Adaptive Variational Multiscale Methods

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Motivation

- Important applications including materials with microstructure, flow in porous media, etc
- These problems are computationally challenging and calls for multiscale methods
- Understanding of propagation and amplification of error in such multiscale methods are important
- Many discretization parameters creates a need for adaptive algorithms for automatic tuning

Outline and Papers

Outline

- Variational Multiscale Method (VMS)
- Adaptive VMS
- Symmetric VMS
- Extension to mixed problems
- Adaptive Symmetric VMS with application
- Conclusions and Outlook

Papers

- A. Målqvist, *Adaptive Variational Multiscale Methods*, PhD Thesis September 2005, Chalmers Universiy of Technology, Sweden
- M.G. Larson and A. Målqvist, *Adaptive Variational Multiscale Methods Based on A Posteriori Error Estimation: Energy Norm Estimates for Elliptic Problems*, CMAME 2007
- M.G. Larson and A. Målqvist, *A Mixed Adaptive Variational Multiscale Method with Applications in Oil Reservoir Simulation* M3AS 2008

Model Problem

Poisson Equation. Find $u : \Omega \to \mathbf{R}$ such that

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

where $a(x) \geq a_0 > 0$ bounded with multiscale features, $f \in L^2$, and Ω is a domain in $\mathbf{R}^d$, $d = 1, 2, 3$

Weak Form. Find $u \in H_0^1(\Omega)$ such that

$$a(u, v) = (a\nabla u, \nabla v) = (f, v) \quad \text{for all } v \in H_0^1(\Omega),$$

where $(v, w) = \int_\Omega v \cdot w \, dx$.

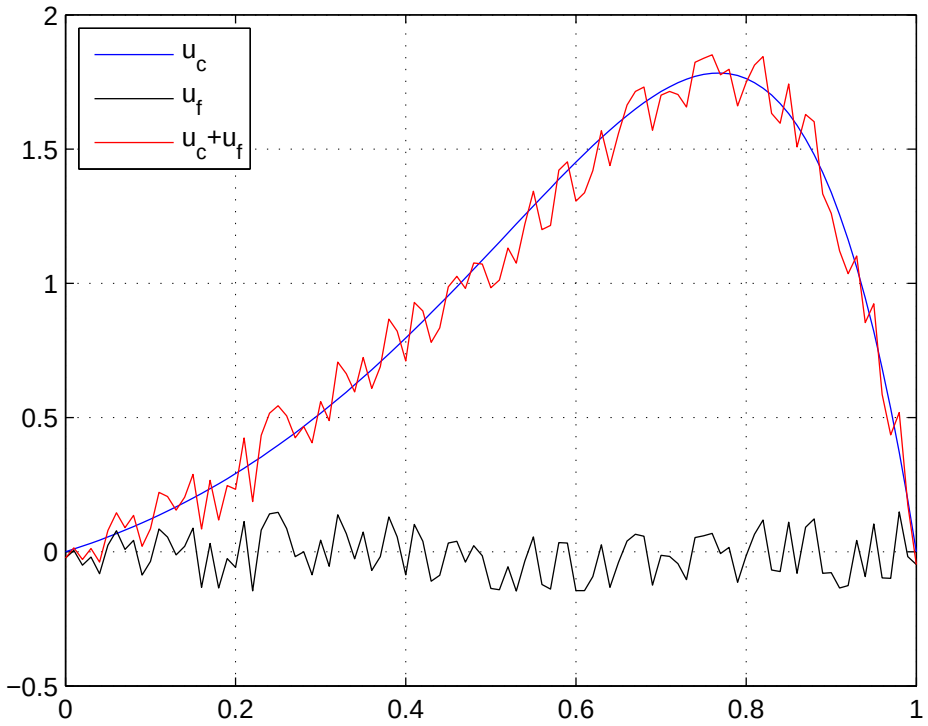
Variational Multiscale Method

We introduce two spaces $\mathcal{V}_c$ and $\mathcal{V}_f$ such that

$$\boxed{\mathcal{V}_c \oplus \mathcal{V}_f = H_0^1(\Omega)}$$

- $\mathcal{V}_c$ is a finite dimensional approximation of $H_0^1(\Omega)$. (finite element space)
- $\mathcal{V}_f$ can be chosen in different ways
  - Hierarchical basis
  - $L^2(\Omega)$-orthogonal to $\mathcal{V}_c$
  - Wavelet modified hierarchical basis

