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A posteriori error estimates and adaptation for multiscale problems

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› Outline

Motivation: Multi-Scale and Multi-Physics Problems

Introduction to a posteriori error estimation

- Error control for stationary variational problems
- Adaptive schemes/ equal distribution strategy

Error control and adaptivity for numerical multiscale methods

- Linear elliptic multiscale problems
- Nonlinear elliptic multiscale problems

Model reduction and multiscale methods

- Reduced Basis Methods
- A new reduced basis DG multiscale method

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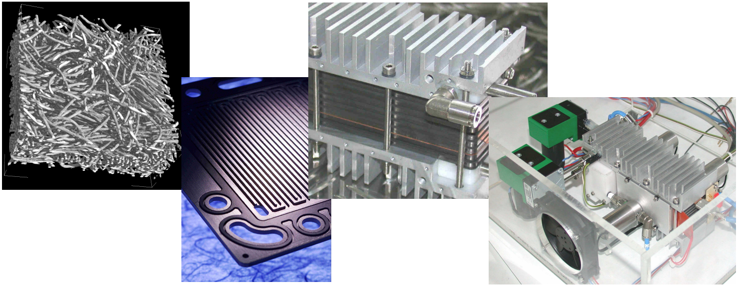
› Example: PEM fuel cells

Pore Cell Stack System



[BMBF-Project PEMDesign: Fraunhofer ITWM and Fraunhofer ISE]

› Example: PEM fuel cells

Porous layers:
- Two phase flow with phase transition
- Species transport with reaction for O_2, H_2, H_2O
- Potential flow for electrons
- Energy balance

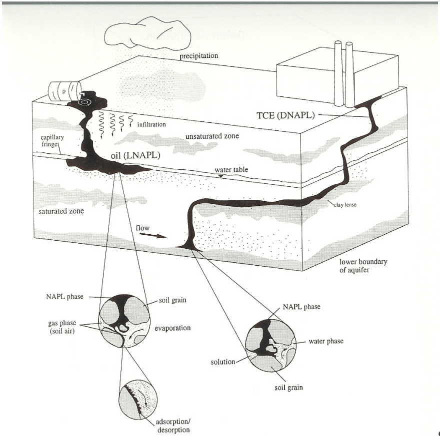
Membrane:
- Two phase water transport
- Potential flow for protons
- Energy balance

Gas channels:
- flow, species transport and energy balance

Bipolar plates:
- electron flow and energy balance

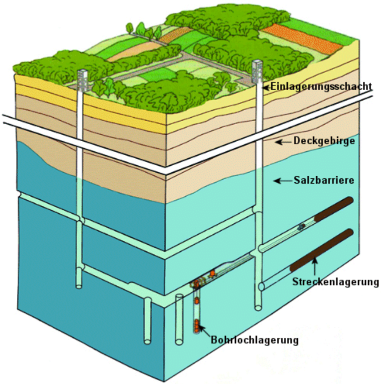
Coupling through interface conditions

› Example: Environmental Problems

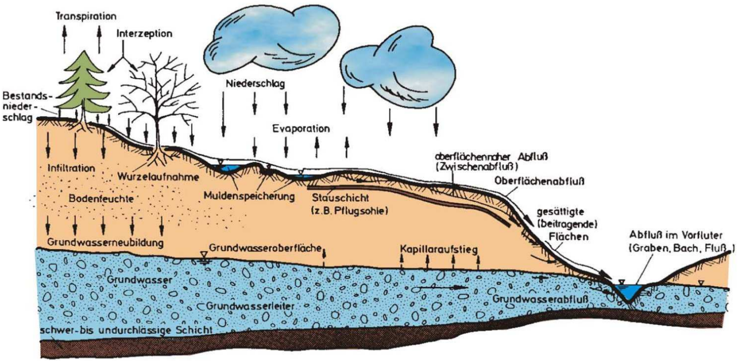


Source: [Helmig '97]

› Security behavior of nuclear waste disposals

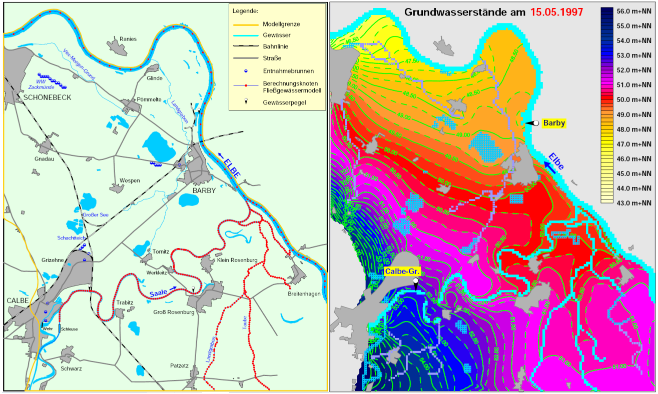


› Example: Hydrological Modeling



[BMBF-Project AdaptHydroMod: Bronstert et al., Potsdam]

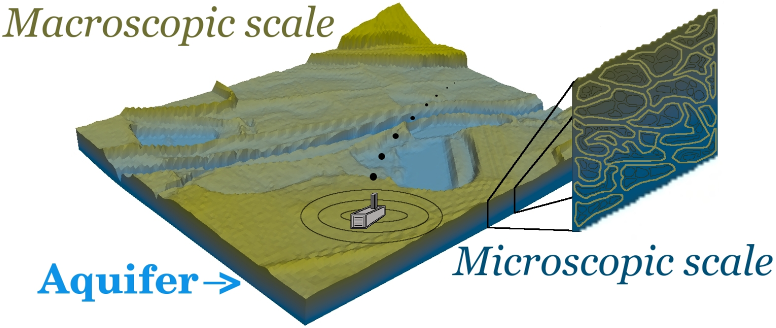
› Example: Hydrological Modeling



[BMBF-Project AdaptHydroMod: Wald & Corbe, Hügelsheim]

› Multiscale problems in subsurface flow

Application scenario



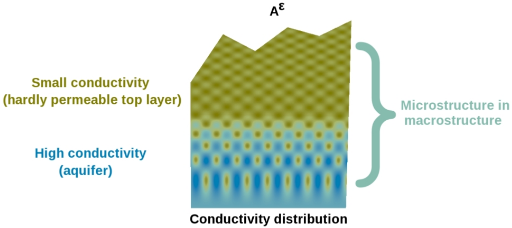
Groundwater: important source of drinking water.

Simple approaches to modelling:

Linear elliptic multiscale problem.

$$\nabla \cdot (A^\epsilon(x)\nabla u^\epsilon(x)) = f(x) \quad \text{in } \Omega,$$
$$u^\epsilon(x) = 0 \quad \text{on } \partial\Omega.$$

- u^ϵ: concentration of pollutant,
- ϵ: indicator for (representative) size of small scale,
- A^ϵ: conductivity / diffusion operator.



Simple approaches to modelling:

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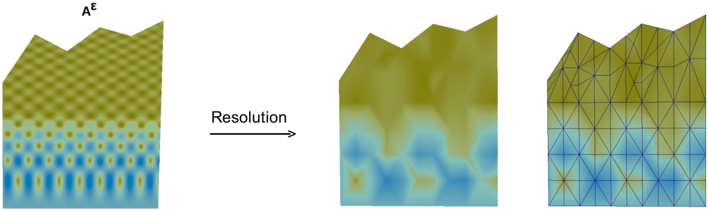

Conductivity distribution
(Still relatively coarse!)

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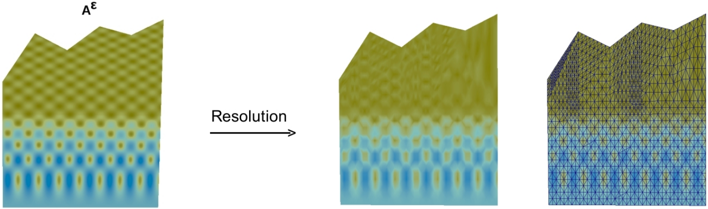

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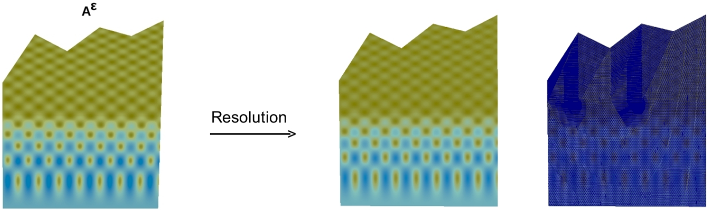

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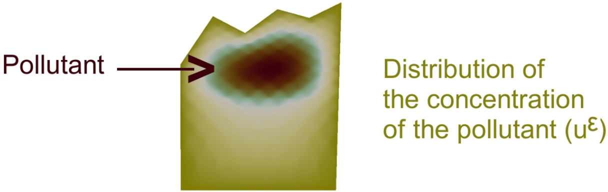


› Mathematical Modelling and Model Reduction

Increasing Efficiency

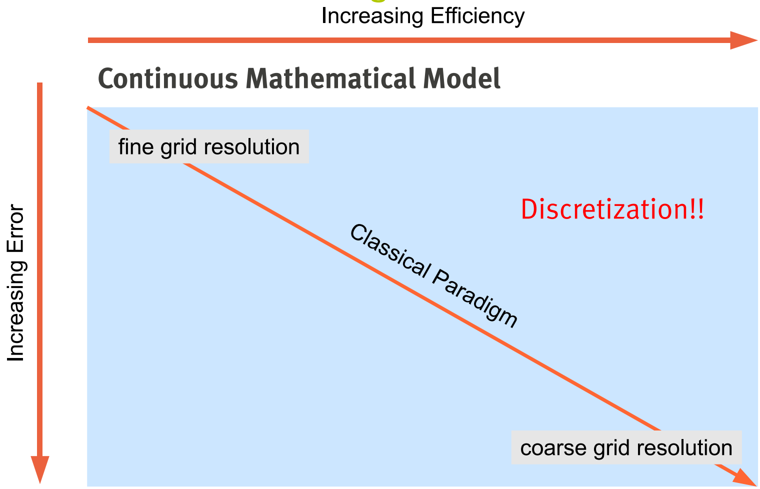
Increasing Error

Real World Problem

Continuous Mathematical Model

- Here: system of partial differential equations
- Problem: infinite dimensional solution space
- no solutions in closed form

› Mathematical Modelling and Model Reduction



› Mathematical Modelling and Model Reduction

Increasing Efficiency →

Increasing Error ↓

Continuous Mathematical Model

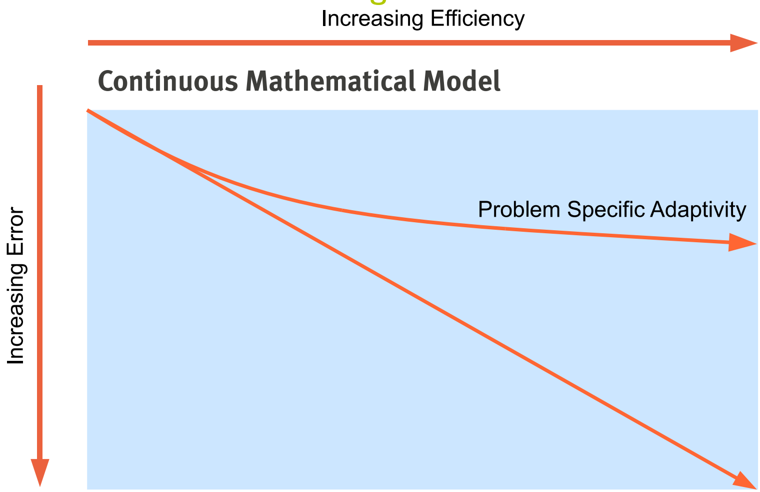
Discrete model on uniform grid (FEM, FV, DG, ...)

- Typical error estimates:

$$||u - u_h|| \leq c \inf_{v_h \in X_h} ||u - v_h||$$

- Error related to approximation property of X_h
- $\Longrightarrow$ Very general approach, but in particular cases not very efficient!!

› Mathematical Modelling and Model Reduction



› Mathematical Modelling and Model Reduction

Increasing Efficiency →

Increasing Error ↓

Continuous Mathematical Model

Problem specific: Adaptive Mesh Refinement

- Typical error estimates:

$$||u - u_h|| \leq c\,\eta(u_h)$$

- Error related to approximate solution!
- $\Longrightarrow$ Construct optimal mesh!
- Problem: Grid construction for every solve!
  Resulting system is still high-dimensional!

› Mathematical Modelling and Model Reduction

Increasing Efficiency

Increasing Error

Continuous Mathematical Model

Problem class specific: Reduced Basis Method

- Typical error estimates:

$$||(u - u_N)(\boldsymbol{\mu})|| \leq c\, \eta(u_N(\boldsymbol{\mu}))$$

- Error related to reduced solution!
- $\Longrightarrow$ Construct optimal reduced space for problem class!!
  Resulting system is low dimensional!

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› Variational Problems

Let X denote a Hilbert space, $B : X \times X \to \mathbb{R}$ a continuous (c_1) and coercive (c_0) bilinear form and $f \in X'$, i.e.

$$\begin{aligned} B(u,v) &\leq c_1||u||\,||v||, \forall u, v \in X, \\ B(u,u) &\geq c_0||u||^2. \end{aligned}$$

We then denote $u \in X$ the unique solution of a corresponding variational problem if it satisfies

$$B(u,\phi) = f(\phi), \quad \forall \phi \in X.$$

Note: Existence and uniqueness is guaranteed by the Lax-Milgram Lemma.

› Galerkin Approximation

Let $X_h \subset X$ denote a finite dimensional subspace of X, where the dimension $\dim(X_h)$ is correlated to the parameter h. We define a unique Galerkin approximation $u_h \in X_h$ through

$$B(u_h, \phi_h) = f(\phi_h), \quad \forall \phi_h \in X_h.$$

From Cea's Lemma we know, that u_h is a nearly optimal approximation of u in X_h. More specific it holds

$$||u - u_h|| \leq \frac{c_1}{c_0} \inf_{v_h \in X_h} ||u - v_h||.$$

However: This result gives only asymptotic information and no computable error bounds!!

› Goal: Adaptivity based on error control

Situation: u exact solution, u_h approximate solution.

First step: A posteriori error estimate.

$$||u - u_h|| \leq \eta(u_h).$$

Second step: Definition of local error indicators.

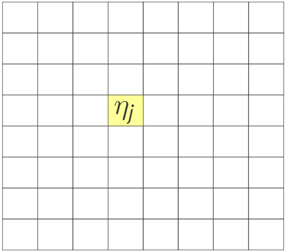
$$\eta(u_h) = \sum_j \eta_j(u_h).$$

› Goal: Adaptivity based on error control

Third step: Equidistribution strategy.

Choose local mesh size such that all $\eta_j(u_h)$ are approximately of the same size, and $\eta(u_h) \leq TOL$!

This is done by an estimate–mark–adapt algorithm:



"estimate"

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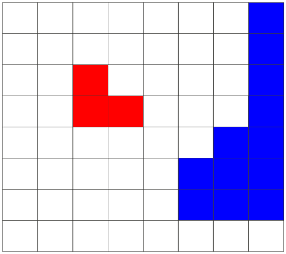

”mark”

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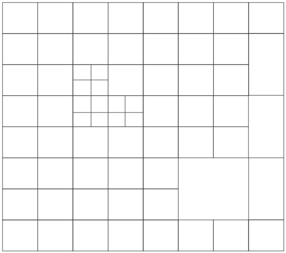


”refine”

Definition (Robust and efficient error estimator)

We say that an error estimator $\eta_h(u_h)$ is robust if it is an upper bound of the error $||u - u_h||$, i.e.

$$||u - u_h|| \leq K_1 \eta_h(u_h).$$

The estimator is efficient with efficiency index $\frac{K_1}{K_0} \geq 1$, if it also satisfies

$$K_0 \, \eta_h(u_h) \leq ||u - u_h||.$$

› Residual based error estimation

For any $v_h \in X_h$ let us define the residual $R[v_h] \in X'$ through

$$R[v_h](\phi) := B(v_h, \phi) - f(\phi) \quad \forall \phi \in X.$$

Theorem (Residual error estimate)

Let us define the error estimator

$$\eta_h(u_h) := ||R[u_h]||_{X'}.$$

Then $\eta_h(u_h)$ is robust and efficient with constants

$$K_1 = \frac{1}{c_0}, K_0 = \frac{1}{c_1} \quad \longrightarrow \quad \text{efficiency} = \frac{c_1}{c_0}$$

› Residual based error estimation

Proof. With the coercivity of B it holds

$$\begin{aligned} c_0 ||u - u_h||^2 &\leq B(u - u_h, u - u_h) = |B(u_h, u - u_h) - f(u - u_h)| \\ &= |R[u_h](u - u_h)| \leq ||R[u_h]||_{X'} ||u - u_h||. \end{aligned}$$

This yields robustness.On the other hand, we have

$$\begin{aligned} ||R(u_h)||_{X'} &= \sup_{\phi \in X \setminus \{0\}} \frac{|R[u_h](\phi)|}{||\phi||} = \sup_{\phi \in X \setminus \{0\}} \frac{|B(u_h, \phi) - f(\phi)|}{||\phi||} \\ &= \sup_{\phi \in X \setminus \{0\}} \frac{|B(u_h, \phi) - B(u, \phi)|}{||\phi||} \leq c_1 ||u - u_h||. \end{aligned}$$

Hence, the estimator is also efficient. □

› Residual based error estimation

Problem:

- $\eta_h(u_h) := ||R(u_h)||_{X'}$ is not computable, as it is a dual norm of an infinite dimensional space!!
- $\eta_h(u_h)$ is not localized and hence not suitable for adaptive mesh adaptation.

Idea: Estimate $\eta_h(u_h)$ by a localized computable upper bound!

