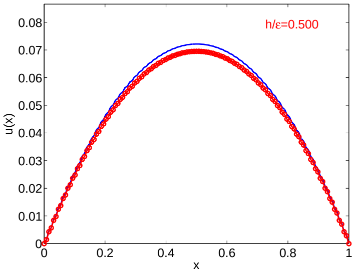
Motivation: simple numerical example

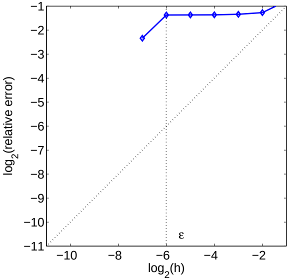
Find: u with $u(0) = u(1) = 0$ and

$$-\big(A(x)\, u'(x)\big)' = 1 \quad \text{in} \quad (0,1),$$

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

Standard $P1$-FEM estimate: $||u - u_h||_{H^1(0,1)} \lesssim h\|u\|_{H^2(0,1)}$





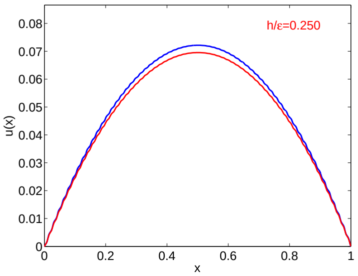
Motivation: simple numerical example

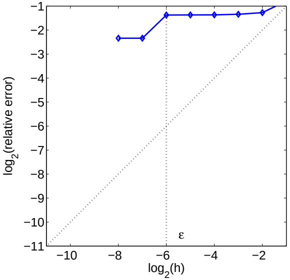
Find: u with $u(0) = u(1) = 0$ and

$$-\left(A(x)\, u'(x)\right)' = 1 \quad \text{in} \quad (0,1),$$

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

Standard $P1$-FEM estimate: $\|u - u_h\|_{H^1(0,1)} \lesssim h \|u\|_{H^2(0,1)}$





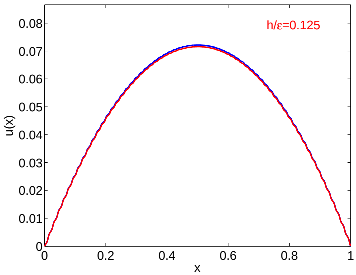
Motivation: simple numerical example

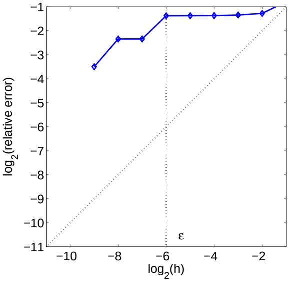
Find: u with $u(0) = u(1) = 0$ and

$$-\big(A(x)\, u'(x)\big)' = 1 \quad \text{in} \quad (0,1),$$

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

Standard $P1$-FEM estimate: $||u - u_h||_{H^1(0,1)} \lesssim h\|u\|_{H^2(0,1)}$





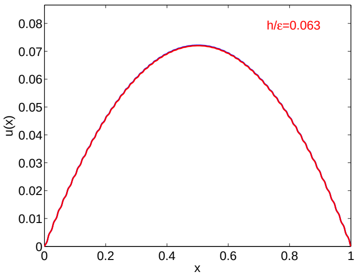
Motivation: simple numerical example

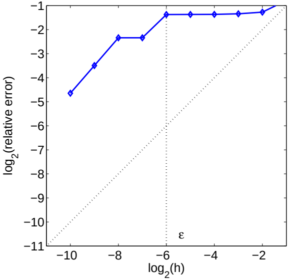
Find: u with $u(0) = u(1) = 0$ and

$$-\left(A(x)\, u'(x)\right)' = 1 \quad \text{in} \quad (0,1),$$

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

Standard $P1$-FEM estimate: $||u - u_h||_{H^1(0,1)} \lesssim h\|u\|_{H^2(0,1)}$





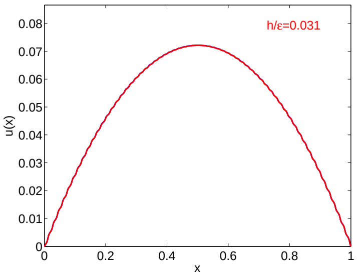
Motivation: simple numerical example

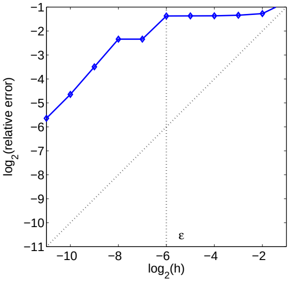
Find: u with $u(0) = u(1) = 0$ and

$$-\left(A(x)\,u'(x)\right)' = 1 \quad \text{in} \quad (0,1),$$

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

Standard $P1$-FEM estimate: $||u - u_h||_{H^1(0,1)} \lesssim h\|u\|_{H^2(0,1)}$





Problem setting and notation

Notation - Let

- $\mathcal{D} \subset \mathbb{R}^d$ bounded Lipschitz-domain ($d \in \{1, 2, 3\}$),
- $A \in L^\infty(\mathcal{D}, \mathbb{R}^{d\times d})$ multiscale coefficient
  - matrix-valued;
  - possibly non-symmetric;
  - and elliptic, i.e. there is $\alpha > 0$ so that for a.e. $x \in \mathcal{D}$

$$\alpha|\xi|^2 \leq A(x)\xi \cdot \xi \qquad \text{for all } \xi \in \mathbb{R}^d.$$

  - highly oscillatory and not smooth;
  - possibly heterogenous (no scale separation);

Elliptic model problem (multiscale)

Find $u : \mathcal{D} \to \mathbb{R}$ with $u = 0$ on $\partial\mathcal{D}$ such that

$$-\nabla \cdot (A\nabla u) = F$$

for some $F \in H^{-1}(\mathcal{D})$.

Differential operator expressed as coercive and bounded bilinear form on $H_0^1(\mathcal{D})$

$$a(u, v) = \int_{\mathcal{D}} A\nabla u \cdot \nabla v.$$

Problem in variational form:

Find $u \in H_0^1(\mathcal{D})$ such that

$$a(u, v) = \langle F, v \rangle \quad \text{for all } v \in H_0^1(\mathcal{D}).$$

Galerkin method

Find $u \in H_0^1(\mathcal{D})$ such that

$$a(u, v) = \langle F, v \rangle \quad \text{for all } v \in H_0^1(\mathcal{D}).$$

Numerical approximation?

Idea of Galerkin methods: Replace infinite dim space $H_0^1(\mathcal{D})$ by finite dim subspace $V_H \subset H_0^1(\mathcal{D})$.

Find $u_H \in V_H$ such that

$$a(u_H, v_H) = \langle F, v_H \rangle \quad \text{for all } v_H \in V_H.$$

Galerkin method

Find $u \in H_0^1(\mathcal{D})$ such that

$$a(u, v) = \langle F, v \rangle \quad \text{for all } v \in H_0^1(\mathcal{D}).$$

Find $u_H \in V_H$ such that

$$a(u_H, v_H) = \langle F, v_H \rangle \quad \text{for all } v_H \in V_H.$$

How big is the error $e_H = u - u_H$? Galerkin orthogonality

$$a(u - u_H, v_H) = 0 \quad \text{for all } v_H \in V_H,$$

implies (Céa's lemma):

$$\|u - u_H\|_{H^1(\mathcal{D})} \leq \frac{\beta}{\alpha} \inf_{v_H \in V_H} \|u - v_H\|_{H^1(\mathcal{D})},$$

i.e. u_H is always the H^1-quasi best approximation of u in V_H.

L^2-error estimates

RUB

Theorem (Aubin-Nitsche lemma)

In our setting we have

$$\|u - u_H\|_{L^2(\mathcal{D})} \le \beta \|u - u_H\|_{H^1(\mathcal{D})} \sup_{r \in L^2(\mathcal{D})\setminus\{0\}} \frac{\inf_{z_H \in V_H} \|z^{(r)} - z_H\|_{H^1(\mathcal{D})}}{\|r\|_{L^2(\mathcal{D})}},$$

where $z^{(r)} \in H^1_0(\mathcal{D})$ is the solution to the dual problem

$$a(v, z^{(r)}) = (v, r)_{L^2(\mathcal{D})} \qquad \text{for all } v \in H^1_0(\mathcal{D}).$$

For $F \in L^2(\mathcal{D})$ and $P1$-FEM, the theorem says roughly

$$\|u - u_H\|_{L^2(\mathcal{D})} \simeq \|u - u_H\|^2_{H^1(\mathcal{D})}.$$

Message:

If u_H is a poor H^1-approximation, then it is also a poor L^2-approximation.

Finite element approximations

Quantified error estimates

Galerkin method (summary)

Find $u \in H_0^1(\mathcal{D})$ such that

$$a(u, v) = \langle F, v \rangle \quad \text{for all } v \in H_0^1(\mathcal{D}).$$

Galerkin approximation in $V_H \subset H_0^1(\mathcal{D})$:

Find $u_H \in V_H$ such that

$$a(u_H, v_H) = \langle F, v_H \rangle \quad \text{for all } v_H \in V_H.$$

Abstract error estimate:

$$\|u - u_H\|_{H^1(\mathcal{D})} \leq \frac{\beta}{\alpha} \inf_{v_H \in V_H} \|u - v_H\|_{H^1(\mathcal{D})} \; = ?.$$

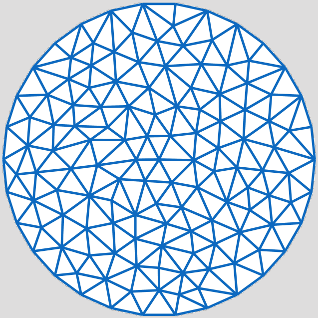
(H^1-quasi-best approximation)

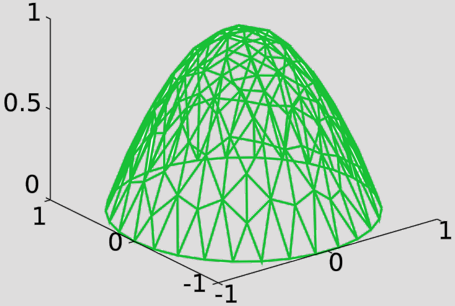
$P1$-FEM - A typical choice for V_H

Let $\mathcal{T}_H$ be a regular quasi-uniform triangulation of $\mathcal{D}$.