Variational Multiscale Method



Lines are u_c, u_f, and $u_c + u_f$

Variational Multiscale Method

Find $u_c \in \mathcal{V}_c$ and $u_f \in \mathcal{V}_f$ such that

$$a(u_c, v_c) + a(u_f, v_c) = (f, v_c) \quad \text{for all } v_c \in \mathcal{V}_c$$

$$a(u_f, v_f) = (f, v_f) - a(u_c, v_f)$$

$$:= (R(u_c), v_f) \quad \text{for all } v_f \in \mathcal{V}_f$$

Fine scale information is used to modify the coarse scale equation: Find $u_c \in \mathcal{V}_c$ such that

$$a(u_c, v_c) + a(\mathcal{T}R(u_c), v_c) = (f, v_c) \;\; \forall v_c \in \mathcal{V}_c$$

where $\mathcal{T}$ is the solution operator defined by

$$a(\mathcal{T}R(u_c), v_f) = (R(u_c), v_f) \quad \text{for all } v_f \in \mathcal{V}_f$$

Adaptive VMS

The Adaptive Variational Multiscale Method (AVMS) builds on the following ingredients:

- Systematic technique for computing u_f. We approximate u_f by a sum

$$u_f = \sum_i u_{f,i}$$

  of solutions to localized (subdomain-subgrid) problems
- Error estimation framework
- Adaptive strategy for tuning of critical discretization parameters

Decoupled Fine Scale Equations

Recall the fine scale equations:

$$a(u_f, v_f) = (R(u_c), v_f), \quad \text{for all } v_f \in \mathcal{V}_f$$

Include a partition of unity $\sum_{i=1}^{n} \varphi_i = 1$,

$$a(u_f, v_f) = (R(u_c), v_f) = \sum_{i=1}^{n} (\varphi_i R(u_c), v_f)$$

let $u_f = \sum_{i=1}^{n} u_{f,i}$ where

$$\boxed{a(u_{f,i}, v_f) = (\varphi_i R(u_c), v_f)}$$

φ_i is typically a coarse basis function

Solution on Subdomains

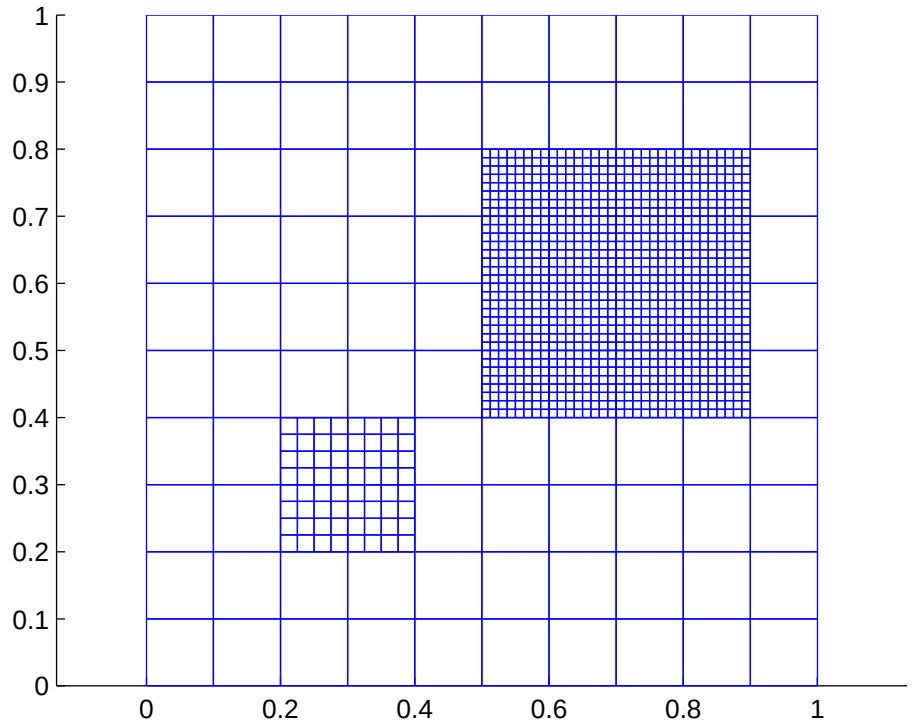
We approximate $u_{f,i}$ by

- Restricting to a localized patch ω_i with supp$(\varphi_i) \subset \omega_i$
- Discretizing using a subgrid on ω_i.
- We expect rapid decay of $u_{f,i}$ and therefore we use Dirichlet conditions $u_{f,i} = 0$ on $\partial\omega_i$.