› Localized upper bound for the Poisson problem

Consider $X := H^1_0(\Omega)$, $f \in L^2(\Omega)$, and $B(u,v) := \int_\Omega \nabla u \cdot \nabla v$. Let $X_h := \{v_h \in X | v_h|_T \in \mathbb{P}^k(T) \forall T \in \mathcal{T}_h\}$ and $u_h \in X_h$ solution of

$$B(u_h, \phi_h) = (f, \phi_h) \ \ \forall \phi_h \in X_h.$$

Then, the following upper bound holds true

$$||R(u_h)||_{X'} \leq C \Big(\sum_{T \in \mathcal{T}_h} \eta_T(u_h)^2 \Big)^{1/2}$$

with the local error indicators $\eta_T(u_h)$ defined through

$$\eta_T(u_h)^2 := h_T^2 ||f + \Delta u_h||^2_{L^2(T)} + \frac{1}{2} \sum_{S \in \partial T \setminus \partial\Omega} ||[\nabla u_h \cdot n]||^2_{L^2(S)}.$$

Here, $[\nabla u_h \cdot n]$ denotes the jump of the normal derivative across S.

› Localized upper bound for the Poisson problem

Proof. By definition of the residual, we have

$$\begin{aligned} R[u_h](\phi) &= \int_\Omega \nabla u_h \cdot \nabla \phi - f\phi = \sum_{T \in \mathcal{T}_h} \int_T \nabla u_h \cdot \nabla \phi - f\phi \\ &= \sum_{T \in \mathcal{T}_h} \int_T -(\Delta u_h + f)\phi + \int_{\partial T} \nabla u_h \cdot n\phi \end{aligned}$$

With $R[u_h](\phi_h) = 0 \ \forall \phi_h \in X_h$, we thus obtain

$$\begin{aligned} R[u_h](\phi) &= R[u_h](\phi) - R[u_h](\phi_h) = R[u_h](\phi - \phi_h) \\ &= \sum_{T \in \mathcal{T}_h} \int_T -(\Delta u_h + f)(\phi - \phi_h) + \frac{1}{2} \sum_{S \in \partial T \setminus \partial\Omega} \int_S [\nabla u_h \cdot n](\phi - \phi_h) \\ &\leq \sum_{T \in \mathcal{T}_h} h_T ||\Delta u_h + f||_{L^2(T)} ||\frac{1}{h_T}\phi - \phi_h||_{L^2(T)} \\ &\quad \sum_{T \in \mathcal{T}_h} \frac{1}{2} \sum_{S \in \partial T \setminus \partial\Omega} h_T^{1/2} ||[\nabla u_h \cdot n]||_{L^2(S)} ||h_T^{-1/2}(\phi - \phi_h)||_{L^2(S)}. \end{aligned}$$

› H^1-interpolant

The result now follows by choosing ϕ_h as an H^1-interpolant of ϕ and corresponding interpolation error estimates.

Theorem (H_0^1 interpolation)

Let $\mathcal{T}$ denote a regular grid of a polygonally bounded domain Ω and $X_h := S^k_{h,0} \subset H^1_0(\Omega)$. Then, there exists an interpolation operator

$$I_{h,0} \in L(H_0^1(\Omega), X_h),$$

such that for all $v \in H_0^1(\Omega)$ we have

$$\begin{aligned} ||v - I_{h,0}v||_{L^2(\Omega)} &\leq ch||\nabla v||_{L^2(\Omega)}, \\ ||\nabla(v - I_{h,0}v)||_{L^2(\Omega)} &\leq c||\nabla v||_{L^2(\Omega)}. \end{aligned}$$

Furthermore, with the trace theorem, it holds

$$||v - I_{h,0}v||_{L^2(S)} \leq c\Big(h(T)^{-1/2}||v - I_{h,0}v||_{L^2(T)} + h(T)^{1/2}||\nabla(v - I_{h,0}v)||_{L^2(T)}\Big)$$

Theorem (A posteriori error estimate)

For the solution u and the FE approximation u_h of the Poisson problem, we have

$$||\nabla(u - u_h)||_{L^2(\Omega)} \leq K_1 ||R(u_h)||_{H^{-1}(\Omega)} \leq c\, \eta_h(u_h).$$

with

$$\eta_h(u_h)^{:} = \sum_{T \in \mathcal{T}} \eta_T(u_h)^2$$

and the local indicators $\eta_T(u_h)$ defined as

$$\eta_T(u_h)^2 = h(T)^2 ||f + \Delta u_h||^2_{L^2(T)} + \frac{1}{2} h(T) \sum_{S \subset \partial T \setminus \partial\Omega} \left|\left| \left[\nabla u \cdot n \right] \right|\right|^2_{L^2(S)}.$$

› Efficiency of the localized error estimate

Question: Did we loose efficiency through the localization of the residual?

Goal: Derive a localized lower bound of the error in terms of the error estimator!

› Cut-off functions for localization

Lemma (Element bubbles)

Let T denote a d-dimensional simplex in $\mathbb{R}^d$ and $\lambda_i(x), i = 0, \ldots, d$ the barycentric coordinates of $x \in T$. We define the element bubble function $\psi_T : \mathbb{R}^d \to \mathbb{R}$ as

$$\psi_T(x) := \begin{cases} c_0 \prod_{i=0}^{d} \lambda_i(x), & \text{if } x \in T, \\ 0, & \text{else}, \end{cases}$$

with $c_0 := (d+1)^{d+1}$. Then ψ_T satisfies

1. $\operatorname{supp} \psi_T \subset T, \quad \psi_T|_T \in \mathbb{P}^{d+1}(T), \quad 0 \le \psi_T \le 1, \quad \max_{x \in T} \psi_T(x) = 1,$
2. $\int_T \psi_T(x)dx = c_d|T|$, with $c_d := \frac{d!(d+1)^{d+1}}{(2d+1)!}$,
3. $||\nabla \psi_T||_{L^2(T)} \le \frac{c}{h(T)} ||\psi_T||_{L^2(T)}$.

› Proof.

With the definition of ψ_T we have $\psi_T|_{\partial T} = 0$, i.e. supp $\psi_T \subset T$.
Furthermore, $\psi_T|_T \in \mathbb{P}^{d+1}(T)$ and $0 \leq \psi_T$ is clear from the definition.
Because of the symmetry, the maximum of ψ_T is attained at the center of gravity of T which yields with the definition of c_0:

$$\psi_T(x_s) = c_0\Big(\frac{1}{d+1}\Big)^{d+1} = 1.$$

The second property now follows:

$$\int_T \psi_T = (d+1)^{d+1} \int_T \lambda_0(x) \cdots \lambda_d(x)\,\mathrm{d}x = (d+1)^{d+1} \frac{d!}{(2d+1)!}|T|.$$

The third property can be obtained with a scaling argument. □

› Cut-off functions for localization

Lemma (Face bubbles)

Let T, T' denote d-simplices in $\mathbb{R}^d$ with face $S = T \cap T'$ and let $\lambda_i(x), i = 0, \dots, d$, $\lambda_i'(x), i = 0, \dots, d$ denote barycentric coordinates of $x \in T$, $x \in T'$. Let the enumeration of the nodes be such that a_0 and a_0' are opposite to the face S, i.e. $\lambda_0(x) = \lambda_0'(x) = 0 \; \forall x \in S$. We define the face bubble function $\psi_S : \mathbb{R}^d \to \mathbb{R}$ as

$$\psi_S(x) := c_0 \begin{cases} \prod_{i=1}^d \lambda_i(x), & \text{if } x \in T, \\ \prod_{i=1}^d \lambda_i'(x), & \text{if } x \in T', \\ 0, & \text{else}, \end{cases}$$

with $c_0 := d^d$. Then ψ_S satisfies

1. $\operatorname{supp} \psi_S \subset T \cup T'$, $\psi_S|_T \in \mathbb{P}^d(T)$, $\psi_S|_{T'} \in \mathbb{P}^d(T')$, $0 \le \psi_S \le 1$, $\max_{x \in T \cup T'} \psi_S(x) = 1$,
2. $\int_S \psi_S(x) dx = \tilde{c}_d |S|$, with $\tilde{c}_d := \frac{d!(d)^d}{(2d)!}$,
3. $||\nabla \psi_S||_{L^2(T \cup T')} \le \frac{c}{h(S)} ||\psi_T||_{L^2(T \cup T')}$.

Lemma (Local lower bound by the element estimator)

Let $u_h \in S^1_{h,0}$ *denote the linear FE approximation of the Poisson problem. For* $T \in \mathcal{T}$ *and* $f \in L^2(\Omega)$ *we define the average*

$$f_T := \frac{1}{|T|} \int_T f(x)\,\mathrm{d}x\,.$$

Then the following estimate holds

$$\eta_T(u_h) \leq c||\nabla(u-u_h)||_{L^2(\omega(T))} + \sum_{T' \in \omega(T)} h(T')||f - f_{T'}||_{L^2(T')},$$

where $\omega(T)$ *is given as* $\omega(T) := \bigcup_{T' \in \mathcal{T} | T \cap T' = S} T'$.

› Proof.

The proof will be split into three steps.
First step: Local bound of the element residual by the error.

Second step: Local bound of the jump residual by the error.

Third step: Global lower bound by summing up local contributions.

1. Step: Bound on $h(T)||f + \Delta u_h||_{L^2(T)}$

u_h being piecewise linear, we have

$$||f + \Delta u_h||_{L^2(T)} = ||f||_{L^2(T)} \leq ||f - f_T||_{L^2(T)} + ||f_T||_{L^2(T)}.$$

With the element bubble ψ_T we get

$$c_d||f_T||^2_{L^2(T)} = c_d|f_T|^2|T| = |f_T|^2 \int_T \psi_T = \int_T (f_T)^2\psi_T.$$

With $v_T := f_T\psi_T$ it follows

$$c_d||f_T||^2_{L^2(T)} = \int_T f_T v_T = \int_T f v_T + \int_T (f_T - f) v_T.$$

As v_T vanishes on ∂T, we further get

$$0 = \int_T \Delta u_h v_T = \int_T \nabla u_h \cdot \nabla v_T = \int_\Omega \nabla u_h \cdot \nabla v_T.$$

› 1. Step: Bound on $h(T)||f + \Delta u_h||_{L^2(T)}$ (cont.)

In addition, we have $\int_\Omega \nabla u \cdot \nabla \phi = \int_\Omega f\phi$. Thus with $\phi = v_T$:

$$\int_T \nabla u \cdot \nabla v_T = \int_\Omega \nabla u \cdot \nabla v_T = \int_\Omega f v_T = \int_T f v_T.$$

Using this relation, we obtain

$$\begin{aligned} c_d ||f_T||^2_{L^2(T)} &= \int_T \nabla u \cdot \nabla v_T - \int_T \nabla u_h \cdot \nabla v_T + \int_T (f_T - f) v_T \\ &= \int_T \nabla (u - u_h) \cdot \nabla v_T + \int_T (f_T - f) v_T \\ &\leq ||\nabla (u - u_h)||_{L^2(T)} ||\nabla v_T||_{L^2(T)} + ||f - f_T||_{L^2(T)} ||v_T||_{L^2(T)}. \end{aligned}$$

› 1. Step: Bound on $h(T)||f + \Delta u_h||_{L^2(T)}$ (cont.)

With the properties of the bubble function, it holds

$$\begin{aligned} ||\nabla v_T||_{L^2(T)} &= |f_T|||\nabla\psi_T||_{L^2(T)} \leq \frac{c}{h(T)}|f_T|||\psi_T||_{L^2(T)} \\ &\leq \frac{c}{h(T)}|f_T||T|^{1/2} = \frac{c}{h(T)}||f_T||_{L^2(T)}. \end{aligned}$$

and

$$||v_T||_{L^2(T)} \leq |f_T|||\psi_T||_{L^2(T)} \leq |f_T||T|^{1/2} = ||f_T||_{L^2(T)}.$$

› 1. Step: Bound on $h(T)||f + \Delta u_h||_{L^2(T)}$ (cont.)

From

$$c_d ||f_T||^2_{L^2(T)} \leq ||\nabla(u - u_h)||_{L^2(T)} ||\nabla v_T||_{L^2(T)} + ||f - f_T||_{L^2(T)} ||v_T||_{L^2(T)}.$$

we hence obtain

$$c_d ||f_T||^2_{L^2(T)} \leq \left(\frac{c}{h(T)} ||\nabla(u - u_h)||_{L^2(T)} + ||f - f_T||_{L^2(T)} \right) ||f_T||_{L^2(T)}.$$

It thus follows after multiplying with $h(T)/(c_d ||f_T||_{L^2(T)})$

$$h(T)||f_T||_{L^2(T)} \leq c\Big(||\nabla(u - u_h)||_{L^2(T)} + h(T)||f - f_T||_{L^2(T)} \Big).$$

› 2. Step: Bound on $h(T)^{1/2}||[\nabla u_h \cdot n]||_{L^2(S)}$

We proceed similar to the first step and define

$$v_S := [\nabla u_h \cdot n]\psi_S.$$

With the properties of the bubble and $[\nabla u_h \cdot n]$ being constant on S, we get

$$\begin{aligned} ||[\nabla u_h \cdot n]||^2_{L^2(S)} &= [\nabla u_h \cdot n]^2 |S| = \frac{1}{\tilde{c}_d}[\nabla u_h \cdot n]^2 \int_S \psi_S \\ &= \frac{1}{\tilde{c}_d} \int_S [\nabla u_h \cdot n] v_S. \end{aligned}$$

In addition, with $\omega(S) := T \cup T'$ we have for the exact solution

$$\int_{\omega(S)} f v_S = \int_\Omega f v_S = \int_\Omega \nabla u \cdot \nabla v_S = \int_{\omega(S)} \nabla u \cdot \nabla v_S.$$

› 2. Step: Bound on $h(T)^{1/2}||[\nabla u_h \cdot n]||_{L^2(S)}$ (cont.)

On the other hand, it holds

$$\begin{aligned}\int_\Omega \nabla u_h \cdot \nabla v_S &= \int_{\omega(S)} \nabla u_h \cdot \nabla v_S = \int_T \nabla u_h \cdot \nabla v_S + \int_{T'} \nabla u_h \cdot \nabla v_S \\ &= \int_{\partial T} \nabla u_h \cdot n v_S + \int_{\partial T'} \nabla u_h \cdot n v_S = \int_S [\nabla u_h \cdot n] v_S.\end{aligned}$$

Altogether we thus have

$$\begin{aligned}\tilde{c}_d ||[\nabla u_h \cdot n]||^2_{L^2(S)} &= \int_{\omega(S)} \nabla u_h \cdot \nabla v_S = \int_{\omega(S)} \nabla(u_h - u) \cdot \nabla v_S + \int_{\omega(S)} f v_S \\ &\leq ||\nabla(u-u_h)||_{L^2(\omega(S))} ||\nabla v_S||_{L^2(\omega(S))} + ||f||_{L^2(\omega(S))} ||v_S||_{L^2(\omega(S))}.\end{aligned}$$

› 2. Step: Bound on $h(T)^{1/2}||[\nabla u_h \cdot n]||_{L^2(S)}$ (cont.)

With the properties of the bubble function, we further have

$$\begin{aligned} ||v_S||_{L^2(\omega(S))} &= |[\nabla u_h \cdot n]|||\psi_S||_{L^2(\omega(S))} \leq |[\nabla u_h \cdot n]||\omega(S)|^{1/2} \\ &= ||[\nabla u_h \cdot n]||_{L^2(S)}|S|^{-1/2}|\omega(S)|^{1/2} \leq ch(T)^{1/2}||[\nabla u_h \cdot n]||_{L^2(S)} \end{aligned}$$

and

$$||\nabla v_S||_{L^2(\omega(S))} \leq \frac{c}{h(T)}||v_S||_{L^2(\omega(S))} \leq ch(T)^{-1/2}||[\nabla u_h \cdot n]||_{L^2(S)}.$$

In these estimates we have used the regularity of the triangulation $\mathcal{T}$, i.e.

$$|\omega(S)| = |T \cup T'| \leq c|T|, \qquad |T| \leq c|S|h(T).$$

Using these estimates we obtain for the jump residual

$$\begin{aligned} h(T)^{1/2}||[\nabla u_h \cdot n]||_{L^2(S)} &\leq c||\nabla(u - u_h)||_{L^2(\omega(S))} \\ &\quad + ch(T)(||f||_{L^2(T)} + ||f||_{L^2(T')}). \end{aligned}$$

› 3. Step: Global lower bound

With the local bounds from step one and two, we get by summation

$$
\begin{aligned}
\eta_T(u_h) &\leq ch(T)||f||_{L^2(\Omega)} + ch(T)^{1/2} \sum_{S\subset\partial T\setminus\partial\Omega} \left|\left|\left[\nabla u\cdot n\right]\right|\right|_{L^2(S)} \\
&\leq c\Big(||\nabla(u-u_h)||_{L^2(T)} + h(T)||f-f_T||_{L^2(T)}\Big) \\
&\quad + c\sum_{T'\cap T=S}\Big(||\nabla(u-u_h)||_{L^2(\omega(S))} + h(T)(||f||_{L^2(T)} + ||f||_{L^2(T')})\Big) \\
&\leq c\Big(||\nabla(u-u_h)||_{L^2(T)} + h(T)||f-f_T||_{L^2(T)}\Big) \\
&\quad + c\sum_{T'\cap T=S}||\nabla(u-u_h)||_{L^2(T')} + c\sum_{T'\cap T=S} h(T')||f-f_{T'}||_{L^2(T')}.
\end{aligned}
$$

With the definition of $\omega(T)$ this yields the result. □

› Adaptive schemes based on error estimates

Let us now suppose that we are given a localized error estimator of the form

$$||u - u_h||^2 \leq \eta_h(u_h)^2 := \sum_{T \in \mathcal{T}} \eta_T(u_h)^2.$$

Goal: Define an algorithm, such that for a given tolerance *TOL* the computational grid is constructed such the error satisfies

$$||u - u_h||^2 \leq TOL.$$

Definition (Equal distribution strategy)

Let $\Omega \subset R^d$, $\mathcal{T}_0$, TOL > 0, and $\Theta \in (0,1)$ be given.

EqualDistribution($\mathcal{T}_0, TOL, \Theta$)

$\mathcal{T} := \mathcal{T}_0$
repeat
  $[u_h, \eta_h] :=$ FEM($\mathcal{T}$)
  if $\eta_h > TOL$
   then
    for $T \in \mathcal{T}$
    do (compute marks)
     if $\eta_T^2 > \frac{TOL^2}{\#(\mathcal{T})}$
      then $M_h(T) :=$ MarkRefine
      else if $\eta_T^2 < \Theta \frac{TOL^2}{\#(\mathcal{T})}$
       then $M_h(T) :=$ MarkCoarsen
    $\mathcal{T} :=$ Adapt($M_h, \mathcal{T}$)
 until $\eta_h \leq TOL$
return $(\mathcal{T}, u_h, \eta_h)$

› Equal distribution strategy (cont.)