On the mesh $\mathcal{T}_H$ we define the $P1$ finite element space as

$$V_H := \{v \in C^0(\mathcal{D}) \cap H^1_0(\mathcal{D}) | \\ \forall K \in \mathcal{T}_H : \ v_{|K} \text{ is polynomial of degree 1}\}.$$





The L^2-projection

We consider the L^2-projection

$$P_H : H^1_0(\mathcal{D}) \to V_H.$$

It yields the L^2-best approximation and is defined by

$$(P_H(v), v_H)_{L^2(\mathcal{D})} = (v, v_H)_{L^2(\mathcal{D})} \qquad \text{for all } v_H \in V_H.$$

On quasi-uniform meshes it fulfils the estimates for all $v \in H^1_0(\mathcal{D})$

$$\|P_H(v) - v\|_{L^2} \leq CH\|v\|_{H^1} \qquad \text{and} \qquad \|P_H(v) - v\|_{H^1} \leq C\|v\|_{H^1}$$

and for all $v \in H^1_0(\mathcal{D}) \cap H^2(\mathcal{D})$:

$$\|P_H(v) - v\|_{L^2} \leq CH^2\|v\|_{H^2} \qquad \text{and} \qquad \|P_H(v) - v\|_{H^1} \leq CH\|v\|_{H^2}.$$

[Bank, Yserentant, Numer. Math. 126 (2014)]

Quantified error estimates - $H^2(\mathcal{D})$ case

RUB

Conclusion:

Let V_H be the $P1$-FEM space, then we have the error estimate

$$\|u - u_H\|_{H^1(\mathcal{D})} \leq \frac{\beta}{\alpha} \inf_{v_H \in V_H} \|u - v_H\|_{H^1(\mathcal{D})} \leq \frac{\beta}{\alpha} \|u - P_H(u)\|_{H^1(\mathcal{D})}.$$

If $u \in H^1_0(\mathcal{D}) \cap H^2(\mathcal{D})$ we have $\|u - P_H(u)\|_{H^1(\mathcal{D})} \leq C\, H \|u\|_{H^2(\mathcal{D})}$ and hence

$$\|u - u_H\|_{H^1(\mathcal{D})} \leq C\, H \|u\|_{H^2(\mathcal{D})}.$$

Quantified error estimates - $H^1(\mathcal{D})$ case

Conclusion:

Let V_H be the $P1$-FEM space, then we have the error estimate

$$\|u - u_H\|_{H^1(\mathcal{D})} \leq \frac{\beta}{\alpha} \inf_{v_H \in V_H} \|u - v_H\|_{H^1(\mathcal{D})} \leq \frac{\beta}{\alpha} \|u - P_H(u)\|_{H^1(\mathcal{D})}.$$

If only $u \in H^1_0(\mathcal{D})$ we have by density

$$\lim_{H \to 0} \|u - u_H\|_{H^1(\mathcal{D})} \leq \frac{\beta}{\alpha} \lim_{H \to 0} \inf_{v_H \in V_H} \|u - v_H\|_{H^1(\mathcal{D})} = 0.$$

But with $\|u - P_H(u)\|_{H^1(\mathcal{D})} \leq C \|u\|_{H^1(\mathcal{D})}$ and Aubin-Nitsche

$$\|u - u_H\|_{H^1} \leq C \|u\|_{H^1} \quad \text{and} \quad \|u - u_H\|_{L^2} \leq C \|u\|_{H^1}.$$

Quantified error estimates - $H^1(\mathcal{D})$ case

Observation:

If $u \in H_0^1(\mathcal{D})$ we have

$$\|u - u_H\|_{L^2} \leq C\,\|u\|_{H^1}$$

but

$$\|u - P_H(u)\|_{L^2} \leq C\,H\,\|u\|_{H^1}.$$

Contradiction?

Quantified error estimates - $H^1(\mathcal{D})$ case

Summary:

If only $u \in H^1_0(\mathcal{D})$ we have

$$\|u - u_H\|_{H^1} \leq C \, \|u\|_{H^1}$$

and if $u \in H^1_0(\mathcal{D}) \cap H^2(\mathcal{D})$

$$\|u - u_H\|_{H^1} \leq C \, H \, \|u\|_{H^2}.$$

Question:

When do we have $u \in H^2(\mathcal{D})$ and how big is $\|u\|_{H^2}$?

Regularity estimates (without proof)

Let $F \in H^{-1}(\mathcal{D})$, then

$$\|u\|_{H^1(\mathcal{D})} \leq C_{\mathcal{D}} \frac{\|F\|_{H^{-1}(\mathcal{D})}}{\alpha}.$$

- Let $F \in L^2(\mathcal{D})$;
- $\mathcal{D}$ be convex (or a $C^{1,1}$-domain);
- $A \in W^{1,\infty}(\mathcal{D}, \mathbb{R}^{d\times d})$;

then we have $u \in H^2(\mathcal{D})$ and it holds the estimate

$$\|u\|_{H^2(\mathcal{D})} \leq C_{\mathcal{D}} \frac{1}{\alpha^2} \|A\|_{W^{1,\infty}(\mathcal{D})} \|F\|_{L^2(\mathcal{D})}.$$

Effective error estimates

RUB

From

$$\|u - u_H\|_{H^1} \;\leq\; C\, H\, \|u\|_{H^2},$$

we conclude (for somme $C = C(\mathcal{D}, \alpha, \beta)$)

$$\|u - u_H\|_{H^1} \;\leq\; C \,\min\{\, H\, \|A\|_{W^{1,\infty}}\,,\, 1 \,\}\; \|F\|_{L^2}.$$

If A is multiscale and rapidly oscillating on a scale ε, then

$$\|A\|_{W^{1,\infty}} \simeq \|A'\|_{L^\infty} \simeq \varepsilon^{-1}.$$

Hence

$$\|u - u_H\|_{H^1} \;\lesssim\; C \,\min\{\, \frac{H}{\varepsilon}\,,\, 1 \,\}.$$

Consequently, we have only linear convergence of $H < \varepsilon$.

Effective error estimates - Conclusion

If A is a (realistic) multiscale coefficient, then either

$$u \notin H^2(\mathcal{D}) \qquad \text{(if } A \text{ is discontinuous)}$$

or

$$\|u - u_H\|_{H^1} \lesssim C \min\{\frac{H}{\varepsilon}, 1\}.$$

Hence

Galerkin approximations u_H are not reliable for coarse mesh sizes H.

"Paradox": even in worst case scenarios we always have:

$$\inf_{v_H \in V_H} \|u - v_H\|_{L^2} \leq CH \|F\|_{H^{-1}(\mathcal{D})}.$$

Effective error estimates - Conclusion

If A is a (realistic) multiscale coefficient, then either

$$u \notin H^2(\mathcal{D}) \qquad \text{(if } A \text{ is discontinuous)}$$

or

$$\|u - u_H\|_{H^1} \lesssim C \min\{\frac{H}{\varepsilon}, 1\}.$$

We need at least

$$H < \varepsilon,$$

hence, the space V_H needs to have a dimension of at least

$$\dim V_H = \mathcal{O}(H^{-d}) \gtrsim \mathcal{O}(\varepsilon^{-d}).$$

Can exceed computation powers of available computers!

Finite elements and multiscale problems

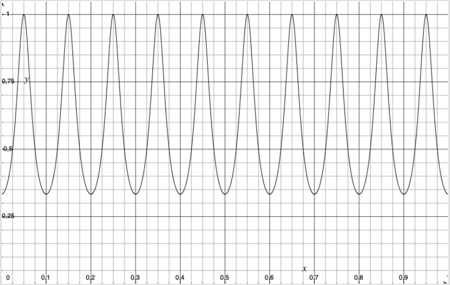
Another numerical experiment

Model problem in $1d$

Consider $\mathcal{D} = (0,1)$ and $F \equiv 1$

and the multiscale coefficient for very small $0 < \varepsilon \ll 1$:

$$A^{\varepsilon}(x) = \left(2 + \cos(2\pi \frac{x}{\varepsilon})\right)^{-1}.$$



Model problem in $1d$

Exact solution (multiscale structure):

$$u^\varepsilon(x) = (1-x)x + \varepsilon\, u_1(x, \frac{x}{\varepsilon}) + \varepsilon^2\, u_2(\frac{x}{\varepsilon})$$

Macroscopic behavior - coarsest level:

$$u_0(x) = (1-x)x.$$

- can be well-approximated in coarse V_H:

$$\inf_{v_H \in V_H} \|u_0 - v_H\|_{L^2} \leq CH^2 \quad \text{and} \quad \inf_{v_H \in V_H} \|u_0 - v_H\|_{H^1} \leq CH.$$

Microscopic behavior - hierarchical fine levels:

$$\varepsilon u_1(x, \frac{x}{\varepsilon}) = \frac{\varepsilon}{2\pi} \sin(2\pi \frac{x}{\varepsilon}) \left(\frac{1}{2} - x\right) \quad \text{and} \quad \varepsilon^2\, u_2(\frac{x}{\varepsilon}) = \frac{\varepsilon^2}{4\pi^2} \left(1 - \cos(2\pi \frac{x}{\varepsilon})\right)$$

- hardly visible $L^2(\mathcal{D})$; important contribution in $H^1(\mathcal{D})$;
- rapidly oscillating (period ε); cannot be captured in coarse V_H;

Model problem in $1d$ - $P1$-FEM

RUB

We solve the problem with $P1$-FEM in V_H and for $\varepsilon = 2^{-7} = 0.0078125$.

- Note: when assembling the integrals in the system matrix, we use a quadrature rule of order 18 (to capture the oscillations).