We get the discrete problem: find $U_{f,i} \in \mathcal{V}_f^h(\omega_i)$ such that

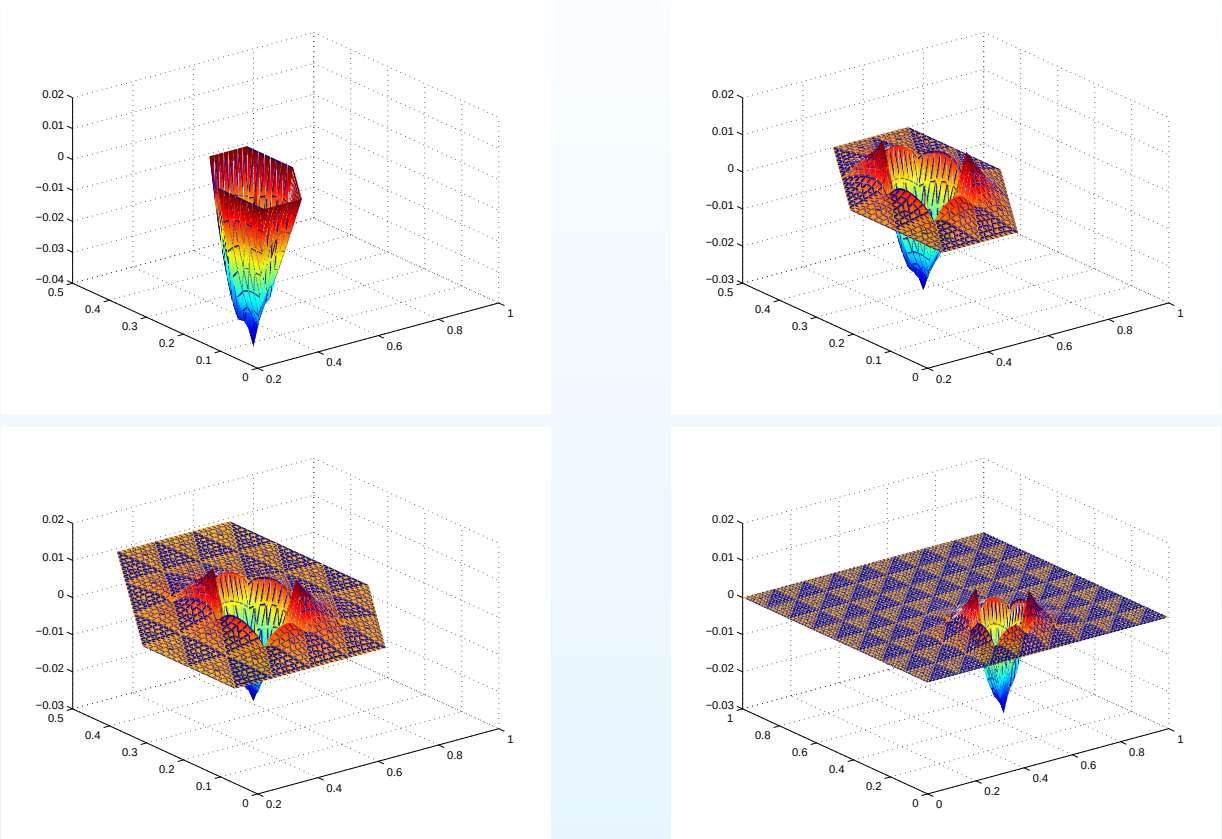
$$a(U_{f,i}, v_f) = (\varphi_i R(U_c), v_f) \quad \text{for all } v_f \in \mathcal{V}_f^h(\omega_i)$$

Refinement and Layers



One and two layer stars.

Localized Fine Scale Solution



The AVMS Method

Find $U_c \in \mathcal{V}_c$ and $\boxed{U_f = \sum_{i=1}^{n} U_{f,i}}$ with $U_{f,i} \in \mathcal{V}_f^h(\omega_i)$ such that