If convergent, the equal distribution strategy results in a triangulation $\mathcal{T}$ with a FE approximation u_h and an error estimator η_h such that $\eta_h \leq$ TOL. This is done in such a way that the local error indicators $\eta_T, T \in \mathcal{T}$ are approximately all of the same size. In particular from

$$\eta_T^2 \leq \frac{TOL^2}{\#(\mathcal{T})}.$$

we get by summation over all elements

$$\eta_h^2 := \sum_{T\in\mathcal{T}} \eta_T^2 \leq \sum_{T\in\mathcal{T}} \frac{TOL^2}{\#(\mathcal{T})} = \#(\mathcal{T}) \frac{TOL^2}{\#(\mathcal{T})} = TOL^2 .$$

› References

The material that I have presented so far is classical and can be found in several text books, e.g.

[AO00] Ainsworth, M. and Oden, J. T.
A posteriori error estimation in finite element analysis.
Pure and Applied Mathematics. Wiley-Interscience, New York, 2000.

[Ver96] R. Verfürth.
A review of a posteriori error estimation and adaptive mesh-refinement techniques.
Wiley-Teubner Series Advances in Numerical Mathematics. Teubner, Stuttgart, 1996.

› Outline

Motivation: Multi-Scale and Multi-Physics Problems

Introduction to a posteriori error estimation

- Error control for stationary variational problems
- Adaptive schemes/ equal distribution strategy

Error control and adaptivity for numerical multiscale methods

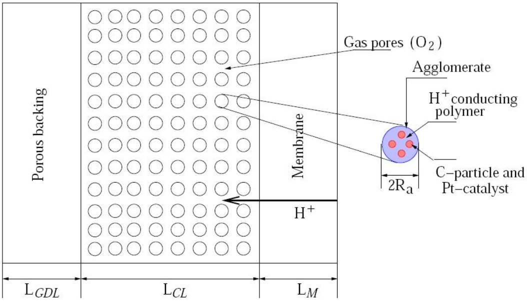
- Linear elliptic multiscale problems
- Nonlinear elliptic multiscale problems

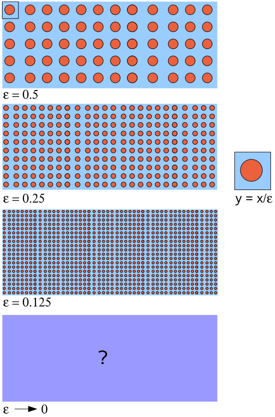
Model reduction and multiscale methods

- Reduced Basis Methods
- A new reduced basis DG multiscale method

› Multiscale Problems / Homogenization

Example: Catalyst layer of a fuel cell





› Numerical multiscale methods

Multiscale methods aim at approximation of multiscale problems, also for problems where there is no homogenization theory!

We distinguish two kind of approaches:

1. Methods that approximate the macroscopic behaviour (u_0), e.g. Heterogeneous Multiscale Method (HMM), ...
2. Methods that approximate the full fine scale solution, e.g. Multiscale Finite Element Method (MFEM), ...

Concerning HMM, we refer to the review article

[E, W.; Engquist, B. et al. Heterogeneous multiscale methods: a review. Commun. Comput. Phys. 2 (2007), no. 3, 367–450.]

Concerning MFEM, there is a recent book:

[Efendiev, Y.; Hou, T. Multiscale finite element methods. Theory and applications. Surveys and Tutorials in the Applied Mathematical Sciences, 4. Springer, 2009.]

› Elliptic multiscale model problem

$$\begin{aligned} -\nabla \cdot (A(x, x/\varepsilon)\nabla u^\varepsilon) &= f \qquad \text{in } \Omega, \\ u^\varepsilon &= 0 \qquad \text{on } \partial\Omega. \end{aligned}$$

We suppose $A(x, y)$ 1-periodic in y and $\varepsilon \ll \operatorname{diam}\Omega$.

Goal

- Robust discretization for $\varepsilon \to 0$ with ε independent complexity
- A posteriori error estimate and self adaptive scheme

$$||u^\varepsilon - u_h|| \leq \eta(u_h, h) + R_h.$$

› Classical Homogenization Result

There exist u^0, A^0, such that $u^\varepsilon \to u^0$ weakly in $H^1_0(\Omega)$, $A^\varepsilon \nabla u^\varepsilon \to A^0 \nabla u^0$ weakly in $L^2(\Omega)^d$ for $\varepsilon \to 0$, and u^0 is a solution of the homogenized problem

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

Furthermore, the homogenized Matrix $A^0(x)$ is given as

$$A^0_{i,j}(x) = \int_Y A_{i,j}(x,y) + \sum_{k,l} \int_Y A_{k,l}(x,y) \nabla_y \chi^x_k(y) \cdot \nabla_y \chi^x_l(y),$$

where $\chi^x_k \in \tilde{H}^1_\#(Y)$ is a solution of the cell problem

$$\int_Y A(x,y) \nabla \chi^x_k \cdot \nabla \varphi = \int_Y A(x,y) e_k \nabla \varphi, \quad \forall \varphi \in \tilde{H}^1_\#(Y).$$

› Two scale convergence (see [Allaire ’92])

Definition

A sequence $u^\epsilon \in L^2(\Omega)$ is two scale convergent to a limit $u_0 \in L^2(\Omega \times Y)$, if for any function $\phi \in \mathcal{D}(\Omega; C^\infty_\#)(Y))$ it holds

$$\lim_{\epsilon \to 0} \int_\Omega u^\epsilon(x)\phi(x, \frac{x}{\epsilon})dx = \int_\Omega \int_Y u_0(x,y)\phi(x,y)dxdy.$$

Theorem (L^2-Compactness)

Let $(u^\epsilon)_\epsilon$ denote a bounded sequence in $L^2(\Omega)$. Then there exists a limit function $u_0 \in L^2(\Omega \times Y)$ such that a subsequence of $(u^\epsilon)_\epsilon$ converges two scale against u_0.

Definition (Two scale homogenized equation [Allaire '92])

A pair $(u^0, u^1) \in H^1_0(\Omega) \times L^2(\Omega; \tilde{H}^1_{\#}(Y))$ is called the two scale homogenized solution of the multiscale problem, if it satisfies

$$\int_\Omega \int_Y A(x,y) \quad (\nabla_x u^0(x) + \nabla_y u^1(x,y))(\nabla_x \Phi(x) + \nabla_y \varphi(x,y))$$
$$= \int_\Omega f(x)\Phi(x), \quad \forall\, (\Phi, \varphi) \in H^1_0(\Omega) \times L^2(\Omega; \tilde{H}^1_{\#}(Y)).$$

Theorem (Two scale convergence)

Let $u^\epsilon \in H^1(\Omega)$ denote the solution of our elliptic homogenization problem. Then u^ϵ converges two scale to u_0 and ∇u^ϵ converges two scale to $\nabla_x u_0 + \nabla_y u_1$ where $(u^0, u^1) \in H^1_0(\Omega) \times L^2(\Omega; \tilde{H}^1_{\#}(Y))$ is a solution of the two scale homogenized equation.

› Two scale convergence: error estimate

From the two scale convergence of ∇u^ϵ to $\nabla_x u_0 + \nabla_y u_1$, it is clear that $u_0(x) + \epsilon u_1(x, \frac{x}{\epsilon})$ should be an approximation of u^ϵ. To make this more precise, we have the following error estimate.

Theorem (Error estimate [Hoang, Schwab '03])

If A is regular enough and $u_0 \in H^2(\Omega)$, then it holds

$$||u^\varepsilon - (u^0(x) + \varepsilon u^1(x, \frac{x}{\varepsilon}))||_{H^1(\Omega)} \leq C\sqrt{\varepsilon}.$$

› Numerical multiscale methods

Let look at the following class of problems

$$\begin{aligned} -\nabla \cdot (A^\epsilon(x) \nabla u^\varepsilon) &= f && \text{in } \Omega, \\ u^\varepsilon &= 0 && \text{on } \partial\Omega. \end{aligned}$$

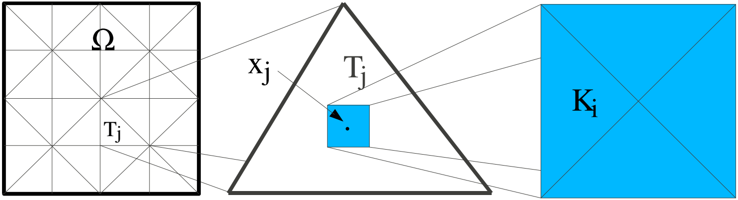
For the time being we make no further assumptions on A^ϵ. Thus ϵ is only a parameter that indications fine scale fluctuations.

Goal

- Robust discretization with ε independent complexity.
- The formulation of the method should not rely on periodicity.

› Heterogeneous Multiscale Method [E, Engquist ’03]

Notation



$$\mathcal{T}_H = \{T_j | j \in J\} \qquad \mathcal{S}_h = \{K_i | i \in I\}$$

$$V_H = \{U_H \in H^1_0(\Omega) |\, U_H|_{T_j} \in \mathbb{P}^l\} \qquad W_h(Y_j^\varepsilon) = \{u_h \in \tilde{H}^1_\#(Y_j^\varepsilon) |\, u_h|_{K_i} \in \mathbb{P}^m\}$$

› Heterogeneous Multiscale Method

The HMM approximation $U_H \in V_H$ is defined as a solution of

$$A_H(U_H, \Phi_H) = (f, \Phi_H), \quad \forall \Phi_H \in V_H$$

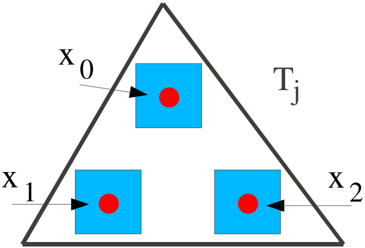
where the discrete bilinear form A_H is given by

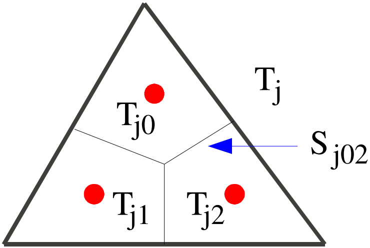
$$A_H(U_H, \Phi_H) \;:=\; \sum_{j \in J} \sum_{k \in Q_j} \frac{q_k}{\varepsilon^d} \int_{Y_k^\varepsilon} A_h^\varepsilon(x) \nabla \mathcal{R}_j(U_H)(x) \cdot \nabla \mathcal{R}_j(\Phi_H)(x) \, \mathrm{dx},$$

with $A_h^\varepsilon|_{K_{i,l}} := A^\varepsilon(y_l)$ for all $K_i \in \mathcal{S}_h(Y_k^\delta), l \in O_i$ and the local reconstructions $\mathcal{R}_j(\Phi_H) \in \Phi_H + W_h^m(Y_k^\delta)$ for given functions $\Phi_H \in V_H^l$ and quadrature points x_k are defined as solutions of the local cell problems

$$\int_{Y_k^\delta} A_h^\varepsilon(x) \nabla_x \mathcal{R}_j(\Phi_H)(x) \cdot \nabla_x \varphi_h(x) \, \mathrm{dx} = 0, \quad \forall \varphi_h \in W_h^m(Y_k^\delta).$$

› Notation





Sketch of the quadrature points $x_k \in T_j$ and shifted unit cells Y_k^δ (left), and notation for a corresponding partition of T_j (right).

› A priori error bound

Theorem (E, Ming and Zhang '03)

Suppose U_H is the HMM approximation where the fine scale cell problems are solved exactly and u^0 the exact solution of the homogenized elliptic problem. Then, if $u^0 \in H^2$, the following estimate holds

$$||u^0 - U_H||_{H^1(\Omega)} \leq C(H + \varepsilon).$$

Problem: In the proof the error is split into

$$||u^0 - U_H|| \leq ||u^0 - U_H^0|| + ||U_H^0 - U_H||.$$

This procedure is not possible for a posteriori type estimates!!

› Setting for a posteriori error analysis

We know how to derive a posteriori error estimates for a variational setting

$$A(u, v) = f(v).$$

Question: Can we recast the HMM in a variational framework!

Ansatz: Try to use the **variational framework of the two scale homogenized equation**!

› Periodicity assumption

Let us suppose that

- $A^\epsilon(x) = A(x, \frac{x}{\epsilon})$, $\quad A(x,y)$ Y – periodic in y.
- $A \in W^{1,\infty}(\Omega \times Y)$ with $0 < c_A \leq A(x,y) \leq C_A \; \forall (x,y) \in \Omega \times Y$.
- Polynomial orders of the approximations spaces $l = m = 1$
- Use one–point quadratures, i.e. $\{(|T_j|, x_j)\}$ for all $T_j \in \mathcal{T}_H$, $\{(|K_i|, y_i)\}$ for all $K_i \in \mathcal{S}_h$, x_j, y_i centers of gravity!
- Choose $\delta = \varepsilon$ and replace $A_h^\epsilon : \Omega \to \mathbb{R}$ in the definition of A_H and $\mathcal{R}_j(\Phi_H)$ by

$$A_h^\epsilon|_{x_j^\varepsilon(K_i)}(x) := A(x_j, \frac{x_j^\varepsilon(y_i)}{\varepsilon}),$$

i.e. we use numerical quadrature on $T_j \times x_j^\varepsilon(K_i)$.

› Heterogeneous Multiscale Method (periodic)

The HMM approximation $U_H \in V_H$ is defined as a solution of

$$A_H(U_H, \Phi_H) = (f, \Phi_H), \quad \forall \Phi_H \in V_H$$

where the discrete bilinear form A_H is given by

$$A_H(U_H, \Phi_H) \;:=\; \sum_{j \in J} |T_j| \fint_{Y_j^\varepsilon} A_h(x, x/\varepsilon) \nabla \mathcal{R}_j(U_H)(x) \cdot \nabla \mathcal{R}_j(\Phi_H)(x)\, dx$$

with $A_h(x,y)|_{T_j \times K_i} := A(x_j, y_i)$ and the local reconstructions $\mathcal{R}_j(\Phi_H) \in \Phi_H + W_h^m(Y_j^\varepsilon)$ are solutions of the local cell problem

$$\int_{Y_j^\varepsilon} A_h(x, x/\varepsilon) \nabla_x \mathcal{R}_j(\Phi_H)(x) \cdot \nabla_x \varphi_h(x)\, dx = 0, \quad \forall \varphi_h \in W_h^m(Y_j^\varepsilon).$$

Lemma (Reformulation of HMM [Ohlberger, MMS 2005])

Define fine scale correction $\mathcal{K}_h(U_H) \in V_H^0(\Omega; W_h^1(Y))$ *of* U_H *through*

$$\mathcal{K}_h(U_H)(x,y)|_{T_j \times Y} := \frac{1}{\varepsilon}\,\mathcal{K}_j(U_H)(\varepsilon\, y), \qquad \mathcal{K}_j(U_H) := \mathcal{R}_j(U_H) - U_H$$

Then, $(U_H, \mathcal{K}_h(U_H)) \in V_H^1 \times V_H^0(\Omega; W_h^1(Y))$ *is a solution of*

$$\int_\Omega \int_Y A_h(x,y) \quad (\nabla_x U_H(x) + \nabla_y \mathcal{K}_h(U_H)(x,y))(\nabla_x \Phi_H(x) + \nabla_y \varphi_h(x,y))\,dxdy$$
$$= \int_\Omega f(x)\Phi_H(x)\,dx, \quad \forall\,(\Phi_H, \varphi_h) \in V_H^1 \times L^2(\Omega; W_h^1(Y))$$

where $A_h : \Omega \times Y \to \mathbb{R}$ *is given by* $A_h(x,y)|_{T_j \times K_i} := A(x_j, y_i)$.

› Result of this observation

In the periodic case, HMM can be seen as a direct Finite Element Approximation of the two-scale homogenized equation with quadrature!

$\Longrightarrow$ **Standard numerical analysis techniques can be applied, as we are now in a nice variational framework!**

› Proof of the reformulation Lemma

We deduce from the discrete cell problems for all $\varphi_h \in W_h^1(Y_j^\varepsilon)$

$$\int_{Y_j^\varepsilon} A_h^\varepsilon(x)\nabla_x(U_H(x) + \mathcal{R}_j(U_H)(x) - U_H(x)) \cdot \nabla_x\varphi_h(x)\, \mathrm{dx} = 0.$$

As $U_H \in V_h^1$, $\nabla_x U_H$ is constant on each simplex T_j which yields after substituting $x = x_j^\varepsilon(y)$, and using the definition of $\mathcal{K}_j(U_H)$,

$$\int_Y A(x_j, \frac{x_j^\varepsilon(y)}{\varepsilon})(\nabla_x U_H(x_j) + \nabla_x\mathcal{K}_j(U_H)(x_j^\varepsilon(y))) \cdot \nabla_x\varphi_h(x_j^\varepsilon(y))\, \varepsilon^d\, \mathrm{dy} = 0.$$

Using the definition of $\mathcal{K}_h(U_H)$ and defining $\tilde{\varphi}_h \in W_h^1(Y)$ as $\tilde{\varphi}_h(y) = \frac{1}{\varepsilon}\varphi_h(\varepsilon y)$ we get

$$\varepsilon^d \int_Y A_h(x_j, \frac{x_j^\varepsilon(y)}{\varepsilon})(\nabla_x U_H(x_j) + \nabla_y\mathcal{K}_h(U_H)(x_j, \frac{x_j^\varepsilon(y)}{\varepsilon})) \cdot \nabla_y\tilde{\varphi}_h(\frac{x_j^\varepsilon(y)}{\varepsilon})\, \mathrm{dy} = 0.$$

› Proof of the reformulation Lemma (cont.)