H^1-error estimates: Since

$$(A^\varepsilon)'(x) = \frac{2\pi}{\varepsilon}\left(2 + \cos(2\pi\frac{x}{\varepsilon})\right)^{-2} \sin(2\pi\frac{x}{\varepsilon}),$$

we have

$$\|A^\varepsilon\|_{W^{1,\infty}} = \|(A^\varepsilon)'\|_{L^\infty} = \mathcal{O}(\varepsilon^{-1}).$$

The previously derived H^1-estimate becomes in this case

$$\begin{aligned} \|u^\varepsilon - u_H\|_{H^1} &\leq C \min\{ H \|A^\varepsilon\|_{W^{1,\infty}} , 1 \} \|F\|_{L^2} \\ &\simeq C \min\{ \frac{H}{\varepsilon} , 1 \}. \end{aligned}$$

Model problem - L^2- and H^1-error estimates

H^1-error estimate:

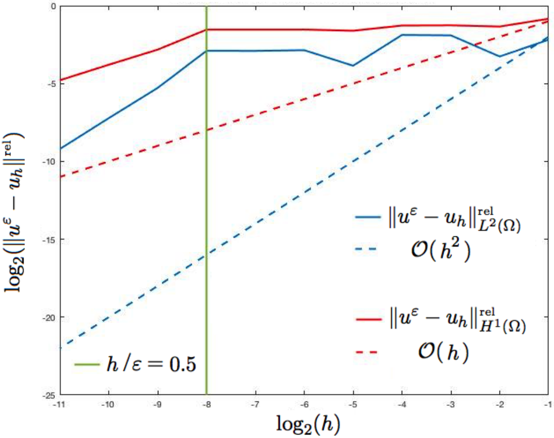
$$\|u^\varepsilon - u_H\|_{H^1} \leq C \begin{cases} \frac{H}{\varepsilon} & \text{if } H < \varepsilon \\ 1 & \text{if } H \geq \varepsilon. \end{cases}$$

L^2-error estimate:

$$\|u^\varepsilon - u_H\|_{L^2} \leq C \begin{cases} \left(\frac{H}{\varepsilon}\right)^2 & \text{if } H < \varepsilon \\ 1 & \text{if } H \geq \varepsilon. \end{cases}$$

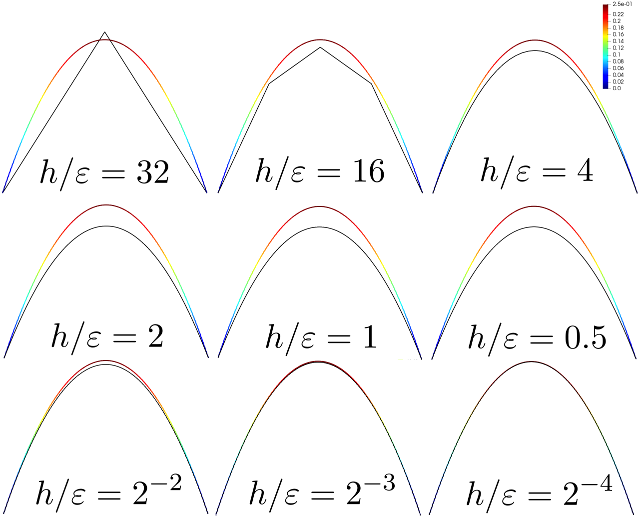
Asymptotic vs. pre-asymptotic regime!

Model problem in $1d$



Relative L^2- and H^1-errors for the model problem solved with Galerkin $P1$-FEM and for various mesh sizes $H = h$.

Model problem in $1d$ - comparison plots u_H vs u^ε



Model problem in $1d$ - Conclusions

- There is a clearly visible pre-asymptotic regime (for $H \geq \varepsilon$).
- In the asymptotic regime (for $H < \varepsilon$) all errors show the expected convergence rates.
- In the pre-asymptotic regime, we observe (visually) a false convergence, i.e. it looks as if the numerical solutions u_H approach a converged state. !!!
- This "false state" is the solution obtained by replacing A^ε by its arithmetic average.
- Note: the correct coarse part u_0 is obtained by replacing A^ε by the harmonic average.

Disclaimer

There is a vast literature on different approaches for tackling multiscale problems.

A (biased) list of important examples contains (in alphabetic order):

- Approximate Component Mode Synthesis,
  Hetmaniuk, Lehoucq, Klawonn, Rheinbach ...
- Classical Multiscale Finite Element Method (MsFEM),
  Efendiev, Hou, Le Bris, Legoll, Wu ...
- Generalized MsFEM (GMsFEM), Chung, Efendiev, Hou, ...
- Heterogenous Multiscale Method (HMM), Abdulle, E, Engquist, Ohlberger, ...
- Localized Orthogonal Decomposition (LOD), Henning, Målqvist, Peterseim, ...
- Operator-adapted wavelets (gamblets), Owhadi, Scovel, ...
- Optimal local subspaces, Babuska, Lipton, Patera, Scheichl, Smetana, ...
- Rough polyharmonic splines, Owhadi, Zhang, ...

In the following we only follow one of the paths.

2. Idealized numerical homogenization of ellliptic multiscale problems

Back to the general problem

We follow a special case of the general framework described in:

R. Altmann, P. Henning and D. Peterseim.
Numerical homogenization beyond scale separation.
Acta Numerica, 30:1–86, 2021.

Reminder

For realistic (discontinuous) multiscale coefficients A, we typically have $u \notin H^2(\mathcal{D})$ and

$$\|u - u_H\|_{L^2} \lesssim C \min\{ \left(\frac{H}{\varepsilon}\right)^{\delta}, 1 \} \|F\|_{L^2(\mathcal{D})} \quad \text{for some } 0 < \delta \ll 2.$$

- "Paradox": even in worst case scenarios we always have:

$$\inf_{v_H \in V_H} \|u - v_H\|_{L^2} \leq CH\|F\|_{H^{-1}(\mathcal{D})}.$$

- But: Galerkin methods in V_H fail to find these approximations, because they aim for H^1-quasi best approximations.
- Since the variations of u are invisible (unresolved) in V_H, a H^1-quasi best approximation is a meaningless function.
- Question: Is it possible to formulate a variational method that yields the L^2-best approximation?

Corrector Green's Operators

An equation for the L^2-projection

Analytical setting

RUB

Recall the setting:

- $\mathcal{D} \subset \mathbb{R}^d$ bounded Lipschitz domain;
- $F \in H^{-1}(\mathcal{D})$;
- differential operator

$$a(u, v) = \int_{\mathcal{D}} A\nabla u \cdot \nabla v,$$

  is a coercive and bounded on $H_0^1(\mathcal{D})$
- Find $u \in H_0^1(\mathcal{D})$ with $a(u, v) = \langle F, v\rangle$ for all $v \in H_0^1(\mathcal{D})$.
- A is multiscale and admits no regularity.

Discrete setting

RUB

Recall the setting:

- $\mathcal{T}_H$ is a regular and quasi-uniform triangulation of $\mathcal{D}$;
- $V_H \subset H_0^1(\mathcal{D})$ is corresponding $P1$-FEM space on $\mathcal{T}_H$;
- H is the mesh size (max diameter of $\mathcal{T}_H$-elements),

---

- L^2-projection $P_H : H_0^1(\mathcal{D}) \to V_H$ (L^2-best approx.), i.e.

$$(P_H(u), v_H)_{L^2(\mathcal{D})} = (u, v_H)_{L^2(\mathcal{D})} \qquad \text{for all } v_H \in V_H.$$

- Note: the L^2-projection on V_H is H^1-stable (in this case):

$$\|P_H(v)\|_{H^1(\mathcal{D})} \leq C\|v\|_{H^1(\mathcal{D})} \qquad \text{for all } v \in H_0^1(\mathcal{D}).$$

(with C independent of H)

Goal

RUB

The space V_H defines a coarse scale of our problem.

The best-coarse scale approximation (in the L^2-sense) to the exact solution u is $P_H(u) \in V_H$.

Goal: Construct a homogenized differential operator $a_0(\cdot, \cdot)$, so that the unique solution $u_H \in V_H$ with

$$a_0(u_H, v_H) = \langle F_0, v_H \rangle \qquad \text{for all } v_H \in V_H$$

just gives the L^2-best coarse scale approximation, i.e.

$$u_H = P_H(u).$$

Recall: $\|P_H(u) - u\|_{L^2(\mathcal{D})} \leq CH\|F\|_{H^{-1}(\mathcal{D})}$.

Corrector Green's Operator Theory

Corrector Green's Operator Theory

Consider the (exact) fine-scale problem:

$$a(u, v) = \langle F, v \rangle \qquad \text{for all } v \in H_0^1(\mathcal{D}).$$

Goal: express u explicitly in terms of its coarse part $\mathcal{P}_H(u)$ and the data A and F.

Tool: Corrector Green's Operators.

Definition: Corrector Green's Operator

RUB

We define the kernel of the L^2-projection $\mathcal{P}_H$ by

$$W := \{w \in H_0^1(\mathcal{D}) | \ \mathcal{P}_H(w) = 0\}.$$

With this, the Corrector Green's Operator

$$\mathcal{G} : H^{-1}(\mathcal{D}) \to W$$

with $\mathcal{G}(\mathcal{F}) \in W$ for $\mathcal{F} \in H^{-1}(\mathcal{D})$ is given by

$$a(\mathcal{G}(\mathcal{F}), w) = \langle \mathcal{F}, w \rangle \qquad \text{for all } w \in W.$$

The image of dual operator $\mathcal{G}^*$ is given by

$$a(w, \mathcal{G}^*(\mathcal{F})) = \langle \mathcal{F}, w \rangle \qquad \text{for all } w \in W.$$

Corrector Green's Operator

RUB

Note:

$$W := \{w \in H_0^1(\mathcal{D})|\ \mathcal{P}_H(w) = 0\}$$

is a closed subspace, because it is the kernel of a linear, H^1-continuous operator.

Hence, the Corrector Green's Operator $\mathcal{G} : H^{-1}(\mathcal{D}) \to W$ with

$$\mathcal{G}(\mathcal{F}) \in W : \qquad a(\mathcal{G}(\mathcal{F}), w) = \langle \mathcal{F}, w \rangle \qquad \text{for all } w \in W$$

is well-defined by the Lax-Milgram theorem.

Corrector Green's Operator Theory

With $W := \{w \in H_0^1(\mathcal{D}) | \mathcal{P}_H(w) = 0\}$, $\mathcal{G}(\mathcal{F}) \in W$ solves

$$a(\mathcal{G}(\mathcal{F}), w) = \langle \mathcal{F}, w \rangle \qquad \text{for all } w \in W.$$

The following representation of $u \in H_0^1(\mathcal{D})$ holds true.