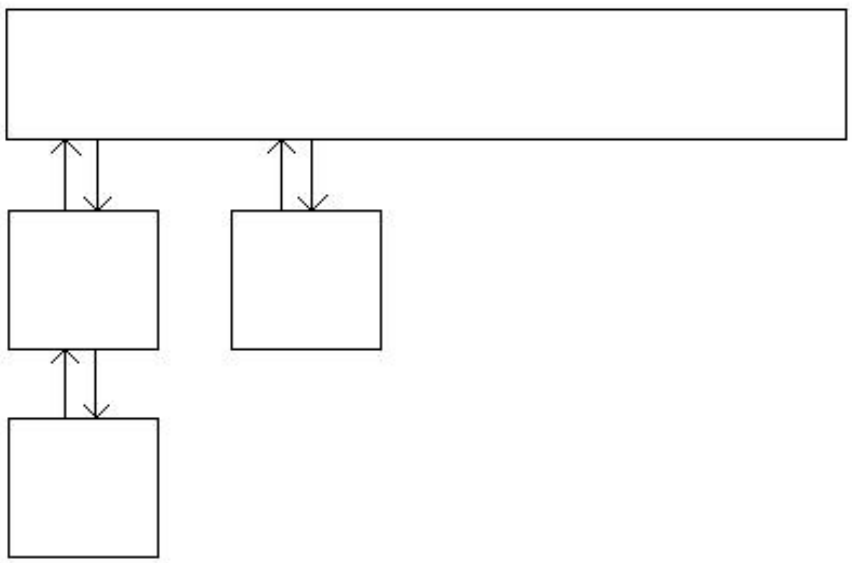
$$a(U_c, v_c) + a(U_f, v_c) = (f, v_c) \quad \text{for all } v_c \in \mathcal{V}_c$$

and

$$a(U_{f,i}, v_f) = (\varphi_i R(U_c), v_f) \quad \text{for all } v_f \in \mathcal{V}_f^h(\omega_i)$$

Can be solved iteratively or directly by replacing U_c in RHS of fine scale with φ_j.

Parallel Structure of AVMS



- No communication between subgrid problems
- Multiple levels possible
- Different physics in subgrid model possible. Need transfer operator.

Error Estimates

The method is designed so that:

$$\boxed{\text{error} \to 0 \text{ when } h \to 0 \text{ and } L \to \infty}$$

- A priori error estimates in progress.
- To circumvent difficulties with choosing discretization parameters h and L we use an adaptive algorithm based on a posteriori error estimates

Energy Norm Error Estimate

$$\|\sqrt{a}\nabla e\|^2 \leq \sum_{i\in\mathcal{C}} C_i \|H\mathcal{R}(U_c)\|^2_{\omega_i}$$
$$+ \sum_{i\in\mathcal{F}} C_i \left(\|\sqrt{H}\Sigma(U_{f,i})\|^2_{\partial\omega_i} + \|h\mathcal{R}_i(U_{f,i})\|^2_{\omega_i} \right)$$

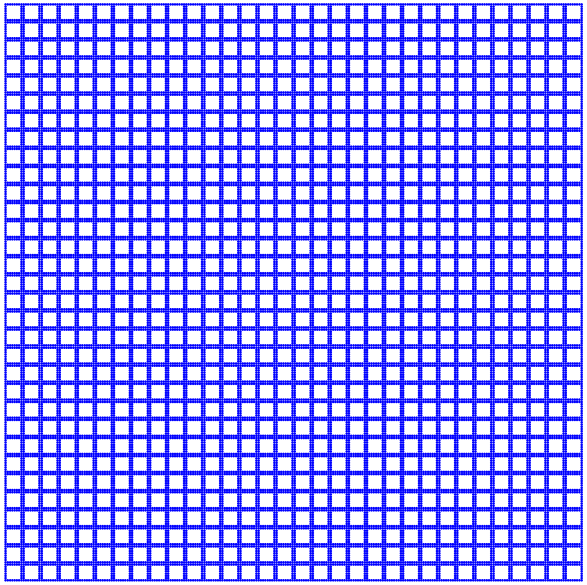
- The first term measures the coarse mesh error
- The second term is the normal derivative of the fine scale solutions on $\partial\omega_i$ and measures the error due to restriction to subdomains
- The third term measures the fine scale error caused by discretization

Adaptive Strategy

$$\|\sqrt{a}\nabla e\|^2 \leq \sum_{i\in\mathcal{C}} C_i \|H\mathcal{R}(U_c)\|^2_{\omega_i}$$
$$+ \sum_{i\in\mathcal{F}} C_i \left(\|\sqrt{H}\Sigma(U_{f,i})\|^2_{\partial\omega_i} + \|h\mathcal{R}_i(U_{f,i})\|^2_{\omega_i} \right)$$

- Calculate residuals for each $i \in \{\text{coarse fine}\}$
- Large values $i \in$ coarse $\rightarrow$ solve local problems
- Large values $i \in$ fine $\rightarrow$ more layers or smaller h