As the integrand of this equation is $Y-$periodic and $\frac{x_j^\varepsilon(y)}{\varepsilon} = y + \frac{x_j}{\varepsilon}$ we get the following orthogonality relation

$$\varepsilon^d \int_Y A_h(x_j, y)(\nabla_x U_H(x_j) + \nabla_y \mathcal{K}_h(U_H)(x_j, y)) \cdot \nabla_y \tilde{\varphi}_h(y) \, dy = 0.$$

Furthermore, from the definition of U_H and A_h we deduce in the same way

$$\begin{aligned}\int_\Omega f(x)\Phi_H(x) &= \sum_{j\in J} |T_j| \int_Y A(x_j, \frac{x_j^\varepsilon(y)}{\varepsilon})(\nabla_x U_H(x_j) + \nabla_y \mathcal{K}_h(U_H)(x_j, \frac{x_j^\varepsilon(y)}{\varepsilon})) \\ &\qquad \cdot (\nabla_x \Phi_H(x_j) + \nabla_y \mathcal{K}_h(\Phi_H)(x_j, \frac{x_j^\varepsilon(y)}{\varepsilon})) \, dy \\ &= \int_\Omega \int_Y A_h(x, y)(\nabla_x U_H(x) + \nabla_y \mathcal{K}_h(U_H)(x, y)) \\ &\qquad \cdot (\nabla_x \Phi_H(x) + \nabla_y \mathcal{K}_h(\Phi_H)(x, y)) \, dy \, dx.\end{aligned}$$

› Proof of the reformulation Lemma (cont.)

$$\int_\Omega f(x)\Phi_H(x) = \int_\Omega \int_Y A_h(x,y)(\nabla_x U_H(x) + \nabla_y \mathcal{K}_h(U_H)(x,y)) \cdot (\nabla_x \Phi_H(x) + \nabla_y \mathcal{K}_h(\Phi_H)(x,y))\,\mathrm{d}y\,\mathrm{d}x.$$

Using the orthogonality relation, we are allowed to replace $\mathcal{K}_h(\Phi_H)$ by any $\varphi_h \in L^2(\Omega; W_h^1(Y))$. This yields

$$\int_\Omega f(x)\Phi_H(x) = \int_\Omega \int_Y A_h(x,y)(\nabla_x U_H(x) + \nabla_y \mathcal{K}_h(U_H)(x,y)) \cdot (\nabla_x \Phi_H(x) + \nabla_y \varphi_h(x,y))\,\mathrm{d}y\,\mathrm{d}x.$$

□

› Variational formulation

Definition (Bilinear forms $\mathcal{A}$, $\mathcal{A}_h$, and residuals)

Let us define $\mathcal{A}, \mathcal{A}_h : (H^1_0(\Omega) \times L^2(\Omega; \tilde{H}^1_\#(Y)))^2 \to \mathbb{R}$ as

$$\mathcal{A}((\Psi,\psi),(\Phi,\varphi)) := \int_\Omega \int_Y A(x,y)\Big(\nabla_x\Psi(x) + \nabla_y\psi(x,y)\Big)\cdot\Big(\nabla_x\Phi(x) + \nabla_y\varphi(x,y)\Big)\,dx\,dy,$$

$$\mathcal{A}_h((\Psi,\psi),(\Phi,\varphi)) := \int_\Omega \int_Y A_h(x,y)\Big(\nabla_x\Psi(x) + \nabla_y\psi(x,y)\Big)\cdot\Big(\nabla_x\Phi(x) + \nabla_y\varphi(x,y)\Big)\,dx\,dy.$$

Define the residual $\mathrm{Res}_h : H^1_0(\Omega) \times L^2(\Omega; \tilde{H}^1_\#(Y)) \to H^{-1}_0(\Omega) \times L^2(\Omega; \tilde{H}^{-1}_\#(Y))$:

$$\Big\langle \mathrm{Res}_h(\Psi,\psi),(\Phi,\varphi)\Big\rangle := \mathcal{A}_h((\Psi,\psi),(\Phi,\varphi)) - (f,\Phi)_\Omega.$$

› Variational formulation (cont.)

With the definition of the bilinear forms $\mathcal{A}, \mathcal{A}_h$, the exact two scale solution $(u_0, u_1) \in H^1_0(\Omega) \times L^2(\Omega; \tilde{H}^1_\#(Y))$ and the HMM approximation $(U_H, \mathcal{K}_h(U_H)) \in V^1_H \times V^0_H(\Omega; W^1_h(Y))$ can be written as solution of

$$\begin{aligned} \mathcal{A}((u_0, u_1), (\Phi, \varphi)) &= (f, \Phi)_\Omega \ \ \forall (\Phi, \varphi) \in H^1_0(\Omega) \times L^2(\Omega; \tilde{H}^1_\#(Y)), \\ \mathcal{A}_h((U_H, \mathcal{K}_h(U_H)), (\Phi_H, \varphi_h)) &= (f, \Phi_H)_\Omega \ \ \forall (\Phi_H, \varphi_h) \in V^1_H \times V^0_H(\Omega; W^1_h(Y)). \end{aligned}$$

Note that for the residual Res_h it holds

$$\left\langle \mathrm{Res}_h(U_H, \mathcal{K}_h(U_H), (\Phi_H, \varphi_h) \right\rangle = 0 \quad \forall (\Phi_H, \varphi_h) \in V^1_H \times V^0_H(\Omega; W^1_h(Y))$$

Theorem (A–posteriori error estimate)

Set $e^0 := u^0 - U_H$, $e^1 := u^1 - \mathcal{K}_h(U_H)$. *Then the following error estimate holds:*

$$
\begin{aligned}
\|\nabla_x e^0 + \nabla_y e^1\|_{L^2(\Omega\times Y)} \le\; & C_1\Big(\sum_{j\in J}\eta_j^2\Big)^{1/2} + C_2\Big(\sum_{(j,l)\in\mathcal{E}(\mathcal{T}_H)}\eta_{jl}^2\Big)^{1/2} \\
& + C_3\Big(\sum_{j\in J}\sum_{(i,k)\in\mathcal{E}(\mathcal{S}_h)}\eta_{j,ik}^2\Big)^{1/2} + C_1\Big(\sum_{j\in J}\zeta_j^2\Big)^{1/2} + \Big(\sum_{j\in J}\sum_{i\in I}\zeta_{ji}^2\Big)^{1/2}
\end{aligned}
$$

The local indicators are defined as

$$
\begin{aligned}
\eta_j &:= H_j\|f_H\|_{L^2(T_j)}, \\
\eta_{jl} &:= H_{jl}^{1/2}\Big\|\Big[\int_Y\Big(A_h\big(\nabla_x U_H + \nabla_y\mathcal{K}_h(U_H)\big)\Big)\cdot\mathbf{n}\Big]_{S_{jl}}\Big\|_{L^2(S_{jl})}, \\
\eta_{j,ik} &:= h_{ik}^{1/2}\Big\|\Big[\Big(A_h\big(\nabla_x U_H + \nabla_y\mathcal{K}_h(U_H)\big)\Big)\Big|_{T_j}\cdot\mathbf{n}\Big]_{\tilde{S}_{ik}}\Big\|_{L^2(T_j\times\tilde{S}_{ik})}, \\
\zeta_j &:= H_j\|f_H - f\|_{L^2(T_j)}, \\
\zeta_{ji} &:= \|(A_h - A)(\nabla_x U_H + \nabla_y\mathcal{K}_h(U_H))\|_{L^2(T_j\times K_i)}.
\end{aligned}
$$

› Sketch of the proof

Lemma (A posteriori error identity)

The error satisfies the following a–posteriori error identity for all $(\Phi_H,\varphi_h)\in V_h^1\times L^2(\Omega;W_h^1(Y))$ *and all* $(\Phi,\varphi)\in H_0^1(\Omega)\times L^2(\Omega;\tilde H_\#^1(Y))$.

$$\begin{aligned}\mathcal{A}((e^0,e^1),(\Phi,\varphi)) &= -\langle \mathrm{Res}_h(U_H,\mathcal{K}_h(U_H)),(\Phi-\Phi_H,\varphi-\varphi_h)\rangle \\ &+ \mathcal{A}_h((U_H,\mathcal{K}_h(U_H)),(\Phi,\varphi))-\mathcal{A}((U_H,\mathcal{K}_h(U_H)),(\Phi,\varphi)).\end{aligned}$$

Proof. With the variational formulation and the definition of e^0, e^1 we have

$$\begin{aligned}\mathcal{A}((e^0,e^1),(\Phi,\varphi)) &= \mathcal{A}((u^0,u^1),(\Phi,\varphi))-\mathcal{A}((U_H,\mathcal{K}_h(U_H)),(\Phi,\varphi))\\ &= (f,\Phi)_\Omega-\mathcal{A}_h((U_H,\mathcal{K}_h(U_H)),(\Phi,\varphi))\\ &\quad +\mathcal{A}_h((U_H,\mathcal{K}_h(U_H)),(\Phi,\varphi))-\mathcal{A}((U_H,\mathcal{K}_h(U_H)),(\Phi,\varphi))\\ &= -\langle \mathrm{Res}_h(U_H,\mathcal{K}_h(U_H)),(\Phi,\varphi)\rangle+\langle \mathrm{Res}_h(U_H,\mathcal{K}_h(U_H)),(\Phi_H,\varphi_h)\rangle\\ &\quad +\mathcal{A}_h((U_H,\mathcal{K}_h(U_H)),(\Phi,\varphi))-\mathcal{A}((U_H,\mathcal{K}_h(U_H)),(\Phi,\varphi)).\end{aligned}$$ □

› Sketch of the proof (cont.)

Corollary (Abstract a posteriori error estimate)

$$||\nabla_x e^0 + \nabla_y e^1||_{L^2(\Omega\times Y)} \leq C_0 \inf_{\substack{(\Phi_H,\varphi_h)\in \\ V_h^1\times L^2(\Omega;W_h^1(Y))}} \sup_{\substack{(\Phi,\varphi)\in H_0^1(\Omega)\times L^2(\Omega;\tilde{H}^1_\#(Y)),\\ ||\nabla_x\Phi+\nabla_y\varphi||_{L^2(\Omega\times Y)}=1}} \Big\{ \Big| \langle \mathrm{Res}_h(U_H,\mathcal{K}_h(U_H)),(\Phi-\Phi_H,\varphi-\varphi_h)\rangle \Big| + \Big| \mathcal{A}_h((U_H,\mathcal{K}_h(U_H)),(\Phi,\varphi)) - \mathcal{A}((U_H,\mathcal{K}_h(U_H)),(\Phi,\varphi)) \Big| \Big\}.$$

Proof. Using duality and uniform ellipticity of A we get

$$c_A||\nabla_x e^0 + \nabla_y e^1||_{L^2(\Omega\times Y)} \leq \sup_{\substack{(\Phi,\varphi)\in H_0^1(\Omega)\times L^2(\Omega;\tilde{H}^1_\#(Y)),\\ ||\nabla_x\Phi+\nabla_y\varphi||_{L^2(\Omega\times Y)}=1}} \mathcal{A}((e^0,e^1),(\Phi,\varphi)).$$

Together with the error identity and taking the infimum with respect to (Φ_H, φ_h) this yields the result! □

› Sketch of the proof (cont.)

The proof is now concluded by localization and using estimates of appropriate H^1 interpolation operators, i.e.

Lemma (Error estimates for H^1 interpolation)

Let us denote by $I_H : L^2(\Omega) \to V_h^1$ *and* $\tilde{I}_h : L^2(Y) \to W_h^1(Y)$ *the Clément interpolation operators. Furthermore, let us define*
$I_h : L^2(\Omega; L^2(Y)) \to L^2(\Omega; W_h^1(Y))$ *as* $I_h\varphi(x,y) := \tilde{I}_h(\varphi(x,\cdot))(y)$, for all $x \in \Omega$.
Then, the following estimates hold for all $\Phi \in H^1(\Omega)$ *and* $\varphi \in L^2(\Omega; \tilde{H}_\#^1(Y))$

$$
\begin{aligned}
||\Phi - I_H\Phi||_{L^2(T)} &\le C_{I_1} H_T ||\nabla_x \Phi||_{L^2(\omega_T)}, \\
||\Phi - I_H\Phi||_{L^2(S_{jl})} &\le C_{I_2} H_{jl}^{1/2} ||\nabla_x \Phi||_{L^2(\omega_{S_{jl}})}, \\
||\varphi - I_h\varphi||_{L^2(T\times K)} &\le C_{I_3} h_K ||\nabla_y \varphi||_{L^2(T\times\omega_K)}, \\
||\varphi - I_h\varphi||_{L^2(T\times S_{ik})} &\le C_{I_4} h_{ik}^{1/2} ||\nabla_y \varphi||_{L^2(T\times\omega_{S_{ik}})}.
\end{aligned}
$$

› Further results

Theorem (Lower bound on the error)

$$\Big(\sum_{j\in J}\eta_j^2\Big)^{1/2} + \Big(\sum_{(j,l)\in\mathcal{E}(\mathcal{T}_H)}\eta_{jl}^2\Big)^{1/2} + \Big(\sum_{j\in J}\sum_{(i,k)\in\mathcal{E}(\mathcal{S}_h)}\eta_{j,ik}^2\Big)^{1/2}$$

$$\leq \quad C\Big(||\nabla_x e^0 + \nabla_y e^1||_{L^2(\Omega\times Y)} + \Big(\sum_{j\in J}\zeta_j^2\Big)^{1/2} + \Big(\sum_{j\in J}\sum_{i\in I}\zeta_{ji}^2\Big)^{1/2}\Big).$$

Theorem (A–priori error estimate)

Let us assume $(u^0, u^1) \in H^2(\Omega) \times L^2(\Omega; H^2_\#(Y))$*. The error* (e^0, e^1) *then satisfies the following a–priori error estimate*

$$||\nabla_x e^0 + \nabla_y e^1||_{L^2(\Omega\times Y)} \leq C(H+h).$$

› Numerical experiments

Quasi one dimensional periodic problem

We start with the following model problem [Hoang, Schwab '03]

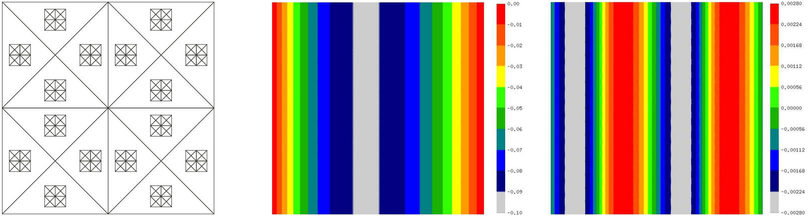
$$\begin{aligned}
-\nabla \cdot (A^\varepsilon(x)\nabla u^\varepsilon) &= f(x) && \text{in } \Omega := (0,1)^2,\\
u^\varepsilon &= 0 && \text{on } \Gamma_D := \{0\} \times (0,1) \cup \{1\} \times (0,1),\\
A^\varepsilon(x)\nabla u^\varepsilon &= 0 && \text{on } \Gamma_N := \partial\Omega \setminus \Gamma_D
\end{aligned}$$

with

- $f(x) = -1$,
- $A^\varepsilon(x) = a_0(x_1)a_1(\frac{x_1}{\varepsilon})$,
- $a_0(x_1) = 1 + x_1$,
- $a_1(y_1) = 2/3(1 + \cos^2(2\pi y_1))$.

› Numerical experiments

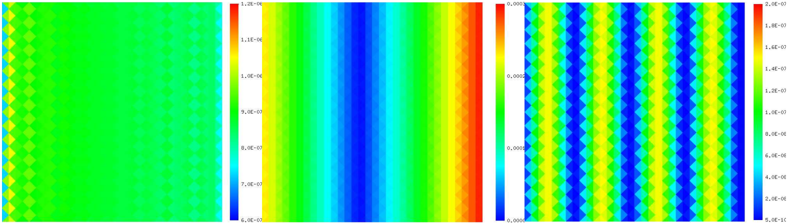
Quasi one dimensional periodic problem



Coarse computational grids for the macro and micro scale (left), HM–FEM solution (middle) and solution of one of the cell problems (right).

› Numerical experiments

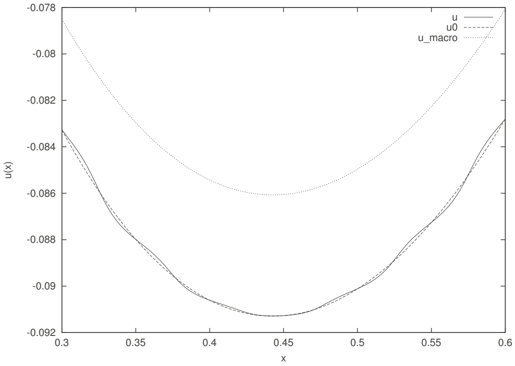
Quasi one dimensional periodic problem



Local distribution of the error indicators. Macroscopic indicator (left), macroscopic distribution of the microscopic indicator (middle), microscopic indicator on one of the micro cells (right).

› Numerical experiments

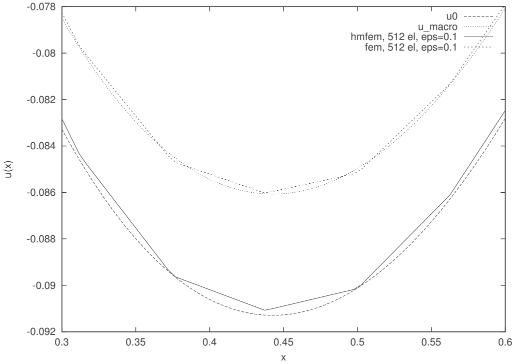
Quasi one dimensional periodic problem



Exact solution u for $\varepsilon = 0.1$, homogenized solution u^0, and solution of the problem with $a_2 = 1$.

› Numerical experiments

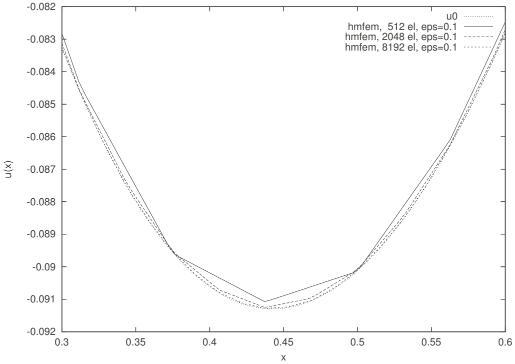
Quasi one dimensional periodic problem



Comparison of the HM-FEM solution with the standard finite element solutions on a coarse macro grid with 512 elements.