Lemma (Representation of exact solution)

With $\mathcal{A} := -\nabla \cdot (A\nabla\, \cdot)$ (in the sense of distributions) it holds

$$u = u_H - (\mathcal{G} \circ \mathcal{A})u_H + \mathcal{G}(F),$$

where $u_H \in V_H$ is the L^2-projection of u in the coarse space, i.e.

$$u_H := \mathcal{P}_H(u).$$

Proof of Representation of fine-scale solution

Since $\mathcal{P}_H : H_0^1(\mathcal{D}) \to V_H$ is a projection, we can write

$$u \in H_0^1(\mathcal{D}) = V_H \oplus W$$

uniquely as

$$u = u_H + u_{\mathrm{f}}, \qquad \text{where } u_H := \mathcal{P}_H(u) \text{ and } u_{\mathrm{f}} := u - \mathcal{P}_H(u) \in W.$$

By definition we have

$$a(u_H + u_{\mathrm{f}}, w) = \langle F, w \rangle \qquad \text{for all } w \in W.$$

Together with the definition of $\mathcal{G}$ (and $\mathcal{A}(u_H) = a(u_H, \cdot)$) we have

$$a(u_{\mathrm{f}}, w) = \langle F - \mathcal{A}(u_H), w \rangle = a(\mathcal{G}(F) - (\mathcal{G} \circ \mathcal{A})(u_H), w).$$

Since $u_{\mathrm{f}} \in W$ and $\mathcal{G}(F) - (\mathcal{G} \circ \mathcal{A})(u_H) \in W$, we conclude

$$u_{\mathrm{f}} = \mathcal{G}(F) - (\mathcal{G} \circ \mathcal{A})(u_H),$$

which finishes the proof. □

Proof of Representation of fine-scale solution

Since $\mathcal{P}_H : H_0^1(\mathcal{D}) \to V_H$ is a projection, we can write

$$u \in H_0^1(\mathcal{D}) = V_H \oplus W$$

uniquely as

$$u = u_H + u_{\mathrm{f}}, \qquad \text{where } u_H := \mathcal{P}_H(u) \text{ and } u_{\mathrm{f}} := u - \mathcal{P}_H(u) \in W.$$

By definition we have

$$a(u_H + u_{\mathrm{f}}, w) = \langle F, w \rangle \qquad \text{for all } w \in W.$$

Together with the definition of $\mathcal{G}$ (and $\mathcal{A}(u_H) = a(u_H, \cdot)$) we have

$$a(u_{\mathrm{f}}, w) = \langle F - \mathcal{A}(u_H), w \rangle = a(\mathcal{G}(F) - (\mathcal{G} \circ \mathcal{A})(u_H), w).$$

Since $u_{\mathrm{f}} \in W$ and $\mathcal{G}(F) - (\mathcal{G} \circ \mathcal{A})(u_H) \in W$, we conclude

$$u_{\mathrm{f}} = \mathcal{G}(F) - (\mathcal{G} \circ \mathcal{A})(u_H),$$

which finishes the proof. $\square$

Proof of Representation of fine-scale solution

Since $\mathcal{P}_H : H_0^1(\mathcal{D}) \to V_H$ is a projection, we can write

$$u \in H_0^1(\mathcal{D}) = V_H \oplus W$$

uniquely as

$$u = u_H + u_{\mathrm{f}}, \qquad \text{where } u_H := \mathcal{P}_H(u) \text{ and } u_{\mathrm{f}} := u - \mathcal{P}_H(u) \in W.$$

By definition we have

$$a(u_H + u_{\mathrm{f}}, w) = \langle F, w \rangle \qquad \text{for all } w \in W.$$

Together with the definition of $\mathcal{G}$ (and $\mathcal{A}(u_H) = a(u_H, \cdot)$) we have

$$a(u_{\mathrm{f}}, w) = \langle F - \mathcal{A}(u_H), w \rangle = a(\mathcal{G}(F) - (\mathcal{G} \circ \mathcal{A})(u_H), w).$$

Since $u_{\mathrm{f}} \in W$ and $\mathcal{G}(F) - (\mathcal{G} \circ \mathcal{A})(u_H) \in W$, we conclude

$$u_{\mathrm{f}} = \mathcal{G}(F) - (\mathcal{G} \circ \mathcal{A})(u_H),$$

which finishes the proof. □

Proof of Representation of fine-scale solution

Since $\mathcal{P}_H : H_0^1(\mathcal{D}) \to V_H$ is a projection, we can write

$$u \in H_0^1(\mathcal{D}) = V_H \oplus W$$

uniquely as

$$u = u_H + u_{\mathrm{f}}, \qquad \text{where } u_H := \mathcal{P}_H(u) \text{ and } u_{\mathrm{f}} := u - \mathcal{P}_H(u) \in W.$$

By definition we have

$$a(u, w) = \langle F, w \rangle \qquad \text{for all } w \in W.$$

Together with the definition of $\mathcal{G}$ (and $\mathcal{A}(u_H) = a(u_H, \cdot)$) we have

$$a(u_{\mathrm{f}}, w) = \langle F - \mathcal{A}(u_H), w \rangle = a(\mathcal{G}(F) - (\mathcal{G} \circ \mathcal{A})(u_H), w).$$

Since $u_{\mathrm{f}} \in W$ and $\mathcal{G}(F) - (\mathcal{G} \circ \mathcal{A})(u_H) \in W$, we conclude

$$u_{\mathrm{f}} = \mathcal{G}(F) - (\mathcal{G} \circ \mathcal{A})(u_H),$$

which finishes the proof. $\square$

Representation: $u = u_H - (\mathcal{G} \circ \mathcal{A}) u_H + \mathcal{G}(F)$

We define the corrector operator $\mathcal{C} : V_H \to W$ as

$$\mathcal{C} := -(\mathcal{G} \circ \mathcal{A}).$$

Let $v_H \in V_H$. Observe that $\mathcal{C}(v_H) \in W$ solves

$$\begin{aligned} a(\mathcal{C}(v_H), w) &= -a((\mathcal{G} \circ \mathcal{A}) v_H, w) = -\langle \mathcal{A} v_H, w \rangle \\ &= -a(v_H, w) \end{aligned}$$

for all $w \in W$. Hence, $\mathcal{C}(v_H) \in W$ solves

$$a(v_H + \mathcal{C}(v_H), w) = 0 \qquad \text{for all } w \in W.$$

Note similarity to homogenization theory!

Corrector Green's Operator Theory

RUB

Plug representation $u = (\mathrm{I} + \mathcal{C})u_H + \mathcal{G}(F)$ into problem formulation and test only with coarse functions $v_H \in V_H$:

Lemma

The (coarse) L^2-projection $u_H = \mathcal{P}_H(u) \in V_H$ can be characterized as the solution to the coarse scale problem

$$a((\mathrm{I} + \mathcal{C})u_H, v_H) = \langle F, v_H \rangle - a(\mathcal{G}(F), v_H) \qquad \text{for all } v_H \in V_H.$$

As a matter of fact:

$$\begin{aligned}\|u - u_H\|_{L^2(\mathcal{D})} &= \|u - \mathcal{P}_H(u)\|_{L^2(\mathcal{D})} \\ &\leq CH\|\nabla u\|_{L^2(\mathcal{D})} \leq CH\alpha^{-1}\|F\|_{H^{-1}(\mathcal{D})}.\end{aligned}$$

Corrector Green's Operator Theory

RUB

We have

$$a((\mathrm{I}+\mathcal{C})u_H, v_H) = \langle F, v_H\rangle - a(\mathcal{G}(F), v_H) \qquad \text{for all } v_H \in V_H.$$

Next step: reformulate coarse-scale equation in more convenient way.

1. Observe that for any $v_H \in V_H$ we have

$$a(\mathcal{G}(F), v_H) = -a(\mathcal{G}(F), \mathcal{C}^*(v_H)) = -\langle F, \mathcal{C}^*(v_H)\rangle, \qquad (*)$$

with $\mathcal{C}^*(v_H) \in W$ given by

$$a(w, \mathcal{C}^* v_H) = -a(w, v_H) \qquad \text{for all } w \in W.$$

2. It obviously holds

$$a((\mathrm{I}+\mathcal{C})u_H, v_H) = a(u_H, (\mathrm{I}+\mathcal{C}^*)v_H), \qquad (**)$$

From **$(*)$** and **$(**)$** we have

$$a(u_H, (\mathrm{I}+\mathcal{C}^*)v_H) = \langle F, (\mathrm{I}+\mathcal{C}^*)v_H\rangle \qquad \text{for all } v_H \in V_H.$$

Corrector Green's Operator Theory

We have seen $u_H = \mathcal{P}_H(u) \in V_H$ solves

$$a((\mathrm{I} + \mathcal{C})u_H, v_H) = \langle F, v_H \rangle - a(\mathcal{G}(F), v_H) \qquad \text{for all } v_H \in V_H$$

but also

$$a(u_H, (\mathrm{I} + \mathcal{C}^*)v_H) = \langle F, (\mathrm{I} + \mathcal{C}^*)v_H \rangle \qquad \text{for all } v_H \in V_H.$$

We define

$$V_H^{\mathrm{ms},*} := \{(\mathrm{I} + \mathcal{C}^*)v_H | \; v_H \in V_H\}$$

and obtain

$$a(u_H, v_H^{\mathrm{ms}}) = \langle F, v_H^{\mathrm{ms}} \rangle \qquad \text{for all } v_H^{\mathrm{ms}} \in V_H^{\mathrm{ms},*}.$$

Hence:

Petrov-Galerkin characterisation of the L^2-projection

RUB

Theorem (Multiscale Finite Element Method 1)

Let $u_H \in V_H$ denote the coarse interpolation of u into V_H, then it is a solution to the Petrov-Galerkin problem

$$a(u_H, v_H^{\mathrm{ms}}) = \langle F, v_H^{\mathrm{ms}} \rangle \qquad \text{for all } v_H^{\mathrm{ms}} \in V_H^{\mathrm{ms},*},$$

where

$$V_H^{\mathrm{ms},*} := \{(\mathrm{I} + \mathcal{C}^*)v_H |\, v_H \in V_H\}.$$

By the properties of $\mathcal{P}_H$ it holds

$$\|u - u_H\|_{L^2(\mathcal{D})} \leq C H \alpha^{-1} \|F\|_{H^{-1}(\mathcal{D})}.$$

Corrector Green's Operator Theory

What if we want more,

i.e. a H^1-approximation?