› Numerical experiments

Quasi one dimensional periodic problem



Convergence study of the HM-FEM solution on successively refined grids.

› Numerical experiments

Quasi one dimensional periodic problem

Convergence of U_H and $\mathcal{K}_h(U_H)$

H	$\|\|U_H - u^\varepsilon\|\|_{L^2(\Omega)}$	$\|\|U_H - u^0\|\|_{L^2(\Omega)}$	$\|\|\nabla_x(U_H - u^0)\|\|_{L^2(\Omega)}$	η_H
2^{-3}	0.000614	0.000874	0.027522	0.168951
2^{-4}	0.000527	0.000397	0.013717	0.084631
2^{-5}	0.000390	9.19e-05	0.006837	0.042386
2^{-6}	0.000397	2.02e-05	0.003423	0.021217
2^{-7}	0.000416	4.59e-06	0.001733	0.010614

h/ε	$\|\|\mathcal{K}_h(U_H) - u^1\|\|_{L^2(\Omega\times Y)}$	$\|\|\nabla_y(\mathcal{K}_h(U_H) - u^1)\|\|_{L^2(\Omega\times Y)}$	η_h
2^{-2}	0.000166	0.025736	0.125887
2^{-3}	5.75e-05	0.017562	0.078639
2^{-4}	1.53e-05	0.009240	0.042547
2^{-5}	4.01e-06	0.004617	0.021551
2^{-6}	1.05e-06	0.002308	0.010817

› Numerical experiments

Quasi one dimensional periodic problem

Convergence of the error indicators η_H and η_h

H	$\|\|\nabla_x e^0 + \nabla_y e^1\|\|_{L^2(\Omega\times Y)}$	$\eta_H + \eta_h$	$\frac{\eta_H+\eta_h}{\|\|\nabla_x e^0+\nabla_y e^1\|\|_{L^2(\Omega\times Y)}}$	EOC$(\eta_H + \eta_h)$
2^{-3}	0.053259	0.294838	5.53596	
2^{-4}	0.031279	0.163270	5.21975	0.853
2^{-5}	0.016077	0.084933	5.28283	0.943
2^{-6}	0.008040	0.042768	5.31934	0.999
2^{-7}	0.004041	0.021431	5.30343	0.997

› Numerical experiments

Two dimensional problem with corner singularity

Define the non-convex domain Ω as

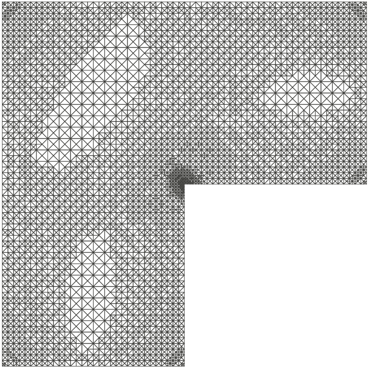
$$\Omega := (0,1)^2 \setminus \left((0,0.5)^2 + (0.5,0)^\top \right).$$

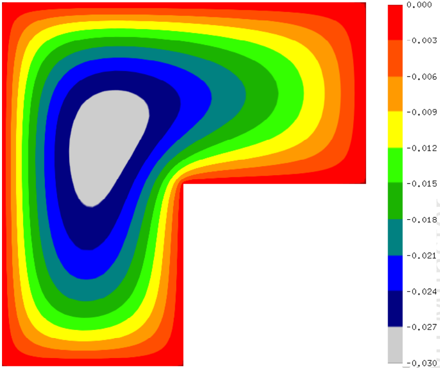
Let A, f be given as in the previous example. We then look at the problem

$$\begin{aligned} -\nabla \cdot (A^\varepsilon(x) \nabla u^\varepsilon) &= f(x) && \text{in } \Omega, \\ u^\varepsilon &= 0 && \text{on } \partial\Omega. \end{aligned}$$

› Numerical experiments

Two dimensional problem with corner singularity

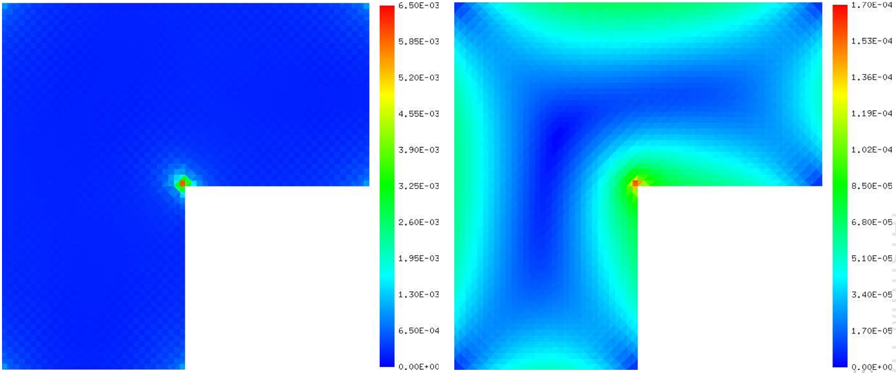




Adaptive macroscopic grid and adaptive HM–finite element solution.

› Numerical experiments

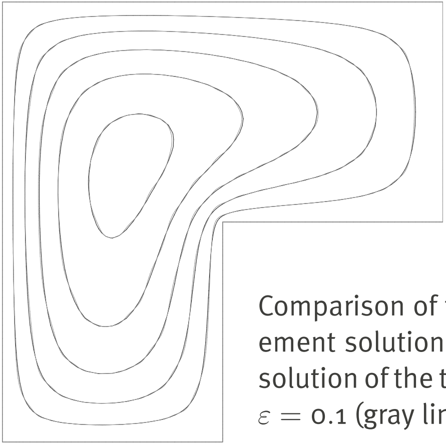
Two dimensional problem with corner singularity



Distribution of the error indicators η_H (left) and η_h (right) on a uniform macroscopic grid.

› Numerical experiments

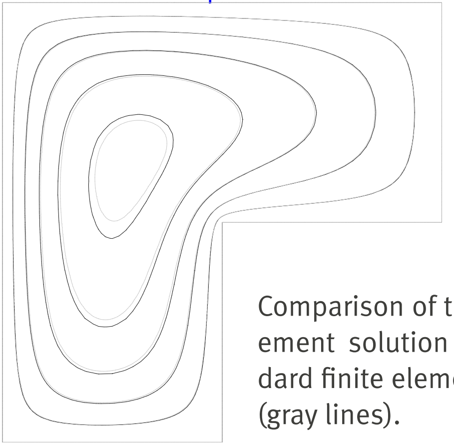
Two dimensional problem with corner singularity



Comparison of the isolines of HM–finite element solution (black lines) with the exact solution of the two dimensional problem for $\varepsilon = 0.1$ (gray lines).

› Numerical experiments

Two dimensional problem with corner singularity



Comparison of the isolines of HM–finite element solution (black lines) with a standard finite element solution for $\varepsilon = 0.0001$ (gray lines).

› Nonlinear elliptic multiscale problems

[Henning, Ohlberger 2011]

$$\nabla \cdot A^\epsilon(x, \nabla u_\epsilon(x)) = f(x) \quad \text{in } \Omega,$$
$$u_\epsilon(x) = 0 \quad \text{on } \partial\Omega.$$

where we assume uniformly in x:

- $A^\epsilon(x, \cdot)$ is strongly monotone,
- $A^\epsilon(x, \cdot) \in \left(H^{1,\infty}(\mathbb{R}^d)\right)^d$ and
- $A^\epsilon(x, 0) = 0$.

Note: With further assumptions this can be generalized for '$A^\epsilon(x, u_\epsilon(x), \nabla u_\epsilon(x))$'!

› Nonlinear elliptic multiscale problems

Assumption (Continuity and monotonicity of A^ϵ)

We assume that there exist two constants $0 < \alpha \leq \beta < \infty$ such that uniformly $\forall x \in \Omega$:

$$(A^\epsilon(x,\xi_1) - A^\epsilon(x,\xi_2), \xi_1 - \xi_2) \geq \alpha|\xi_1 - \xi_2|^2,$$
$$|A^\epsilon(x,\xi_1) - A^\epsilon(x,\xi_2)| \leq \beta|\xi_1 - \xi_2| \text{ and}$$
$$A^\epsilon(x,0) = 0.$$

$\Longrightarrow$ These assumptions guarantee existence and uniqueness of the nonlinear problem!!

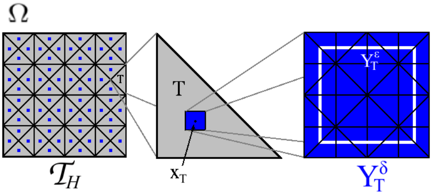
Definition (HMM for monotone elliptic problems)

Find $u_H \in V_H$ with

$$\sum_{T\in\mathcal{T}_H} |T| \fint_{Y_T^\epsilon} A^\epsilon(\nabla R_T(u_H))\cdot\nabla\Phi_H = \int_\Omega f\Phi_H \qquad \forall \Phi_H \in V_H,$$

where $R_T(u_H) \in u_H + W_h(Y_T^\delta)$ solves

$$\int_{Y_T^\delta} A^\epsilon(\nabla R_T(u_H))\cdot\nabla\phi_h = 0 \qquad \forall \phi_h \in W_h(Y_T^\delta) \subset H^1_{per}(Y_T^\delta).$$



› Analysis beyond the periodic setting

Definition (Applicability of the HMM)

We say that HMM is *applicable*, if

$$\lim_{\epsilon \to 0} \lim_{H,h \to 0} \|u_H - u^\epsilon\|_{L^2(\Omega)} = 0,$$

Goal: Derivation of an a posteriori error estimate which only assumes applicability.

Note: From homogenization theory it is clear that HMM is applicable in the periodic setting (see e.g. [Allaire '94, Wall '98])

› Setting for error estimation

Find $u_H \in V_H$

$$\sum_{T \in \mathcal{T}_H} |T| \fint_{Y_T^\epsilon} A^\epsilon \left(\nabla R_T(u_H)\right) \cdot \nabla \Phi_H = \int_\Omega f \Phi_H.$$

We need an analytic reference solution!

Periodic setting

If $period = \epsilon$ and $\delta = k\epsilon$, $k \in \mathbb{N}_{>0}$ then we know:

$$u_H \to u^0 \quad \text{strongly in} \quad H^1(\Omega).$$

What can we do in the generalized setting?

Non-periodic setting

$$u_H \to ? \quad \text{strongly in} \quad H^1(\Omega).$$

Definition (Coarse scale limit problem)

Let us define $u^c \in \mathring{H}^1(\Omega)$ as a solution of

$$\int_\Omega A^0(x, \nabla_x u^c(x)) \cdot \nabla_x \Phi(x)\, dx = \int_\Omega f(x)\Phi(x)\, dx \quad \forall \Phi \in \mathring{H}^1(\Omega).$$

where the effective diffusion coefficient A^0 is given as

$$A^0(x,\xi) := \fint_{\frac{\epsilon}{\delta}Y} A^\epsilon(x + \delta y, \xi + \nabla_y Q(\xi)(x,y))\, dy.$$

The image $Q(\xi)$ under $Q : \mathbb{R}^d \to L^2(\Omega, \tilde{H}^1_\sharp(Y))$ is given as

$$\int_Y A^\epsilon(x + \delta y, \xi + \nabla_y Q(\xi)(x,y)) \cdot \nabla_y \phi(y)\, dy = 0 \quad \forall \phi \in \tilde{H}^1_\sharp(Y).$$

› Coarse scale limit problem

Theorem (Convergence of HMM)

Let u_H denote the HMM approximation. We than have

$$u_H \stackrel{H,h\to 0}{\longrightarrow} u^c \ \text{ strongly in } \ H^1(\Omega),$$

Goal: Derive a posteriori error estimate of the form

$$\|u_H - u^c\|_{L^2(\Omega)} \leq \eta_H(u_H)$$

.

Theorem (A posteriori error estimate)

$$\|u_H - u^c\|^2_{L^2(\Omega)} \leq \sum_{T\in\mathcal{T}_H} H_T^4 \|f\|^2_{L^2(T)} + \sum_{T\in\mathcal{T}_H} \eta_T^{app}(u_H) + \bar{\eta}_T^{app}(u_H) + \sum_{E\in\Gamma(\mathcal{T}_H)} H_E^3\, \eta_E^{res}(u_H) + \sum_{T\in\mathcal{T}_H} \bar{\eta}_T^{res}(u_H) \qquad (1)$$

where $\eta_T^{app}/\eta_T^{res}$ denote approximation/residual error indicators.

For $\Phi_H \in V_H(\Omega)$, the local *approximation error indicators* are defined by

$$\eta_T^{app}(\Phi_H) := \| \int_Y w^{\epsilon_0,\delta}(y) \left(A^{\epsilon,\delta} - A_h^{\epsilon,\delta}\right)(\cdot, y, \nabla_x \Phi_H(x_T) + \nabla_y \mathcal{Q}_h(\Phi_H)(x_T, y))\, dy\|^2_{L^2(T)} \text{ and}$$

$$\bar{\eta}_T^{app}(\Phi_H) := \| \int_Y \left(A^{\epsilon,\delta} - A_h^{\epsilon,\delta}\right)(\cdot, y, \nabla_x \Phi_H(x_T) + \nabla_y \mathcal{Q}_h(\Phi_H)(x_T, y))\, dy\|^2_{L^2(T)}.$$

The local *residual error indicators* are given by

$$\eta_E^{res}(\Phi_H) := H_E^3 \,\| \int_Y [w^{\epsilon_0,\delta}(y) A_h^{\epsilon,\delta}(\cdot, y, \nabla_x \Phi_H + \nabla_y \mathcal{Q}_h(\Phi_H)(\cdot, y))]_E\, dy\|^2_{L^2(E)} \text{ and}$$

$$\bar{\eta}_T^{res}(\Phi_H) := \sum_{E_Y\in\Gamma(\mathcal{T}_h(Y))/\sim_Y} h_{E_Y}^3 \,\|[A_h^{\epsilon,\delta}(\cdot, \cdot, \nabla_x \Phi_H + \nabla_y \mathcal{Q}_h(\Phi_H))]_{E_Y}\|^2_{L^2(T\times E_Y)}.$$

Numerical Experiments

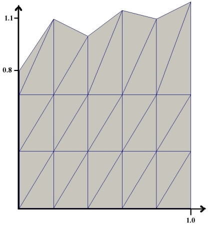
Model Problem (heterogeneous Mikrostruktur)

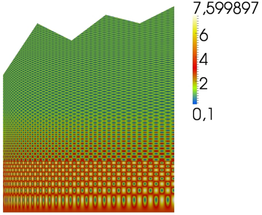
$$-\nabla \cdot A(x, \nabla u(x)) = \begin{cases} \frac{1}{10} & \text{für } x \in \Omega,\ x_2 \leq \frac{1}{10} \\ 1 & \text{für } x \in \Omega,\ x_2 > \frac{1}{10}. \end{cases}$$

$$u(x) = 0 \quad \text{auf } \partial\Omega.$$

with:

$$A(x,\xi) := \begin{pmatrix} \xi_1 + \frac{1}{3}\xi_1^3 \\ \xi_2 + \frac{1}{3}\xi_2^3 \end{pmatrix} \begin{cases} 4 + \frac{18}{5}\sin(40\pi\sqrt{|2x_1|})\sin(90\pi x_2^2) & \text{for } x_2 \leq \frac{3}{10} \\ (3 - \frac{10x_2}{3}) \cdot \left(1 + \frac{9}{10}\sin(40\pi\sqrt{|2x_1|})\sin(90\pi x_2^2)\right) & \text{for } x_2 \in (\frac{3}{10}, \frac{6}{10}) \\ 1 + \frac{9}{10}\sin(40\pi\sqrt{|2x_1|})\sin(90\pi x_2^2) & \text{for } x_2 \geq \frac{6}{10}. \end{cases}$$





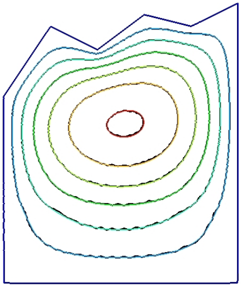
Numerical results:

H	h	ϵ	δ	$\|u_H - u^\epsilon\|_{L^2(\Omega)}$
2^{-2}	2^{-5}	0.15	0.3	$5.2 \cdot 10^{-3}$
2^{-2}	2^{-5}	0.1	0.2	$4.7 \cdot 10^{-3}$
2^{-2}	2^{-6}	0.15	0.3	$4.1 \cdot 10^{-3}$
2^{-3}	2^{-5}	0.05	0.1	$1.7 \cdot 10^{-3}$
2^{-3}	2^{-8}	0.15	0.3	$9.7 \cdot 10^{-4}$
2^{-4}	2^{-6}	0.05	0.1	$4.3 \cdot 10^{-4}$

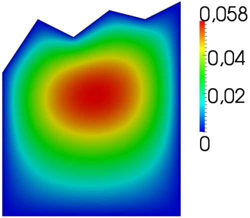
HMM error for increasing resolution of the micro structure through combintations of h, ϵ and δ.

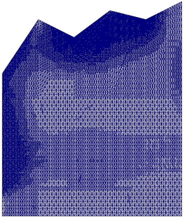
H	h	ϵ	δ	$\|u_H - u^\epsilon\|_{L^2(\Omega)}$	η_H
2^{-2}	2^{-4}	0.05	0.1	$5.1 \cdot 10^{-3}$	$6.0 \cdot 10^{-2}$
2^{-3}	2^{-5}	0.05	0.1	$1.6 \cdot 10^{-3}$	$1.6 \cdot 10^{-2}$
2^{-3}	2^{-7}	0.15	0.3	$1.3 \cdot 10^{-3}$	$1.4 \cdot 10^{-2}$
2^{-4}	2^{-6}	0.05	0.1	$4.3 \cdot 10^{-4}$	$4.4 \cdot 10^{-3}$

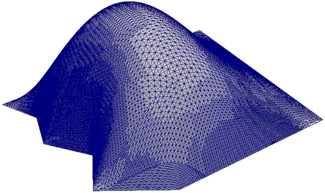
Comparison of error and error estimator.
Observation: Effectivity index is approx. constant at arround 10.



Comparison of isolines for exact and HMM-approximation for $H = 2^{-5}$ and $\delta = \epsilon$.







Exact solution and adaptively refined mesh. The refinement is concentrated at the singularities comming from the re-entering corners.

› Further work

HMM for elliptic problems on perforated domains.

[Henning, Ohlberger: Numer. Math., 2009]

HMM for multi-scale transport with large expected drift

in the context of the BMBF-Project “AdaptHydroMod”
[Henning, Ohlberger: Netw. Heterog. Media. 2010]
[Henning, Ohlberger: J. Anal. Appl. 2011]
[Henning, Ohlberger: submitted to MMS, 2011]

› Outline

Motivation: Multi-Scale and Multi-Physics Problems

Introduction to a posteriori error estimation
- Error control for stationary variational problems
- Adaptive schemes/ equal distribution strategy

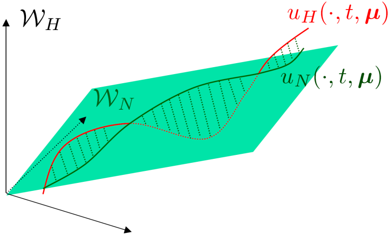
Error control and adaptivity for numerical multiscale methods
- Linear elliptic multiscale problems
- Nonlinear elliptic multiscale problems

Model reduction and multiscale methods
- Reduced Basis Methods
- A new reduced basis DG multiscale method

› Reduced Basis Method for Evolution Equations

Goal: Fast "Online"-Simulation of Complex Evolution Systems for

- Parameter Optimization
- Design Optimization
- Optimal Control
- Integration into System Simulation



Ansatz:

- Reduced Basis Method (RB)

$$\dim(W_N) \ll \dim(W_H)\ !$$

Classical references:

notation RB [Noor, Peters '80], initial value problems [Porsching, Lee '87], method [Nguyen et al. '05], book [Patera, Rozza '07], http://augustine.mit.edu, http://morepas.org

› Model Reduction: Reduced Basis Method

Goal: Find $c(\cdot, t; \boldsymbol{\mu}) \in L^2(\Omega)$ for $t \in [0, T]$, $\boldsymbol{\mu} \in P \subset \mathbb{R}^p$ with

$$\partial_t c(\boldsymbol{\mu}) + L_{\boldsymbol{\mu}}(c(\boldsymbol{\mu})) = 0 \qquad \text{in } \Omega \times [0, T],$$

plus suitable Initial and Boundary Conditions.

Assumption: FV/DG Approximation $c_H(\boldsymbol{\mu}) \in W_H$ for given Parameter $\boldsymbol{\mu}$

Ansatz (RB): Define low dimensional Subspace $W_N \subset W_H$
and project FV/DG Scheme onto the Subspace
$\Longrightarrow$ RB Approximation $c_N(\boldsymbol{\mu}) \in W_N$.

Requirement:
- Efficient Choice of W_N (Exponential Convergence in N)
- Offline–Online Decomposition for all Calculations
- Error Control for $||c_H(\boldsymbol{\mu}) - c_N(\boldsymbol{\mu})||$

› Model Reduction: Reduced Basis Method

Assumption: FV/DG Scheme for Evolution Equations

$$c_H^0 = P[c_0(\mu)], \qquad L_I^k(\mu)[c_H^{k+1}(\mu)] = L_E^k(\mu)[c_H^k(\mu)] + b^k(\mu).$$

with time step counter k and $c_H^k(\mu) \in W_H$.

RB Method: Let $W_N \subset W_H$ be given, $\{\varphi_1, \dots, \varphi_N\}$ a ONB of W_N.

Sought: $c_N^k(\mu) = \sum_{n=1}^{N} \mathbf{a}_n^k(\mu)\varphi_n$ with $\mathbf{L}_I^k(\mu)\mathbf{a}^{k+1} = \mathbf{L}_E^k(\mu)\mathbf{a}^k + \mathbf{b}^k(\mu)$

where

$$(\mathbf{L}_I^k(\mu))_{nm} := \int_\Omega \varphi_n L_I^k(\mu)[\varphi_m], \qquad (\mathbf{L}_E^k(\mu))_{nm} := \int_\Omega \varphi_n L_E^k(\mu)[\varphi_m],$$

$$(\mathbf{a}^0(\mu))_n = \int_\Omega P[c_0(\mu)]\varphi_n, \qquad (\mathbf{b}^k(\mu))_n := \int_\Omega \varphi_n b^k(\mu).$$

› Offline–Online Decomposition

Goal: All Steps for the Calculation of $c_N(\boldsymbol{\mu})$ and for the Calculation of the Error Estimator are split into Two Parts:

- Offline–Step: Complexity depending on $\dim(W_H)$
- Online–Step: Complexity independent of $\dim(W_H)$

Constrained: Affine Parameter Dependency of the Evolution Scheme

$$L_l^k(\boldsymbol{\mu})[\cdot] \;=\; \sum_{q=1}^{Q} \quad L_l^{k,q}[\cdot] \qquad \sigma_{L_l}^q(\boldsymbol{\mu})$$

depending on x — depending on $\boldsymbol{\mu}$

$\Longrightarrow$ Precompute offline: $$(L_l^{k,q})_{nm} := \int_\Omega \varphi_n L_l^{k,q}[\varphi_m]$$

$\Longrightarrow$ Assemble online: $$(L_l^k(\boldsymbol{\mu}))_{nm} := \sum_{q=1}^{Q} (L_l^{k,q})_{nm} \sigma_{L_l}^q(\boldsymbol{\mu})$$

› Example: Convection-Diffusion Problem

$$\partial_t c(\mu) + \nabla \cdot (\mathbf{v}(\mu)c(\mu) - d(\mu)\nabla c(\mu)) = 0 \ \text{ in } \Omega \times [0, T_{\max}],$$

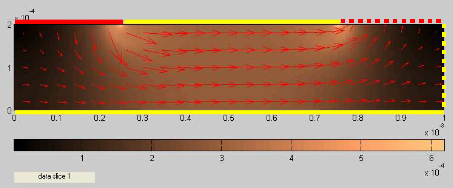
$$\begin{aligned} c(\cdot, 0; \mu) &= c_0(\mu) \ \text{ in } \Omega, \\ c(\mu) &= b_{\mathrm{dir}}(\mu) \ \text{ in } \Gamma_{\mathrm{dir}} \times [0, T_{\max}], \\ (\mathbf{v}(\mu)c(\mu) - d(\mu)\nabla c(\mu)) \cdot \mathbf{n} &= b_{\mathrm{neu}}(u; \mu) \ \text{ in } \Gamma_{\mathrm{neu}} \times [0, T_{\max}]. \end{aligned}$$

Discretization by Finite Volumes $\Longrightarrow$ $c_H(\mu) \in W_H$.

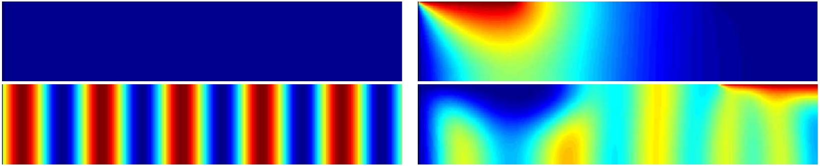
› Example: Convection-Diffusion Problem

Parameter:

- Initial Data
- Boundary Values
- Diffusion Parameter



Possible Variations of the Solution:



› Numerical Experiment

CPU-Time Comparison for a Convection-Diffusion Problem:

Discretization: 40×200 **Elements,** $K = 200$ **time steps**

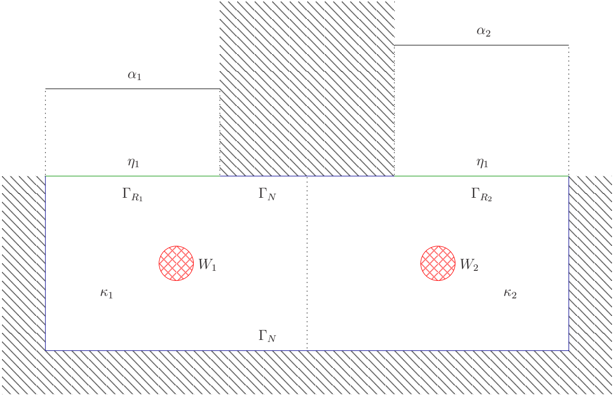
	time dependent data			constant data		
	Reference	RB online	RB offline	Reference	RB online	RB offline
implicit	155.94s	16.67s	447.16s	45.67s	1.02s	2.41s
Factor		**9.44**			**44.77**	
explicit	105.97s	16.53s	437.20s	1.51s	0.79s	2.31s
Factor		**6.41**			**1.91**	

Discretization: 80×400 **Elements,** $K = 1000$ **time steps**

	time dependent data			constant data		
	Reference	RB online	RB offline	Reference	RB online	RB offline
implicit	4043.18s	143.57s	8693.90s	924.91s	6.18s	9.22s
Factor		**28.27**			**149.66**	
explicit	2758.20s	134.00s	8506.60s	17.41s	3.64s	8.83s
Factor		**20.58**			**4.78**	

› Optimization of materials in thermal conductivity

[Schaefer 2010]



› Primal Problem: Thermal Conductivity in a Block

Thermal Conductivity in a Block

$$
\begin{aligned}
-\nabla\cdot(a\nabla u) &= f && (\Omega),\\
a\nabla u\cdot n &= 0 && (\Gamma_N),\\
a\nabla u\cdot n &= \eta\,(g_R - u) && (\Gamma_R),
\end{aligned}
$$

with

$$
\begin{aligned}
a(x) &:= \kappa_1\chi_{[0,0.3)\times[0,0.2]}(x) + \kappa_2\chi_{[0.3,0.6]\times[0,0.2]}(x) && (x\in\Omega),\\
f &:= \vartheta_1\chi_{W_1} + \vartheta_2\chi_{W_2} && (\Omega),\\
\eta &:= \eta_1\chi_{\Gamma_{R_1}} + \eta_2\chi_{\Gamma_{R_2}} && (\Gamma_R),\\
g_R &:= \alpha_1\chi_{\Gamma_{R_1}} + \alpha_2\chi_{\Gamma_{R_2}} && (\Gamma_R).
\end{aligned}
$$

› Parameters

Parameters to be optimized:

- thermal conductivities κ_1, κ_2
- heat transfer coefficients η_1, η_2

Parameters that are kept fix:

- outside temperatures α_1, α_2
- temperatures ϑ_1, ϑ_2 of heat sources W_1, W_2

› A Simple Optimization Problem

Define

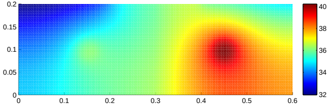
- $J(\mu) := \sum_{i=1}^{4} \mu_i$,
- $\mu_1 = \kappa_1, \mu_2 = \kappa_2, \mu_3 = \eta_1, \mu_4 = \eta_2$,
- $\Omega_1 := [0, 0.3) \times [0, 0.2] \subset \Omega$, $\Omega_2 := \Omega \setminus \Omega_1$,
- $T_i(\mu) := \frac{1}{|\Omega_i|} \int_{\Omega_i} u(\mu)\, \mathrm{dx}$.

Then, the optimization problem reads as follows:

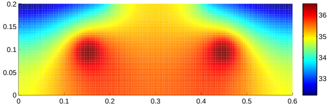
$$\begin{aligned} &\text{Find} \quad \mu^* = \arg\min_{\mu \in \mathcal{P}} J(\mu) \\ &\text{s.t.} \quad T_i(\mu) \leq T_{i,\max} \qquad (i = 1, 2), \end{aligned}$$

for some bound $T_{\max} := (T_{1,\max}, T_{2,\max}) \in \mathbb{R}^2$.

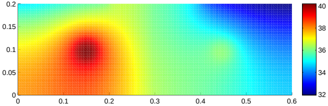
› Optimization Results



(a) $\mu = (.848, .315, .218, .100)$



(b) $\mu = (.624, .624, .166, .166)$



(c) $\mu = (.316, .848, .100, .217)$

Figure: Reduced simulation results for the optimal parameters (grid with 7500 cells): a) $T_{\max} = (35, 50)$, b) $T_{\max} = (35, 35)$, c) $T_{\max} = (50, 35)$

› Comparison of Overall Runtime

T_{max}	runtime [s]	
	detailed	reduced
(35, 50)	338.96	65.24 / 0.34
(35, 35)	179.71	– / 0.22
(50, 35)	283.38	– / 0.39
	$\sum = 802.06$	$\sum = 66.19$

Table: CPU time for different bounds T_{max}.

› A Posteriori Error Estimates [Haasdonk, Ohlberger '08]

Definition: Residual of the FV/DG Method at Time t^k

$$R^{k+1}(\mu)[c_N] := \frac{1}{\Delta t}\left(L_I^k(\mu)[c_N^{k+1}(\mu)] - L_E^k(\mu)[c_N^k(\mu)] - b^k(\mu)\right)$$

Theorem: A Posteriori Error Estimate in $L^\infty L^2$

$$||c_N^k(\mu) - c_H^k(\mu)|| \leq \sum_{l=0}^{k-1} \Delta t\,(C_E)^{k-1-l}\,||R^{l+1}(\mu)[c_N(\mu)]||$$

› Sketch of the proof

Let us denote $e^k := c_N^k - c_H^k$. The definition of the residual and of the exact evolution scheme yields

$$\begin{aligned} L_I^k[e^{k+1}] &= L_I^k[u_N^{k+1}] - L_I^k[u_H^{k+1}] \\ &= \Delta t_k R^{k+1} + L_E^k[u_N^k] + b^k - L_I^k[u_H^{k+1}] \\ &= \Delta t_k R^{k+1} + L_E^k[u_N^k] - L_E^k[u_H^k]. \end{aligned}$$

Thus, the error satisfies the evolution equation

$$L_I^k[e^{k+1}] = \Delta t_k R^{k+1} + L_E^k[e^k].$$

The representation of $L_I^k = Id + \Delta t_k \bar{L}_I^k$ and the positive definiteness of $\bar{L}_I^k$ imply $||(L_I^k)^{-1}|| \leq 1$. Thus, with continuity of the operators we obtain

$$||e^{k+1}|| \leq ||L_I^k||^{-1} \left(\Delta t_k ||R^{k+1}|| + ||L_E^k|| ||e^k|| \right) \leq \Delta t_k ||R^{k+1}|| + C_E ||e^k||.$$

Resolving this recursion yields the proposed a posteriori error estimate. □

› A Posteriori Error Estimates [Haasdonk, Ohlberger '08]

Theorem: A posteriori error estimate in weighted energy norm

$$||c_N(\mu) - c_H(\mu)||_\gamma^2 \leq \frac{1}{4\alpha C(1-\gamma C)} \left(\sum_{l=0}^{k-1} \Delta t ||R^{l+1}[c_N(\mu)]||^2 \right)$$

with weighted energy norm

$$||v||_\gamma^2 := ||v^k||^2 + \gamma \left(\sum_{j=1}^{k} \Delta t \langle v^j, L_I^{j-1}[v^j] \rangle, \right)$$

Here α denotes the coercivity constant of L_I^k,
$C := ((1 - C_E^2)^{1/2} + 1)/2$ and C_E is the continuity constant of L_E^k.

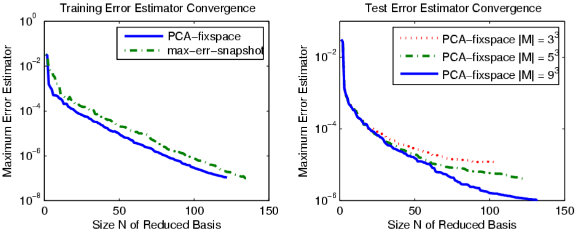
› Efficient Choice of W_N [Haasdonk, Ohlberger '08]

Idea:

- Construct $\tilde{W}_{\tilde{N}}$ as the span of Snapshots $c_H(\boldsymbol{\mu})$, $\boldsymbol{\mu} \in D \subset P$.
- Use Error Estimator for an efficient Choice of the Snapshots with Guaranteed Error Control on a Training Set.
- Reduce $\tilde{W}_{\tilde{N}}$ to W_N with Principal Component Analysis (PCA).

Goal: Exponential Convergence in N!

Preliminary Result: Convergence in N for Training and Test Sets



› Adaptive Basis Enrichment [Haasdonk, Ohlberger '08]

Basis Enrichment Algorithm: Fixed / Adaptive Training Sets

ESGREEDY($\Phi_0, M_{train}, \varepsilon_{tol}, M_{val}, \rho_{tol}$)

$\Phi := \Phi_0$
repeat
  $\boldsymbol{\mu}^* := \arg\max_{\boldsymbol{\mu} \in M_{train}} \Delta(\boldsymbol{\mu}, \Phi)$
  if $\Delta(\boldsymbol{\mu}^*) > \varepsilon_{tol}$
   then
    $\varphi :=$ ONBASISEXT$(u_H(\boldsymbol{\mu}^*), \Phi)$
    $\Phi := \Phi \cup \{\varphi\}$
  $\varepsilon := \max_{\boldsymbol{\mu} \in M_{train}} \Delta(\boldsymbol{\mu}, \Phi)$
  $\rho := \max_{\boldsymbol{\mu} \in M_{val}} \Delta(\boldsymbol{\mu}, \Phi)/\varepsilon$
 until $\varepsilon \leq \varepsilon_{tol}$ **or** $\rho \geq \rho_{tol}$
return Φ, ε

Here, $\mathcal{M}$ denotes a Partition of the Parameter Space,
and $V(\mathcal{M})$ are the Vertices of $\mathcal{M}$.