Corrector Green's Operator Theory

RUB

It holds for all $w \in W$

$$a(w, \mathcal{C}^* v_H) = -a(w, v_H).$$

Hence, with $w = \mathcal{C} u_H$ we have

$$a(\mathcal{C} u_H, v_H + \mathcal{C}^* v_H) = 0.$$

We conclude that $u_H \in V_H$ is also solution to

$$a((\mathrm{I} + \mathcal{C}) u_H, (\mathrm{I} + \mathcal{C}^*) v_H) = a(u_H, (\mathrm{I} + \mathcal{C}^*) v_H).$$

Recalling that $u = u_H + \mathcal{C} u_H + \mathcal{G}(F)$, we summarize the results in the following corollary.

Corollary (Multiscale Finite Element Method 2)

Let

$$V_H^{\mathrm{ms}} := \{ v_H + \mathcal{C}\ v_H |\ v_H \in V_H \} \qquad \text{and}$$
$$V_H^{\mathrm{ms},*} := \{ v_H + \mathcal{C}^* v_H |\ v_H \in V_H \}.$$

Then there exists $u_H^{\mathrm{ms}} \in V_H^{\mathrm{ms}}$ with

$$a(u_H^{\mathrm{ms}}, v_H^{\mathrm{ms}}) = \langle F, v_H^{\mathrm{ms}} \rangle \qquad v_H^{\mathrm{ms}} \in V_H^{\mathrm{ms},*}.$$

Furthermore, it holds

$$u_H^{\mathrm{ms}} = u_H + \mathcal{C} u_H \qquad \text{and} \qquad u - u_H^{\mathrm{ms}} = \mathcal{G}(F),$$

where $u_H \in V_H$ is given by $u_H = \mathcal{P}_H(u)$.

Corrector error estimate

Solving for $u_H^{\mathrm{ms}} \in V_H^{\mathrm{ms}}$ with

$$a(u_H^{\mathrm{ms}}, v_H^{\mathrm{ms}}) = \langle F, v_H^{\mathrm{ms}} \rangle \qquad v_H^{\mathrm{ms}} \in V_H^{\mathrm{ms},*}$$

we obtain a coarse scale solution plus a fine scale corrector $\mathcal{C} u_H$, i.e.

$$u_H^{\mathrm{ms}} = u_H + \mathcal{C} u_H \qquad \text{and} \qquad u - u_H^{\mathrm{ms}} = \mathcal{G}(F).$$

Improved estimates?

Corrector error estimate - $F \in H^{-1}(\mathcal{D})$

We saw the error is precisely given by

$$u - u_H^{\mathrm{ms}} = \mathcal{G}(F).$$

Since $\mathcal{G}(F) \in W$ (i.e. $\mathcal{P}_H(\mathcal{G}(F)) = 0$) we have the L^2-error estimate

$$\begin{aligned} \|u - u_H^{\mathrm{ms}}\|_{L^2(\mathcal{D})} &= \|\mathcal{G}(F)\|_{L^2(\mathcal{D})} \\ &= \|\mathcal{G}(F) - \mathcal{P}_H(\mathcal{G}(F))\|_{L^2(\mathcal{D})} \\ &\leq CH\|\mathcal{G}(F)\|_{H^1(\mathcal{D})} \\ &\leq CH\|F\|_{H^{-1}(\mathcal{D})}. \end{aligned}$$

This is the best we can expect for $F \in H^{-1}(\mathcal{D})$.

Corrector error estimate - $F \in L^2(\mathcal{D})$ or more

RUB

$$\text{error} = u - u_H^{\mathrm{ms}} = \mathcal{G}(F).$$

Let $F = f \in L^2(\mathcal{D})$ $(s = 0)$ or
$F = f \in H_0^1(\mathcal{D}) \cap H^s(\mathcal{D})$ (for $s \in \{1,2\}$)
we have (by definition of $\mathcal{G}$):

$$\begin{aligned}
\alpha \|\nabla \mathcal{G}(f)\|_{L^2(\mathcal{D})}^2 &\leq a(\mathcal{G}(f), \mathcal{G}(f)) = (f, \mathcal{G}(f))_{L^2(\mathcal{D})} \\
&= (f, \mathcal{G}(f) - \mathcal{P}_H(\mathcal{G}(f)))_{L^2(\mathcal{D})} \\
&= (f - \mathcal{P}_H(f), \mathcal{G}(f) - \mathcal{P}_H(\mathcal{G}(f)))_{L^2(\mathcal{D})} \\
&\leq C H^{s+1} \|f\|_{H^s(\mathcal{D})} \|\nabla \mathcal{G}(f)\|_{L^2(\mathcal{D})}.
\end{aligned}$$

Dividing by $\|\nabla \mathcal{G}(f)\|_{L^2(\mathcal{D})}$ yields

$$\|\nabla \mathcal{G}(f)\|_{L^2(\mathcal{D})} \leq C H^{s+1} \alpha^{-1} \|f\|_{H^s(\mathcal{D})}$$

and again with $\mathcal{P}_H(\mathcal{G}(f)) = 0$

$$\|\mathcal{G}(f)\|_{L^2(\mathcal{D})} \leq C H \|\nabla \mathcal{G}(f)\|_{L^2(\mathcal{D})} \leq C H^{s+2} \alpha^{-1} \|f\|_{H^s(\mathcal{D})}.$$

Corrector error estimate

RUB

Summary for multiscale approx.

$$u_H^{\mathrm{ms}} = u_H + \mathcal{C} u_H.$$

If

- $F \in H^s(\mathcal{D})$ for $s \in \{-1, 0, 1, 2\}$ and
- $F \in H_0^1(\mathcal{D})$ **if** $s \in \{1, 2\}$,

we have

$$\|u - u_H^{\mathrm{ms}}\|_{L^2(\mathcal{D})} + H\|u - u_H^{\mathrm{ms}}\|_{H^1(\mathcal{D})} \leq C H^{s+2} \|F\|_{H^s(\mathcal{D})}.$$

and

$$\|u - u_H\|_{L^2(\mathcal{D})} \leq C H \|F\|_{H^{-1}(\mathcal{D})}.$$

From Petrov-Galerkin to Galerkin

Petrov-Galerkin form: find $u_H^{\mathrm{ms}} \in V_H^{\mathrm{ms}}$ with

$$a(u_H^{\mathrm{ms}}, v_H^{\mathrm{ms}}) = (f, v_H^{\mathrm{ms}})_{L^2(\mathcal{D})} \qquad \text{for all } v_H^{\mathrm{ms}} \in V_H^{\mathrm{ms},*},$$

If $a(\cdot,\cdot)$ is symmetric, then $V_H^{\mathrm{ms}} = V_H^{\mathrm{ms},*}$ and we have a Galerkin method.

If $a(\cdot,\cdot)$ is not symmetric, we can still solve for $\tilde{u}_H^{\mathrm{ms}} \in V_H^{\mathrm{ms}}$ with

$$a(\tilde{u}_H^{\mathrm{ms}}, v_H^{\mathrm{ms}}) = (f, v_H^{\mathrm{ms}})_{L^2(\mathcal{D})} \qquad \text{for all } v_H^{\mathrm{ms}} \in V_H^{\mathrm{ms}}.$$

Since Galerkin methods are H^1-quasi optimal, we still have the optimal convergence order (for $s \in \{0, 1, 2\}$) as

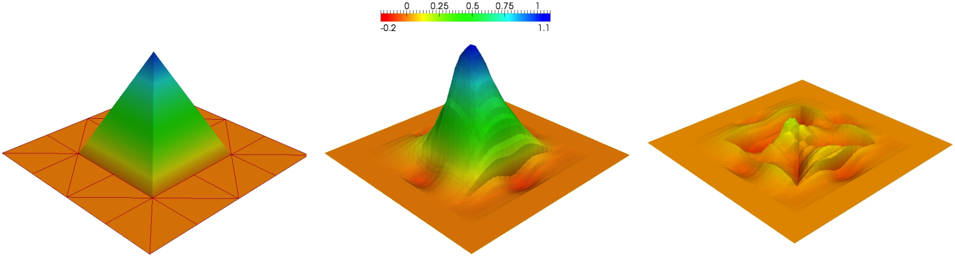
$$\|u - \tilde{u}_H^{\mathrm{ms}}\|_{H^1(\mathcal{D})} \leq C\|u - u_H^{\mathrm{ms}}\|_{H^1(\mathcal{D})} \leq C H^{s+1}\alpha^{-1}\|f\|_{H^s(\mathcal{D})}.$$

This is computationally favorable, since only V_H^{ms} is computed!

Basis functions

We have

$$V_H^{\mathrm{ms}} = (I + \mathcal{C})V_H.$$



Φ_z $(I + \mathcal{C})\Phi_z$ $\mathcal{C}(\Phi_z)$

Summary: Equivalent problem formulations

RUB

Find $u_H \in V_H$ with

$$a(u_H, v_H^{\mathrm{ms}}) = \langle F, v_H^{\mathrm{ms}} \rangle \qquad \text{for all } v_H^{\mathrm{ms}} \in V_H^{\mathrm{ms},*}.$$

Find $u_H \in V_H$ with

$$\underbrace{a(u_H, (I + \mathcal{C}^*)v_H)}_{=:a_0(u_H, v_H)} = \langle F, (I + \mathcal{C}^*)v_H \rangle \qquad \text{for all } v_H \in V_H.$$

Find $u_H^{\mathrm{ms}} \in V_H^{\mathrm{ms}}$ with

$$a(u_H^{\mathrm{ms}}, v_H^{\mathrm{ms}}) = \langle F, v_H^{\mathrm{ms}} \rangle \qquad \text{for all } v_H^{\mathrm{ms}} \in V_H^{\mathrm{ms},*}.$$

Recall $u_H = P_H(u_H^{\mathrm{ms}})$.

Remark: It can be proved that the problems are inf-sup stable (well-posedness).

Localized Orthogonal Decomposition

Question: Can we compute the corrector $\mathcal{C}$ through local problems?

P. Henning and D. Peterseim.
Oversampling for the Multiscale Finite Element Method.
SIAM Multiscale Model. Simul., 11(4):1149–1175, 2013.