› Adaptive Basis Enrichment [Haasdonk, Ohlberger ’08]

Basis Enrichment Algorithm: Fixed / Adaptive Training Sets

ESGREEDY($\Phi_0, M_{train}, \varepsilon_{tol}, M_{val}, \rho_{tol}$)

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  - $\boldsymbol{\mu}^* := \arg\max_{\boldsymbol{\mu} \in M_{train}} \Delta(\boldsymbol{\mu}, \Phi)$
  - **if** $\Delta(\boldsymbol{\mu}^*) > \varepsilon_{tol}$
  - **then**
    - $\varphi := \text{ONBASISEXT}(u_H(\boldsymbol{\mu}^*), \Phi)$
    - $\Phi := \Phi \cup \{\varphi\}$
  - $\varepsilon := \max_{\boldsymbol{\mu} \in M_{train}} \Delta(\boldsymbol{\mu}, \Phi)$
  - $\rho := \max_{\boldsymbol{\mu} \in M_{val}} \Delta(\boldsymbol{\mu}, \Phi)/\varepsilon$
- **until** $\varepsilon \leq \varepsilon_{tol}$ **or** $\rho \geq \rho_{tol}$
- **return** Φ, ε

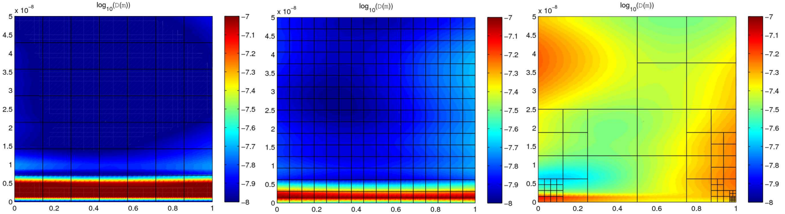
RBADAPTIVE($\Phi_0, \mathcal{M}_0, \varepsilon_{tol}, M_{val}, \rho_{tol}$)

- $\Phi := \Phi_0, \mathcal{M} := \mathcal{M}_0$
- **repeat**
  - $M_{train} := V(\mathcal{M})$
  - $[\Phi, \varepsilon] := \text{ESGREEDY}(\Phi, M_{train}, \varepsilon_{tol}, M_{val}, \rho_{tol})$
  - **if** $\varepsilon > \varepsilon_{tol}$
  - **then**
    - $\boldsymbol{\eta} = \text{ELEMENTINDICATORS}(\mathcal{M}, \Phi, \varepsilon)$
    - $\mathcal{M} := \text{MARK}(\mathcal{M}, \boldsymbol{\eta})$
    - $\mathcal{M} := \text{REFINE}(\mathcal{M})$
- **until** $\varepsilon \leq \varepsilon_{tol}$
- **return** Φ

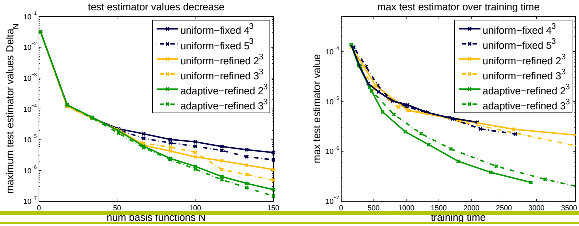
Here, $\mathcal{M}$ denotes a Partition of the Parameter Space, and $V(\mathcal{M})$ are the Vertices of $\mathcal{M}$.

› Adaptive Basis Enrichment [Haasdonk, Ohlberger '08]

Error Distribution for Uniform / Adaptive Training Sets



Exponential Convergence and CPU-Efficiency

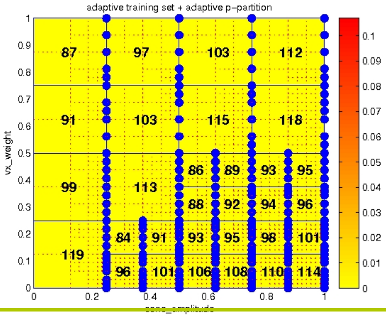


› Adaptive Parameter Domain Partition

[Dihlmann, Haasdonk, Ohlberger ’10]

Idea: Construct a reduced model with prescribed error tolerance and an upper bound for the dimension of the reduced space.

Ansatz: Parameter domain partition and construction of independent reduced spaces in the parameter sub-domains.



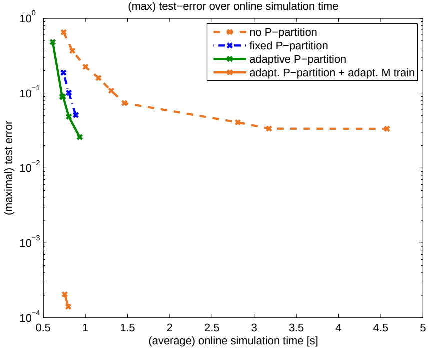
› Adaptive Parameter Domain Partition

$\textsc{AdaptiveParamPartition}(\mathcal{M}_0, \varepsilon_{tol}, N_{max})$

$\mathcal{M} := \mathcal{M}_0, \Phi(e) := \emptyset$ **for** $e \in \mathcal{E}(\mathcal{M})$
repeat
  for $e \in \mathcal{E}(\mathcal{M})$ with $\Phi(e) = \emptyset$
  do $\Phi_0 := \textsc{InitBasis}(e)$
    $M_{train} := \textsc{MTrain}(e)$
    $\eta(e) := 0$
    $[\Phi(e), \varepsilon(e)] := \textsc{EarlyStoppingGreedy}(\Phi, M_{train}, \varepsilon_{tol}, \emptyset, \infty, N_{max})$
    if $\varepsilon(e) > \varepsilon_{tol}$
     then $\eta(e) := 1, \Phi(e) := \emptyset$
  $\eta_{max} := \max_{e \in \mathcal{E}(\mathcal{M})} \eta(e)$
  if $\eta_{max} > 0$
   then $\mathcal{M} := \textsc{Mark}(\mathcal{M}, \boldsymbol{\eta})$
     $\mathcal{M} := \textsc{Refine}(\mathcal{M})$
until $\eta_{max} = 0$
return $\mathcal{M}, \{\Phi(e), \varepsilon(e)\}_{e \in \mathcal{E}(\mathcal{M})}$

› Evaluation of the Online Efficiency

	$\varepsilon_{test,max}$	$\varepsilon_{test,av}$	$\bar{t}_{sim,reduced}$
no p-domain partition	$1.08 \cdot 10^{-1}$	$1.17 \cdot 10^{-2}$	1.31 s
fixed p-domain partition	$1.01 \cdot 10^{-1}$	$1.44 \cdot 10^{-2}$	0.804 s
adaptive p-domain partition	$4.85 \cdot 10^{-2}$	$4.62 \cdot 10^{-3}$	0.804 s
adaptive p-domain partition & training set	$2.06 \cdot 10^{-4}$	$7.90 \cdot 10^{-5}$	0.756 s



see also
hp certified RB approach
[Eftang et al. '10, '11]

› How to treat nonlinear problems?

Current approaches

- Polynomial nonlinearity: Use multi-linear approach
  –› higher order reduced tensors
  [Rozza 05, Jung et al. 09, Nguyen et al. '09]
- Non-affine parameter dependence: Use classical empirical interpolation of functions
  [Barrault et al. '04, Grepl et al. '07, Canuto et al. '09]
- Question: How to deal with general nonlinear problems?
  -› Discrete Empirical Interpolation [Chaturantabut, Sorensen '10]
  -› Empirical Operator Interpolation
  [Haasdonk et al. '08, Drohmann et al. '10]

› How to treat nonlinear problems?

Current approaches

- Polynomial nonlinearity: Use multi-linear approach
  –› higher order reduced tensors
  [Rozza 05, Jung et al. 09, Nguyen et al. ’09]
- Non-affine parameter dependence: Use classical empirical interpolation of functions
  [Barrault et al. ’04, Grepl et al. ’07, Canuto et al. ’09]
- Question: How to deal with general nonlinear problems?
  -› Discrete Empirical Interpolation [Chaturantabut, Sorensen ’10]
  -› Empirical Operator Interpolation
  [Haasdonk et al. ’08, Drohmann et al. ’10]

› Empirical Interpolation of Explicit Operators

Reduced Basis Method for Explicit Finite Volume Approximations of Nonlinear Conservation Laws
[Haasdonk, Ohlberger, Rozza '08], [Haasdonk, Ohlberger '09]

A Simple Model Problem

$$\partial_t c(\mu) + \nabla \cdot (\mathbf{v} c(\mu)^{\mu}) = 0 \qquad \text{in } \Omega \times [0, T], \ \mu \in [1, 2]$$

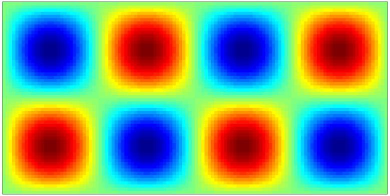
plus suitable Initial and Boundary Conditions.

$\mu = 1 \implies$ Linear Transport

$\mu = 2 \implies$ Burgers Equation

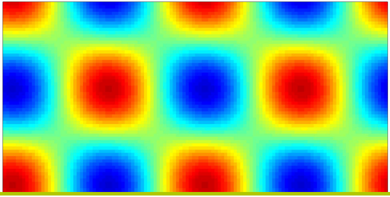
› Numerical Results

Initial values: $c_0(x) = 1/2(1 + \sin(2\pi x_1)\sin(2\pi x_2))$

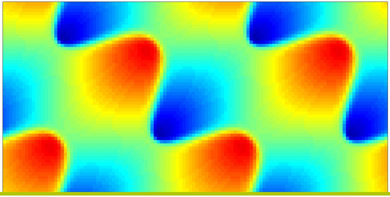


Solution at t = 0.3

Linear Transport



Burgers Equation



› General Framework

Nonlinear Equation

$$\partial_t c(\boldsymbol{\mu}) + L_{\boldsymbol{\mu}}[c(\boldsymbol{\mu})] = 0 \qquad \text{in } \Omega \times [0, T],$$

Explicit Discretization

$$c_H^{k+1}(\boldsymbol{\mu}) = c_H^k(\boldsymbol{\mu}) - \Delta t L_H^k(\boldsymbol{\mu})[c_H^k(\boldsymbol{\mu})].$$

Problem: Non-Affine Parameter Dependency
Non-Linear Evolution Operator

Idea: Linear Affine Approximation through Empirical Interpolation

$$L_H^k(\boldsymbol{\mu})[c_H^k(\boldsymbol{\mu})](x) \approx \sum_{m=1}^{M} y_m(c, \boldsymbol{\mu}, t^k)\xi_m(x)$$

$$y_m(c, \boldsymbol{\mu}, t^k) := L_H^k(\boldsymbol{\mu})[c_H^k(\boldsymbol{\mu})](x_m)$$

Empirical Interpolation of Localized Operators

Idea: Construct a Collateral Reduced Basis Space W_M that approximates the space spanned by $L_H^k(\boldsymbol{\mu})[c_H^k(\boldsymbol{\mu})]$

Ingredients: Collateral Reduced Basis Space:

$$W_M := \text{span}\{L_H^{k_m}(\boldsymbol{\mu}_m)[c_H^{k_m}(\boldsymbol{\mu}_m)] | m = 1, \ldots, M\}$$

Nodal Collateral Reduced Basis:

$$\{\xi_m\}_{m=1}^M \Longrightarrow W_M = \text{span}\{\xi_m | m = 1, \ldots, M\}$$

Interpolation Points:

$$\{x_k\}_{k=1}^M \text{ with } \xi_m(x_k) = \delta_{mk}$$

Empirical Interpolation:

$$\mathcal{I}_M[L_H^k(\boldsymbol{\mu})[c_H^k(\boldsymbol{\mu})]] := \sum_{m=1}^M y_m(c, \boldsymbol{\mu}, t^k)\xi_m(x)$$

Offline: Collateral Basis $\{\xi_m\}_{m=1}^M$ and Interpolation Points $\{x_m\}_{m=1}^M$

Online: Calculate Coefficients $y_m = L_H^k(\boldsymbol{\mu})[c_H^k(\boldsymbol{\mu})](x_m)$

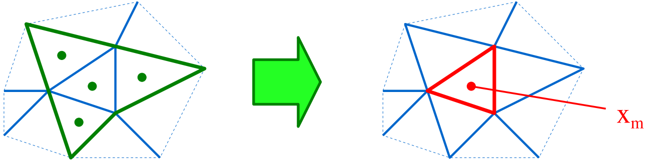
$\Longrightarrow$ Localized operators for H-independent point evaluations

› Local Operator Evaluations and RB Scheme

Local Operator Evaluations in the Online-Phase require:

1.) Local reconstruction of c_N^k from coefficients $\mathbf{a}^k$

2.) Local operator evaluation: $y_m = L_H^k(\boldsymbol{\mu})[c_H^k(\boldsymbol{\mu})](x_m)$



Requires Offline: Numerical subgrids, local basis representation

RB Method: Galerkin projection of interpolated scheme

$$\int_\Omega \left(c_N^{k+1}(\boldsymbol{\mu}) = c_N^k(\boldsymbol{\mu}) - \Delta t \mathcal{I}_M[L_H^k(\boldsymbol{\mu})[c_N^k(\boldsymbol{\mu})]] \right) \varphi, \quad \forall \varphi \in W_N.$$

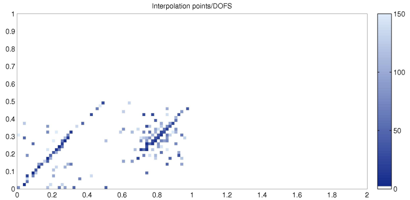
Offline-Online decomposition analog to the linear and affine case!!

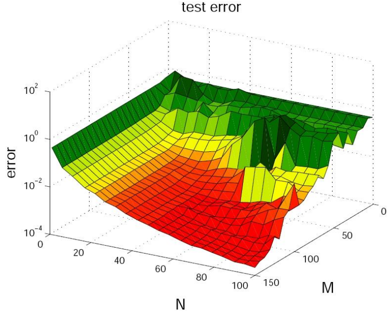
› Numerical Experiment

Empirical Interpolation:

$M_{\max} = 150$ interpolation points

Translation symmetry detected





Test error convergence:

Exponential convergence for simultaneous increase of N and M

› Numerical Experiment

Comparison of Online-Runtimes

Simulation	Dimension	Runtime [s]	Gain Factor
detailed	H = 7200	20.22	
reduced	N=20, M=30	0.91	**22.2**
reduced	N=40, M=60	1.22	**16.6**
reduced	N=60, M=90	1.55	**13.0**
reduced	N=80, M=120	1.77	**11.4**
reduced	N=100, M=150	2.06	**9.8**

› Extension to Nonlinear Implicit Operators

[Drohmann, Haasdonk, Ohlberger 2010]

Evolution Equation

$$\partial_t c(\mu) + L_{\mu}[c(\mu)] = 0 \qquad \text{in } \Omega \times [0, T],$$

Mixed Implicit - Explicit Discretization

$$(Id + \Delta t \, L_I^k(\mu))[c_H^{k+1}(\mu)] = (Id - \Delta t \, L_E^k(\mu))[c_H^k(\mu)].$$

Problem: Non-Affine Parameter Dependency
Non-Linear Evolution Operators
L_I^k involves the solution of a non-linear System

Ansatz: Newton's Method and
Empirical interpolation for the linearized defect equation

Newton's Method and Empirical Interpolation

Define the defect $d_H^{k+1,\nu+1} := c_H^{k+1,\nu+1} - c_H^{k+1,\nu}$.
Solve in each Newton step ν for the defect

$$(Id + \Delta t\, F_I^k(\boldsymbol{\mu}))[c_H^{k+1,\nu}]d_H^{k+1,\nu+1} = (Id - \Delta t\, L_I^k(\boldsymbol{\mu}))[c_H^{k+1,\nu}] + (Id - \Delta t\, L_E^k(\boldsymbol{\mu}))[c_H^k],$$

and update

$$c_H^{k+1,\nu+1} = c_H^{k+1,\nu} + d_H^{k+1,\nu+1}.$$

Here F_I^k is the Frechet derivative of L_I^k.

Problem: F_I^k has Non-Affine Parameter Dependency

L_I^k and L_E^k can be treated as before!

› Empirical Interpolation for the Frechet Derivative

Empirical interpolation for L_l^k

$$\mathcal{I}_M[L_l^k(\boldsymbol{\mu})[c_H]] = \sum_{m=1}^{M} y_m^l(c_H^k, \boldsymbol{\mu})\, \xi_m .$$

Empirical Interpolation for F_l^k

$$\mathcal{I}_M[F_l^k(\boldsymbol{\mu})[c_H]v_H] := \sum_{i=1}^{H}\sum_{m=1}^{M} \partial_i y_m^l(c_H^k, \boldsymbol{\mu}) v_i\, \xi_m \overset{!}{=} \sum_{i\in\tau}\sum_{m=1}^{M} \partial_i y_m^l(c_H^k, \boldsymbol{\mu}) v_i\, \xi_m .$$

Properties:

- $\tau \subset \{1, \ldots, H\}$ is the smallest subset, such that equality holds
  $\Longrightarrow$ $\mathrm{card}(\tau) = \mathcal{O}(M)$, since L_l^k is supposed to be localized!
- $(v_i)_{i\in\tau}$ can be evaluated efficiently in case of a nodal basis of W_H.

› Resulting RB Formulation of one Newton Step

Ansatz: $c_N^{k,\nu}(x) = \sum_{n=1}^N a_n^{k,\nu} \phi_n(x)$, ($\mathbf{a}^{k,\nu}$: coefficient vector)

$$(Id + \Delta t\, G\, A[c_N^{k+1,\nu}])\,\underbrace{(\mathbf{a}^{k+1,\nu+1} - \mathbf{a}^{k+1,\nu})}_{=:\mathbf{d}^{k+1,\nu+1}} = RHS(\mathbf{a}^{k+1,\nu}, \mathbf{a}^k).$$

Thereby the matrices $A[c_N]$, G are given as

$$(A[c_N])_{m,n} := \sum_{i=1}^M \partial_i y_m^I(c_N, \boldsymbol{\mu})\varphi_n(x_i), \qquad G_{n,m} := \int_\Omega \xi_m \varphi_n$$

with a corresponding offline-online splitting.

› A Posteriori Error Estimate

Definition: Residual of the approximated FV/DG Method

$$\Delta t R^{k+1}(\mu)\,[c_N] = (Id + \Delta t \mathcal{I}_M\,[L_I(\mu)])\left[{c_N}^{k+1}\right] - (Id - \Delta t \mathcal{I}_M\,[L_E(\mu)])\left[{c_N}^{k}\right]$$

Theorem: A Posteriori Error Estimate in $L^\infty L^2$

$$||c_N^k(\mu) - c_H^k(\mu)|| \leq \sum_{i=0}^{k-1} C_I^{k-i+1} C_E^{k-1} \left(|| \sum_{m=M}^{M+M'} \Delta t \left(y_m^I\left({c_N}^{i+1}, \mu\right) - y_m^E\left({c_N}^{i}, \mu\right)\right) \xi_m || + \varepsilon^{New} + ||R^{l+1}(\mu)\,[c_N]\,|| \right)$$

› Numerical Experiments

Model Problem: Porous Medium Equation

$$\partial_t c(\boldsymbol{\mu}) + \boldsymbol{\mu}_2 \Delta(c^{\boldsymbol{\mu}_1}(\boldsymbol{\mu})) = 0 \qquad \text{in } \Omega \times [0,T],\ \boldsymbol{\mu} \in [1,5] \times [0, 0.001] \times [0, 0.2]$$

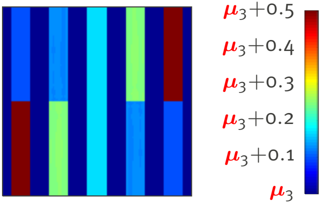
plus suitable initial and boundary conditions.

Nonlinearity:

$\mu_1 > 2 \implies$ adiabatic flow

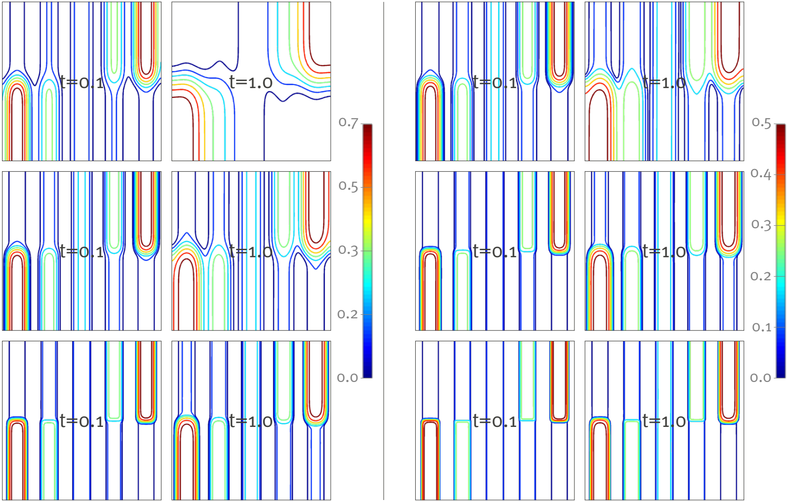
$\mu_1 = 2 \implies$ isothermal case

$\mu_1 = 1 \implies$ linear diffusion

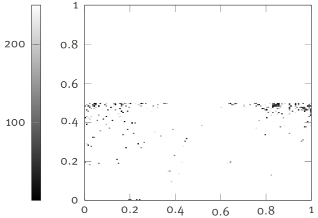


μ_3 dependent initial data

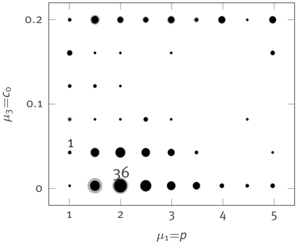
› Reduced solutions for various parameters



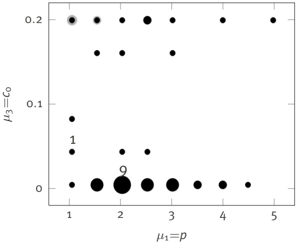
a) Selected interpolation DOFs



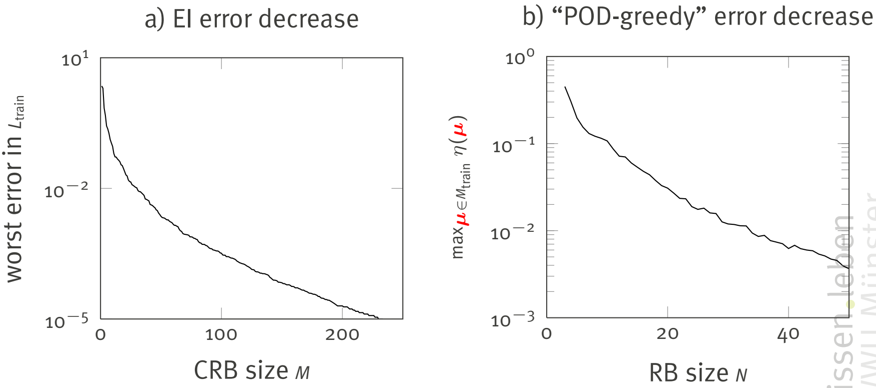
b) Selected parameters during CRB generation



c) Selected parameters during “POD-greedy”



› Error Decrease

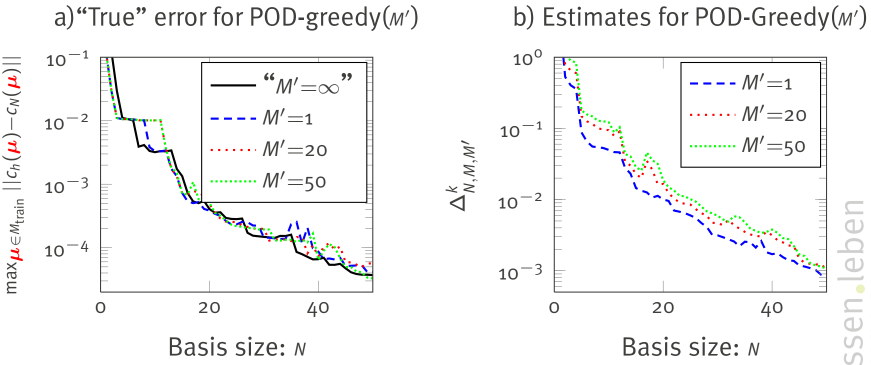


› Averaged Runtime Comparison

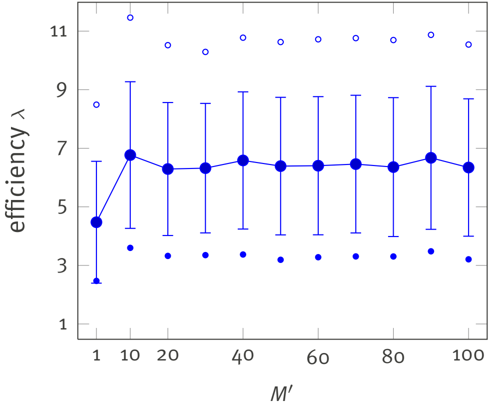
Simulation	Dimensionality	Runtime[s]	Error
Detailed	H=22500	605.66	–
Reduced	N=15, M=75	5.01	$4.93 \cdot 10^{-3}$
Reduced	N=30, M=150	7.14	$1.73 \cdot 10^{-3}$
Reduced	N=40, M=200	8.27	$8.53 \cdot 10^{-4}$
Reduced	N=50, M=250	9.78	$7.59 \cdot 10^{-4}$

Gain Factor about 60 - 120

› Comparison of Error and Estimator



› Error Estimator Efficiency dependent on M'



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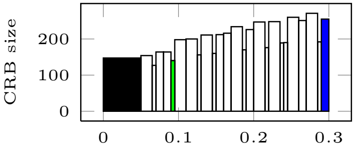
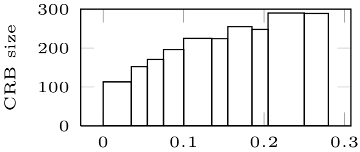
› Time Adaptive Collateral Space [DHO ’11]

adaptation	no. of bases	ø-dim(CRB)	offline time[h]	ø-runtime[s]	max. error
no	1	350	1.47	6.79	$5.88 \cdot 10^{-4}$
yes, $c_{min} = 5$	11	223.09	2.08	4.06	$5.80 \cdot 10^{-4}$
yes, $c_{min} = 1$	26	198.42	8.40	3.38	$5.75 \cdot 10^{-4}$

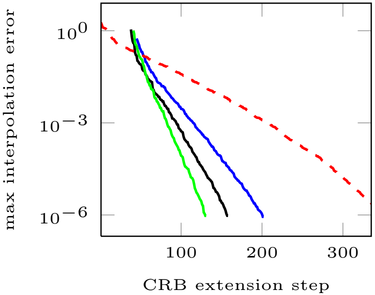
(a)



(b)



(c)



› A new localized RB-DG multiscale method

with Bernard Haasdonk and Sven Kaulmann

Goal: Multiscale problem for two phase flow in porous media:

$$-\nabla \cdot (\lambda(s^\epsilon) k^\epsilon \nabla p^\epsilon) = q,$$
$$\partial_t s^\epsilon - \nabla \cdot A^\epsilon(u^\epsilon, s^\epsilon, \nabla s^\epsilon) = f.$$

First step: Consider the pressure equation as a problem depending on a parameter function $\boldsymbol{\lambda} = \boldsymbol{\lambda}(x, t)$:

$$-\nabla \cdot (\boldsymbol{\lambda} k^\epsilon \nabla p^\epsilon(\boldsymbol{\lambda})) = q,$$

$\Longrightarrow$ Apply ideas from the RB-framework!!

General Idea (see also [Aarnes, Efendiev, Jiang 2008])

Idea: Find a small number of representative fields $\{p_i, i = 1, \dots, N\}$, such that for all admissible parameter functions λ there exists a smooth, non-linear mapping S with

$$||p(\lambda(x); x) - S(p_1, \dots, p_N)(x)|| \leq \text{TOL},$$

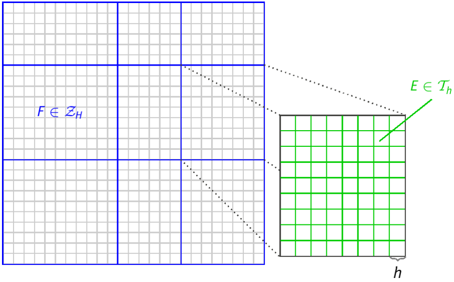
Ansatz: Define mapping S through

$$S(p_1, \dots, p_N)(x) = \sum_{i=1}^{N} a_i(x) p_i(x)$$

If the coefficient functions $a_i(x)$ are assumed to be piecewise constant on a coarse mesh, this leads to our new method.

› RB-DG multiscale method

$$\Phi_F := \{\varphi_F^1, \dots, \varphi_F^{N_F}\},\ \varphi_F^i \in S_{h,k}(F),$$
$$W_N = \{v_N \in L^2(\Omega) |\ v_N|_F \in \mathrm{span}(\Phi_F),\ \forall F \in \mathcal{Z}_H\}.$$



For given $\boldsymbol{\lambda}$, we define $p_N^{\boldsymbol{\lambda}} \in W_N$ as a solution of the RB-M-DGM

$$B_{\mathrm{DG}}(\boldsymbol{\lambda}; p_N^{\boldsymbol{\lambda}}, v_N) = L(\boldsymbol{\lambda}; v_N) \quad \forall v_N \in W_N.$$

with

$$B_{\mathrm{DG}}(\lambda; v, w) = \sum_{F \in \mathcal{Z}_H} \int_F \lambda k \nabla v \cdot \nabla w - \sum_{e \in \Xi} \int_e \{\lambda k \nabla v \cdot \mathbf{n_e}\}[\mathbf{w}] - \sum_{\mathbf{e} \in \ddot{}} \int_{\mathbf{e}} \{\lambda \mathbf{k} \nabla \mathbf{w} \cdot \mathbf{n_e}\}[\mathbf{v}] + \sum_{\mathbf{e} \in \ddot{}} \frac{\sigma}{|\mathbf{e}|^\beta} \int_{\mathbf{e}} [\mathbf{v}][\mathbf{w}],$$

$$L(\lambda; v) = \sum_{F \in \mathcal{Z}_H} \int_F fv + \sum_{e \in \Xi_B} \int_e \left(\frac{\sigma}{|e|^\beta} v - \lambda k \nabla v \cdot \mathbf{n} \right) g_D.$$

› Theorem: A posteriori error estimate

$$\|p^\lambda - p_N^\lambda\|_{0,\Omega} \leq \|\mathcal{R}(p_N^\lambda) - p_N^\lambda\|_{0,\Omega} + \sum_{F\in\mathcal{Z}_H} \eta_1^F(\mathcal{R}(p_N^\lambda)) + \sum_{e\in\Gamma_I} \eta_2^e(\mathcal{R}(p_N^\lambda)) + \sum_{e\in\Xi_B} \eta_3^e(\mathcal{R}(p_N^\lambda))$$

where $\mathcal{R}(p_N^\lambda)$ denotes a higher order reconstruction of p_N^λ and the indicators are given as

$$\eta_1^F(\xi) = \frac{C_o^2}{k_1}\|f + \nabla\cdot(\lambda k\nabla\xi)\|_{0,F} + C_r\left(\frac{C_o k_2}{k_1} + h_e\right)\sum_{e\subset\partial F}\|\mathbf{r}_e(\xi)\|_{0,\Omega},$$

$$\eta_2^e(\xi) = (C_o + h_e)\frac{C_r C_o}{k_1}\|\mathbf{r}_e(\lambda k\nabla\xi\cdot\mathbf{n})\|_{0,\Omega},$$

$$\eta_3^e(\xi) = C_r\left(\frac{C_o k_2}{k_1} + h_e\right)\|\mathbf{r}_e(\xi - g_D)\|_{0,\Omega}.$$

› Adaptive basis construction for W_N

Given: $\mathcal{M}_{\text{train}} := \{\lambda^i, i \in I_{\text{train}}\}$, a tolerance Δ, a maximum basis size $N_{\max}$ and a POD-tolerance Δ_{POD}.

Generate basis Φ of W_N:

0. Set $\tilde{\Phi}_{-1}, \tilde{\Phi}_{-1,F} := \emptyset$ for all $F \in \mathcal{Z}_H$ and choose $\lambda_0 \in \mathcal{M}_{\text{train}}$ for the construction of an initial basis.
1. Let a basis $\tilde{\Phi}_{k-1} = \bigcup_{F\in\mathcal{Z}_H} \tilde{\Phi}_{k-1,F}$ and a parameter function λ_k be given. Perform detailed simulation to obtain $p_h^{\lambda_k}$ and define preliminary basis extension $\tilde{\varphi}_F, F \in \mathcal{Z}_H$ by $\tilde{\varphi}_F := p_h^{\lambda_k}|_F, \forall F \in \mathcal{Z}_H$. Add $\tilde{\varphi}_F, F \in \mathcal{Z}_H$ to the basis $\tilde{\Phi}_{k-1,F}$ and obtain $\tilde{\Phi}_{k,F}$, $\tilde{\Phi}_k = \bigcup_{F\in\mathcal{Z}_H} \tilde{\Phi}_{k,F}$.
2. Compute offline-parts of the DG scheme and of the error estimator for the current basis $\tilde{\Phi}_k$.
3. Compute reduced solutions p_N^{λ} for all $\lambda \in \mathcal{M}_{\text{train}}$ using the current basis. Then evaluate error estimator for all these solutions and find the parameter function $\lambda_{k+1} \in \mathcal{M}_{\text{train}}$ with largest error.
4. If $N < N_{\max}$ and if the error bound for the reduced solution $p_N^{\lambda_{k+1}}$ is larger than Δ, continue with Step (1) with λ_{k+1} from Step (3).

   Else Apply POD with accuracy Δ_{POD} to $\tilde{\Phi}_{k,F}$ on each coarse cell $F \in \mathcal{Z}_H$ and obtain the reduced orthogonalized local bases Φ_F and the global basis $\Phi = \bigcup_{F\in\mathcal{Z}_H} \Phi_F$.

› Numerical Experiment

$$-\nabla \cdot (\lambda k^\epsilon \nabla p^\epsilon(\lambda)) = 0 \qquad \text{on } \Omega = [0, 10]^2$$

with

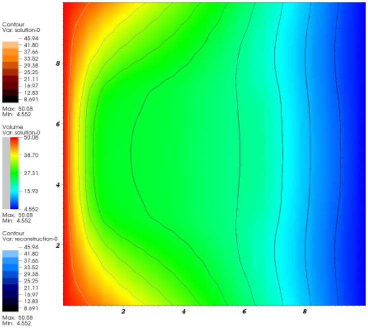
$$k^\epsilon(x) := \frac{2}{3}(1 + x_1)(1 + \cos^2(2\pi \frac{x_1}{\epsilon})),$$

$$\lambda(x) := \frac{1}{\eta_O} - \frac{2}{\eta_O} S(x) + \frac{\eta_O + \eta_W^2}{\eta_W \eta_O} \sum_{m,n=1}^{N_S} \mu_n \mu_m S_n(x) S_m(x),$$

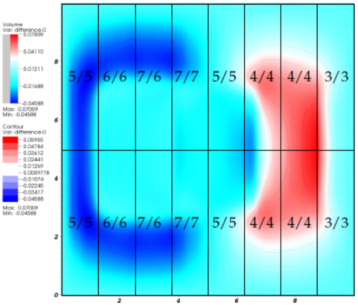
$$S(x) := \sum_{n=1}^{N_S} \mu_n S_n(x) \text{ with } N_S = 3 \text{ and } S_n(x) \text{ given.}$$

$+$ suitable Dirichlet boundary conditions.

› Simulation results



Contour plots of fine scale solution (solid lines) and reconstructed reduced solution (dotted lines) for $\mu_1 = 0.85$, $\mu_2 = 0.5$, $\mu_3 = 0.1$ ($|\mathcal{T}_h| = 32768$).



Difference between fine scale and reduced solution. Coarse triangulation (black) with number of reduced basis functions $|\Phi_F|$ ($|\mathcal{T}_h| = 2048/32768$, respectively).

› CPU times for the new method

$\|\mathcal{T}_h\|$	N	t_{highdim} (s)	t_{lowdim} (ms)	t_{recons} (ms)	Factor	rel. error
2,048	82	0.19	8.54	36.78	**4**	$4.74e{-4}$
8,192	80	2.59	9.93	151.4	**16**	$6.44e{-4}$
32,768	80	22.58	12.24	545.3	**40**	$7.59e{-4}$

Averaged runtimes over 125 simulations: high and low dimensional algorithms (t_{highdim} and t_{lowdim}); the reconstruction (t_{recons}) and mean relative errors ($\|p_h^\lambda - p_N^\lambda\|_{L^2} / \|p_h^\lambda\|_{L^2}$) for different grid sizes.

Thank you for your attention!

Software: DUNE, DUNE-FEM, RBmatlab

http://www.wwu.de/math/num/ohlberger

http://morepas.org