P. Henning and A. Målqvist.
Localized orthogonal decomposition techniques for boundary value problems.
SIAM Journal of Scientific Computing, 36(4):A1609–A1634, 2014.

Localization of $\mathcal{C}$

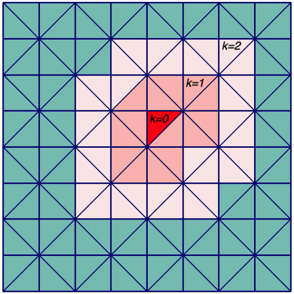
Decoupling idea:

For each triangle $T \in \mathcal{T}_H$, solve for $\mathcal{C}_T^k(v_H) \in W(U_k(T))$ with

$$a(\mathcal{C}_T^k(v_H), w) = \underbrace{-a_T(v_H, w)}_{\text{local source term!}} \qquad \forall w \in W(U_k(T)).$$

and set

$$\mathcal{C}^k(v_H) = \sum_{T \in \mathcal{T}_H} \mathcal{C}_T^k(v_H).$$



Advantage: solution $\mathcal{C}_T(v_H)$ decays (exponentially) outside of T to zero!

Replace $\mathcal{D}$ by $U_k(T)$, a k-layer environment of T.

Approximation with exponential convergence

Theorem

Let $k \in \mathbb{N}_{>0}$, *and* $\mathcal{C}_T^k(v_H) \in W(U_k(T))$ *solve (in parallel)*

$$a(\mathcal{C}_T^k(v_H), w) = a_T(v_H, w) \quad \forall w \in W(U_k(T))$$

and set

$$\mathcal{C}^k(v_H) := \sum_{T \in \mathcal{T}_H} \mathcal{C}_T^k(v_H)$$

then

$$\left\| \mathcal{C}(v_H) - \mathcal{C}^k(v_H) \right\|_{H^1(\mathcal{D})} \lesssim e^{-ck} \|\nabla v_H\|_{L^2(\mathcal{D})}.$$

L^2-projection nicht benötigt for Berechnung; $\ker(I_H|_{V_h})$ äquivalent ausdrückbar durch Quasi-Interpolationsoperator vom Clément-Typ (cf. Carstensen, Verforth, SINUM Vol. 36, '99).

Approximation with exponential convergence

Theorem

Let $k \in \mathbb{N}_{>0}$, *and* $\mathcal{C}_T^k(v_H) \in W(U_k(T))$ *solve (in parallel)*

$$a(\mathcal{C}_T^k(v_H), w) = a_T(v_H, w) \quad \forall w \in W(U_k(T))$$

and set

$$\mathcal{C}^k(v_H) := \sum_{T \in \mathcal{T}_H} \mathcal{C}_T^k(v_H)$$

then

$$\left\| \mathcal{C}(v_H) - \mathcal{C}^k(v_H) \right\|_{H^1(\mathcal{D})} \lesssim e^{-ck} \|\nabla v_H\|_{L^2(\mathcal{D})}.$$

The choice $k \approx s|\ln(H)|$ preserves convergence rate H^s.

Approximation with exponential convergence

RUB

Theorem

Let $k \in \mathbb{N}_{>0}$*, and* $\mathcal{C}_T^k(v_H) \in W(U_k(T))$ *solve (in parallel)*

$$a(\mathcal{C}_T^k(v_H), w) = a_T(v_H, w) \quad \forall w \in W(U_k(T))$$

and set

$$\mathcal{C}^k(v_H) := \sum_{T \in \mathcal{T}_H} \mathcal{C}_T^k(v_H)$$

then

$$\left\| \mathcal{C}(v_H) - \mathcal{C}^k(v_H) \right\|_{H^1(\mathcal{D})} \lesssim e^{-ck} \|\nabla v_H\|_{L^2(\mathcal{D})}.$$

Instead of $V_H^{\mathrm{ms}} := (I + \mathcal{C})V_H$ use $V_{H,k}^{\mathrm{ms}} := (I + \mathcal{C}^k)V_H$.

A priori error estimates for symmetric $a(\cdot,\cdot)$

RUB

Theorem

Let $V_{H,k}^{\mathrm{ms}} := (I + \mathcal{C}^k)V_H$ *and* $k \gtrsim |\ln(H)|$. *Find* $u_{H,k}^{\mathrm{ms}} \in V_{H,k}^{\mathrm{ms}}$ *with*

$$a(u_{H,k}^{\mathrm{ms}}, v) = \langle F, v\rangle \qquad \text{for all } v \in V_{H,k}^{\mathrm{ms}}.$$

Then it holds (generically) for $F \in H_0^1(\mathcal{D}) \cap H^s(\mathcal{D})$ *where* $s \in \{1,2\}$:

$$\|u - u_{H,k}^{\mathrm{ms}}\|_{L^2(\mathcal{D})} + H\|u - u_{H,k}^{\mathrm{ms}}\|_{H^1(\mathcal{D})} \lesssim \|F\|_{H^s(\mathcal{D})} H^{2+s},$$

for $F \in L^2(\mathcal{D})$:

$$\|u - u_{H,k}^{\mathrm{ms}}\|_{L^2(\mathcal{D})} + H\|u - u_{H,k}^{\mathrm{ms}}\|_{H^1(\mathcal{D})} \lesssim \|F\|_{L^2(\mathcal{D})} H^2,$$

and for $F \in H^{-1}(\mathcal{D})$:

$$\|u - u_{H,k}^{\mathrm{ms}}\|_{L^2(\mathcal{D})} + H\|u - u_{H,k}^{\mathrm{ms}}\|_{H^1(\mathcal{D})} \lesssim \|F\|_{H^{-1}(\mathcal{D})} H.$$

Remark: the H^1-estimates remain valid if $a(\cdot,\cdot)$ is non-symmetric. For optimal order L^2-convergence, the test function space $V_{H,k}^{\mathrm{ms}}$ must be replaced by a dual version $V_{H,k}^{\mathrm{ms},*}$.

Localized Orthogonal Decomposition

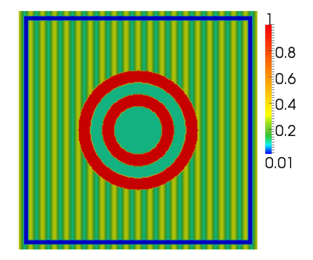
Numerical experiment

Numerical experiment - Model Problem

Let $\mathcal{D} := [0,1]^2$. Find $u \in H^1(\mathcal{D})$ with

$$-\nabla \cdot (A \nabla u) = F \quad \text{in } \mathcal{D},$$
$$u = x_1 \quad \text{on } \partial\mathcal{D}.$$

A given by



and for $c := (\frac{1}{2}, \frac{1}{2})$ and $r := 0.05$

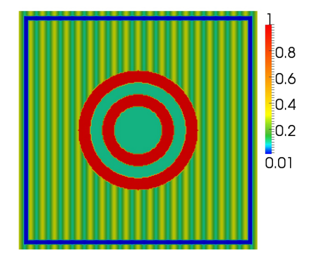
$$F(x) := \begin{cases} 20 & \text{if } |x - c| \leq r \\ 0 & \text{else.} \end{cases}$$

Numerical experiment - Model Problem

Let $\mathcal{D} := [0,1]^2$. Find $u \in H^1(\mathcal{D})$ with

$$-\nabla \cdot (A \nabla u) = F \quad \text{in } \mathcal{D},$$
$$u = x_1 \quad \text{on } \partial\mathcal{D}.$$

A given by



Green/yellow region: $A(x) = \frac{1}{10}(2 + \cos(2\pi \frac{x_1}{\varepsilon}))$ for $\varepsilon = 0.05$.

Isolator (blue region) $A(x) = 0.01$.

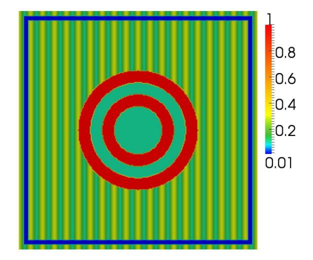
Circular layers in the middle: $A = 1$ (red region) and $A = 0.1$ (cyan region).

Numerical experiment - Model Problem

Let $\mathcal{D} := [0,1]^2$. Find $u \in H^1(\mathcal{D})$ with

$$-\nabla \cdot (A \nabla u) = F \quad \text{in } \mathcal{D},$$
$$u = x_1 \quad \text{on } \partial\mathcal{D}.$$

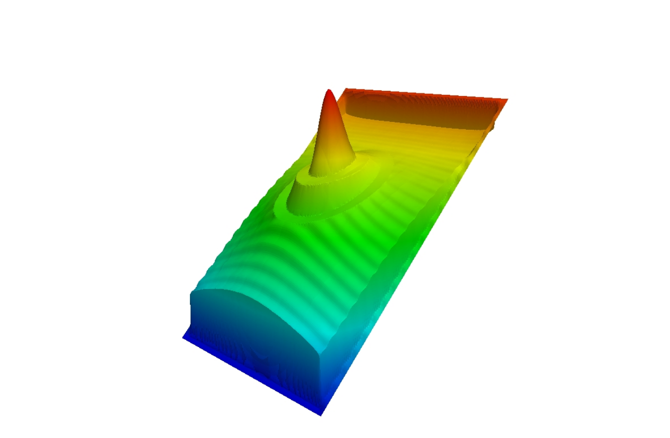
A given by



and for $c := (\frac{1}{2}, \frac{1}{2})$ and $r := 0.05$

$$F(x) := \begin{cases} 20 & \text{if } |x - c| \le r \\ 0 & \text{else.} \end{cases}$$

Numerical experiment - Reference solution



Results

H	k	$\left\Vert u_h - u^{\mathrm{ms}}_{H,k} \right\Vert^{\text{rel}}_{L^2(\mathcal{D})}$	$\left\Vert u_h - u^{\mathrm{ms}}_{H,k} \right\Vert^{\text{rel}}_{H^1(\mathcal{D})}$
2^{-3}	1	0.01708	0.12064
2^{-3}	2	0.00655	0.07400
2^{-3}	3	0.00557	0.06996
2^{-4}	1	0.00908	0.09389
2^{-4}	2	0.00159	0.03066
2^{-4}	3	0.00091	0.02269
2^{-4}	4	0.00074	0.02011

Table: *Reference computations for* $h = 2^{-8}$. k *denotes the number of Coarse Element Layers to create the localization patch.*

Results

H	k	$\left\|u_h - u^{\mathrm{ms}}_{H,k}\right\|^{\text{rel}}_{L^2(\mathcal{D})}$	$\left\|u_h - u^{\mathrm{ms}}_{H,k}\right\|^{\text{rel}}_{H^1(\mathcal{D})}$
2^{-3}	1	0.01708	0.12064
2^{-3}	2	0.00655	0.07400
2^{-3}	3	0.00557	0.06996
2^{-4}	1	0.00908	0.09389
2^{-4}	2	0.00159	0.03066
2^{-4}	3	0.00091	0.02269
2^{-4}	4	0.00074	0.02011

Table: *Reference computations for $h = 2^{-8}$. k denotes the number of Coarse Element Layers to create the localization patch.*

Results

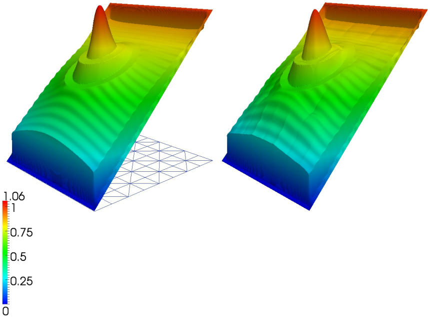


Figure: Fine grid with $h = 2^{-8}$. LOD approximation for $H = 2^{-3}$ and $k = 1$.

Results

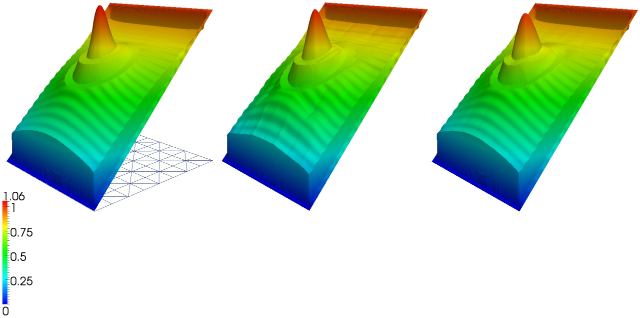


Figure: Fine grid with $h = 2^{-8}$. LOD approximation for $H = 2^{-3}$ and $k = 2$.

Results

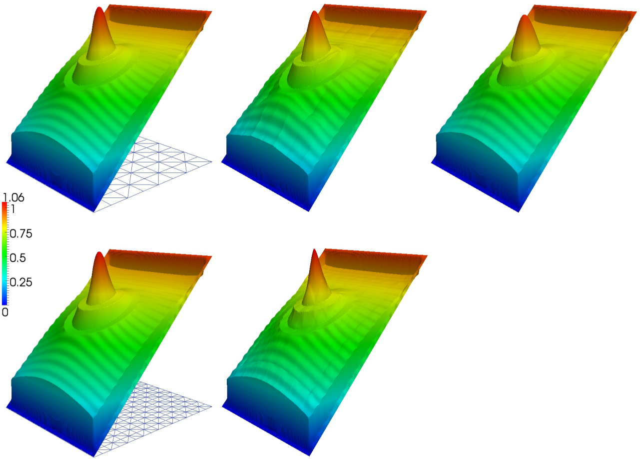


Figure: Fine grid with $h = 2^{-8}$. LOD approximation for $H = 2^{-4}$ and $k = 1$.

Results

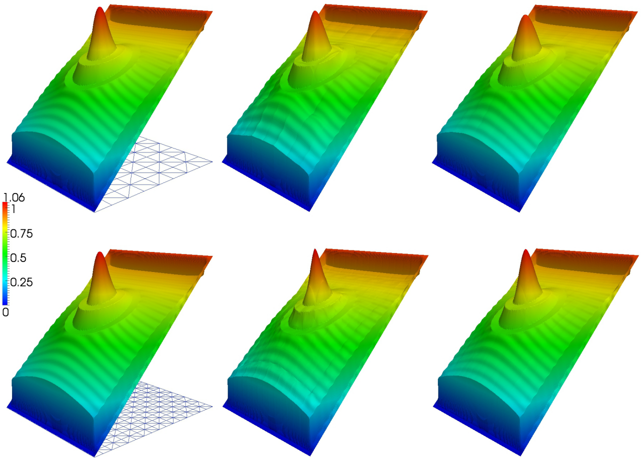


Figure: Fine grid with $h = 2^{-8}$. LOD approximation for $H = 2^{-4}$ and $k = 2$.

3. Some further multiscale problems

Survey and more advanced applications

Localized Orthogonal Decomposition (LOD) - general references

The approach was originally proposed in

A. Målqvist and D. Peterseim.
Localization of elliptic multiscale problems.
Math. Comp., 83:2583–2603, 2014.

and further developed (especially with regard to localization) in

P. Henning and D. Peterseim.
Oversampling for the Multiscale Finite Element Method.
SIAM Multiscale Model. Simul., 11(4):1149–1175, 2013.

P. Henning and A. Målqvist.
Localized orthogonal decomposition techniques for boundary value problems.
SIAM Journal of Scientific Computing, 36(4):A1609–A1634, 2014.

A survey on the methodology is given in:

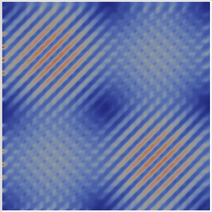
R. Altmann, P. Henning and D. Peterseim.
Numerical homogenization beyond scale separation.
Acta Numerica, 30:1–86, 2021.

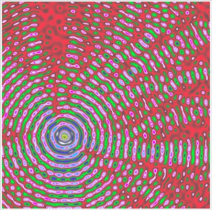
A. Målqvist and D. Peterseim.
Numerical homogenization by localized orthogonal decomposition.
SIAM Spotlights, 5:xii+108 2021.

Some applications – Wave phenomena in multiscale media

- Acoustic wave propagation in heterogenous media.

A. Abdulle and P. Henning. Localized orthogonal decomposition method for the wave equation with a continuum of scales. *Math. Comp.*, 86(304):549–587, 2017.





- Electromagnetic waves (Maxwell's equations, Nédélec FEM)

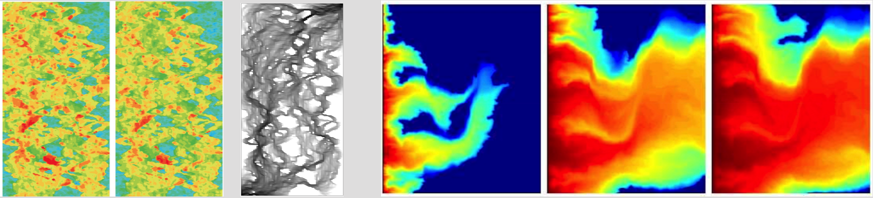
D. Gallistl, P. Henning and B. Verfürth. Numerical homogenization of H(curl)-problems. *SIAM J. Numer. Anal.*, 56(3):1570–1596, 2018.

P. Henning and A. Persson. Computational homogenization of time-harmonic Maxwell's equations. *SIAM J. Sci. Comput.*, 42(3):B581–B607, 2020.

Some applications - Hydrological simulations

- ▷ Darcy flow (problems in mixed formulation, $H(\text{div})$-conforming Raviart-Thomas FEM). Local mass conservation.

  F. Hellman, P. Henning, and A. Målqvist. Multiscale mixed finite elements. *Discrete Contin. Dyn. Syst. Ser. S*, 9(5):1269–1298, 2016.



- ▷ Two-phase flow (Buckley-Leverett equation, DG-FEM)

  D. Elfverson, V. Ginting, and P. Henning. On multiscale methods in Petrov-Galerkin formulation. *Numer. Math.*,131(4):643–682, 2015.

Some applications - Superfluids in complex potentials

Find quantum state of condensate

$$u : \mathcal{D} \times [0, T] \to \mathbb{C}$$

where $u(\cdot, 0) = v$ with $\int_{\mathcal{D}} |v|^2 = 1$ and eigenvalue $\mu \in \mathbb{R}$ solves

$$\boxed{-\triangle v + W v + \mathrm{i}\boldsymbol{\Omega} \cdot (\mathbf{x} \times \nabla) v + \kappa(|v|^2)\, v = \mu\, v.}$$

and $u(\cdot, t)$ (for $t > 0$) solves the nonlinear Schrödinger equation

$$\boxed{\mathrm{i}\partial_t u = -\triangle u + V u + \gamma(|u|^2)\, u.}$$

- V and W are multiscale trapping potentials.

Super-convergence in LOD spaces ($P1$-FEM based) for nonlinear eigenvalue problem: 3rd order in H^1-norm and 4th order in L^2-norm.

P. Henning, A. Målqvist, and D. Peterseim. Two-Level discretization techniques for ground state computations of Bose-Einstein condensates. *SIAM J. Numer. Anal.*,52(4):1525–1550, 2014.

Some applications - Superfluids in complex potentials

Find quantum state of condensate

$$u : \mathcal{D} \times [0, T] \to \mathbb{C}$$

where $u(\cdot, 0) = v$ with $\int_{\mathcal{D}} |v|^2 = 1$ and eigenvalue $\mu \in \mathbb{R}$ solves

$$-\triangle v + W v + \mathrm{i}\boldsymbol{\Omega} \cdot (\mathbf{x} \times \nabla) v + \kappa(|v|^2)\, v = \mu\, v.$$

and $u(\cdot, t)$ (for $t > 0$) solves the nonlinear Schrödinger equation

$$\mathrm{i}\partial_t u = -\triangle u + V u + \gamma(|u|^2)\, u.$$

- V and W are multiscale trapping potentials.

Super-convergence in LOD spaces ($P1$-FEM based) for time-dependent NLS: 6rd order convergence for energy and mass.

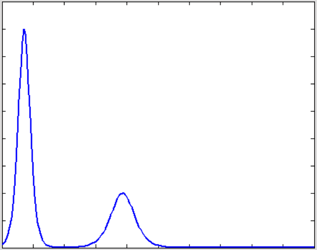
P. Henning and J. Wärnegård. Superconvergence of time invariants for the Gross-Pitaevskii equation. *Math Comp* (early view), 2021.

Motivating example: a multisoliton

Soliton:

- wave (packet) that does not change its shape over time and which propagates with constant velocity;
- can interact with other solitons, and emerge from the collision unchanged (except for a phase shift).

- Nonlinear Schrödinger equations model wave propagation in nonlinear media and have solitons as solutions.



Example: two interacting solitons in 1D

[Aktosun et al. *Exact solutions to the nonlinear Schrödinger equation*. Birkhäuser Verlag, 2010.]

We consider the model equation

$$\mathrm{i}\partial_t u = -\partial_{xx} u - 2|u|^2 u \qquad \text{in } \mathbb{R} \times (0, T].$$

Single soliton solutions to the equation are of the form

$$u(x,t) = \sqrt{\alpha}\, e^{\mathrm{i}(\frac{1}{2}cx - (\frac{1}{4}c^2 - \alpha)t)}\, \mathrm{sech}(\sqrt{\alpha}(x - ct)),$$

where, sech is the hyperbolic secant and

- α: shape parameter of the soliton (also determines amplitude $\sqrt{\alpha}$);
- c: the velocity with which the soliton moves.

However, we consider the problem with a multisoliton solution, that consists of two stationary interacting solitons:

$$u(x,t) = \frac{8e^{4\mathrm{i}t}(9e^{-4x} + 16e^{4x}) - 32e^{16\mathrm{i}t}(4e^{-2x} + 9e^{2x})}{-128\cos(12t) + 4e^{-6x} + 16e^{6x} + 81e^{-2x} + 64e^{2x}}.$$

Example: two interacting solitons in 1D

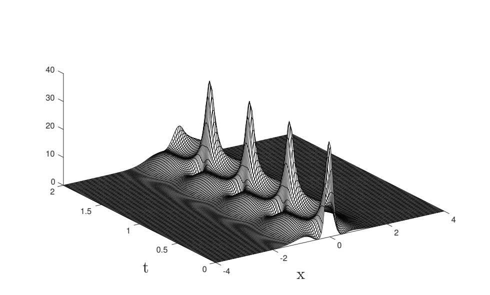
[Aktosun et al. *Exact solutions to the nonlinear Schrödinger equation*. Birkhäuser Verlag, 2010.]

Model equation

$$\mathrm{i}\partial_t u = -\partial_{xx} u - 2|u|^2 u \qquad \text{in } \mathbb{R} \times (0, T].$$

Multisoliton solution consistingg of two stationary interacting solitons:

$$u(x,t) = \frac{8e^{4\mathrm{i}t}(9e^{-4x} + 16e^{4x}) - 32e^{16\mathrm{i}t}(4e^{-2x} + 9e^{2x})}{-128\cos(12t) + 4e^{-6x} + 16e^{6x} + 81e^{-2x} + 64e^{2x}}.$$



Example: two interacting solitons in 1D

$$\mathrm{i}\partial_t u = -\partial_{xx} u - 2|u|^2 u \qquad \text{in } \mathbb{R} \times (0, T].$$

Multisoliton solution consisting of two stationary interacting solitons:

$$u(x,t) = \frac{8e^{4\mathrm{i}t}(9e^{-4x} + 16e^{4x}) - 32e^{16\mathrm{i}t}(4e^{-2x} + 9e^{2x})}{-128\cos(12t) + 4e^{-6x} + 16e^{6x} + 81e^{-2x} + 64e^{2x}}.$$

We can compute the energy and the mass with

$$E(u) = -48 \qquad \text{and} \qquad M(u) = 12.$$

Recall: interacting solitons emerge unchanged from collisions.

From the values of the energy and the formula for single soliton solutions, we find that u is the interaction of the two individual solitons

$$u_1(x,t) = 2e^{4\mathrm{i}t}\,\mathrm{sech}(2x) \qquad \text{and} \qquad u_2(x,t) = 4e^{16\mathrm{i}t}\,\mathrm{sech}(4x).$$

Details: [H. and Wärnegård. *Math Comp* (early view), 2021]

Example: two interacting solitons in 1D

Details: [H. and Wärnegård. *Math Comp* (early view), 2021]

$$\mathrm{i}\partial_t u = -\partial_{xx} u - 2|u|^2 u \qquad \text{in } \mathbb{R} \times (0, T].$$

Consider again the multisoliton consisting of two stationary interacting solitons and assume that we repeat the same calculations with an **energy perturbation** of order ϵ_h (discretization error), i.e.

$$E(u) = -48 + \epsilon_h.$$

In this case we obtain the following two individual solitons:

$$u_1(x,t) = 2\, e^{\mathrm{i}(\frac{1}{2}c_1 x - (\frac{1}{4}c_1^2 - 4)t)}\, \mathrm{sech}(2(x - c_1 t)), \quad \text{where } c_1 = -\sqrt{\tfrac{2}{3}\epsilon_h}$$

and

$$u_2(x,t) = 4\, e^{\mathrm{i}(\frac{1}{2}c_2 x - (\frac{1}{4}c_2^2 - 16)t)}\, \mathrm{sech}(4(x - c_2 t)), \quad \text{where } c_2 = \sqrt{\tfrac{1}{6}\epsilon_h}$$

Hence, both solitons drift apart with a speed proportional to the square root of the energy error.

Example: two interacting solitons in 1D

Details: [H. and Wärnegård. *Math Comp* (early view), 2021]

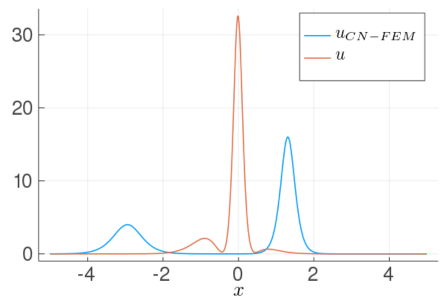
Multisoliton with **energy perturbation** (discretization error)

$$E(u) = -48 + \epsilon_h.$$

We obtain two separate solitons

$$u_1(x,t) = 2\, e^{i(\frac{1}{2} c_1 x - (\frac{1}{4} c_1^2 - 4)t)}\, \mathrm{sech}(2(x - c_1 t)), \quad \text{where } c_1 = -\sqrt{\tfrac{2}{3}\epsilon_h};$$

$$u_2(x,t) = 4\, e^{i(\frac{1}{2} c_2 x - (\frac{1}{4} c_2^2 - 16)t)}\, \mathrm{sech}(4(x - c_2 t)), \quad \text{where } c_2 = \sqrt{\tfrac{1}{6}\epsilon_h}.$$



Example: two interacting solitons in 1D

Details: [H. and Wärnegård. *Math Comp* (early view), 2021]

Problem: split of the multisoliton due to discrete energy errors:

$$E(u) = -48 + \epsilon_h.$$

- Velocity of the drift/separation $\propto \sqrt{\epsilon_h}$.
- If $T \gtrsim \epsilon_h^{-1/2}$ then the error will be of order $\mathcal{O}(1)$.
- Solution: high-order space discretizations/spectral methods?
  Issue: blow up of Sobolev-norms

  $$\|\partial_t^{m-k}\partial_x^k u\|_{L^\infty(L^2)} \simeq p^m \qquad \text{for any } m \in \mathbb{N},$$

  for some $p > 1$. For example:

  $$\|\partial_t^{(6)} u\|_{L^\infty(L^2)} \approx \mathcal{O}(10^{11}) \qquad \text{and} \qquad \|\partial_x^{(9)} u(0)\|_{L^2(\mathcal{D})} = \mathcal{O}(10^{11}).$$

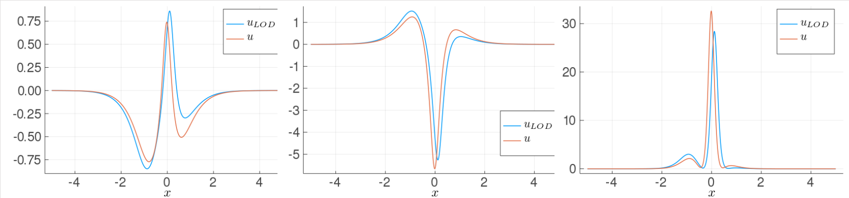
- Experiments in [H. and Wärnegård., Kinet. Relat. Models, 2019]: problem hardly solvable (i.e. can take years) with traditional approaches on long time scales.

Experiment: Comparison Crank–Nicolson

CPU times (in s) **per time step** (5 iterations), $\dim V_H^{\text{ms}} = 1024$

	CN-FEM FPI $h = 40/2^{18}$	CN-FEM LOD $H = 40/2^{10}$, $\ell = 10$
CPU [s]	2	0.014
$E - E_h$	3.33e-5	7.7e-5

$T = 200$; $N = 2^{23}$ time steps: $\approx$ 192 days with CN-FEM FPI and total time $\approx$ 29 hours with CN-FEM LOD.



(a) $\Re u$ (b) $\Im u$ (c) $|u|^2$

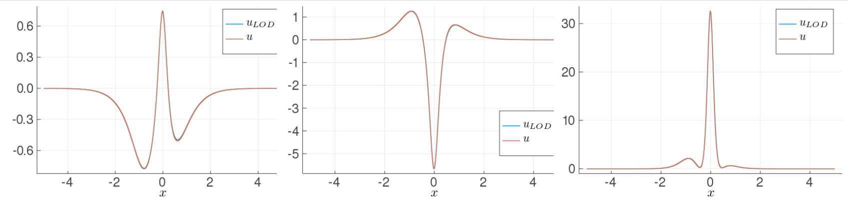
Figure: u_H^{ms} with the above configuration at $T = 200$.

Experiments: Comparison

CPU times (in s) **per time step** (5 iterations), $\dim V_H^{\mathrm{ms}} = 2048$

	CN-FEM FPI $h = 40/2^{21}$	CN-FEM LOD $H = 40/2^{11}$, $\ell = 12$
CPU [s]	15.9	0.032
$E - E_h$	5.2e-7	9.7e-7

$T = 200$; $N = 2^{23}$ time steps: $\approx$ **4.5 years** with CN-FEM FPI and total time $\approx$ 100 hours with CN-FEM LOD.



(a) $\Re u$ (b) $\Im u$ (c) $|u|^2$

Figure: u_H^{ms} with the above configuration at $T = 200$.

Thank you for your attention!