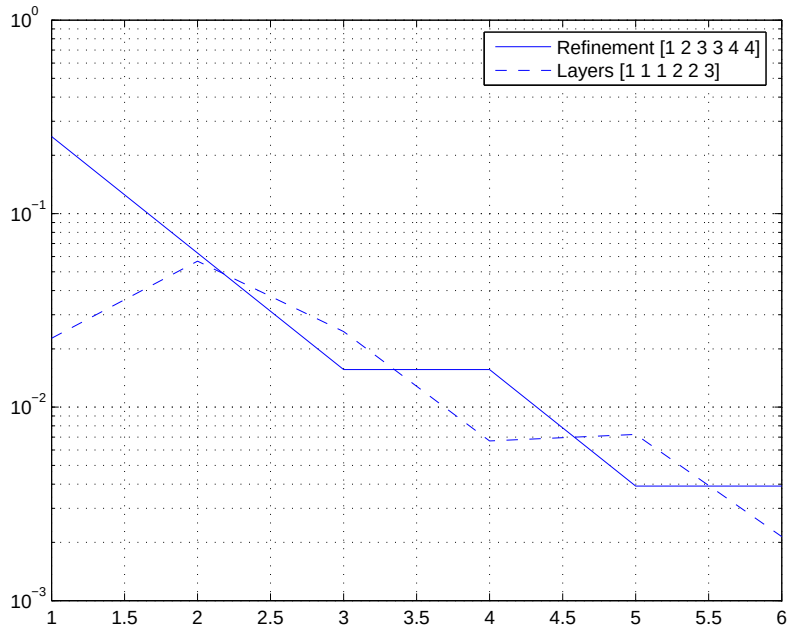
Microstructure Problem



Piece of microstructure.

- $-\nabla \cdot a \nabla u = 1$. $a = 1$ (white) and $a = 0.05$ (blue).
- Coarse grid has $129 \times 129 \approx 16$ kDoF. 3 refinement levels resolves lattice.

Convergence of Residuals



Convergence of subdomain boundary (dashed) and interior residuals (solid) during the adaptive refinement. 4 ref levels correspond to 4.25 MDoF.

Symmetric VMS

Model problem. Find $u \in \mathcal{V}$ such that

$$a(u, v) = l(v) \quad \text{for all } v \in \mathcal{V}$$

Assume the problem is well posed. $a(\cdot, \cdot)$ a bilinear form and $l(\cdot)$ linear form.

Splitting. We introduce two spaces $\mathcal{V}_c$ and $\mathcal{V}_f$ such that

$$\boxed{\mathcal{V} = \mathcal{V}_c \oplus \mathcal{V}_f}$$

Symmetric VMS

Starting from the model problem: find $u \in \mathcal{V}$ such that

$$a(u, v) = l(v) \quad \text{for all } v \in \mathcal{V}$$

and setting

$$u = u_c + u_f \quad v = v_c + v_f$$

we get: find $u_c + u_f \in \mathcal{V}_c \oplus \mathcal{V}_f$ such that

$$a(u_c + u_f, v_c + v_f) = l(v_c + v_f) \quad \text{for all } v_c + v_f \in \mathcal{V}_c \oplus \mathcal{V}_f$$

Note that $u_f \in \mathcal{V}_f$ satisfies the equation

$$a(u_f, v_f) = l(v_f) - a(u_c, v_f) \quad \text{for all } v_f \in \mathcal{V}_f$$

Symmetric VMS

We next write

$$u_f = u_{f,RH} + u_{f,c}$$

with

- $u_{f,RH} \in \mathcal{V}_f$ the contribution from the right hand side

$$a(u_{f,RH}, v_f) = l(v_f) \quad \text{for all } v_f \in \mathcal{V}_f$$

- $u_{f,c} \in \mathcal{V}_f$ the contribution from the coarse scale part

$$a(u_{f,c}, v_f) = -a(u_c, v_f) \quad \text{for all } v_f \in \mathcal{V}_f$$

Symmetric VMS

Let $\mathcal{T} : \mathcal{V}_c \to \mathcal{V}_f$ denote the solution operator to

$$a(u_{f,c}, v_f) = -a(u_c, v_f) \quad \text{for all } v_f \in \mathcal{V}_f$$

i.e.

$$u_{f,c} = \mathcal{T} u_c$$

Using the resulting decomposition

$$u = u_c + \mathcal{T} u_c + u_{f,RH}$$

we get

$$a(u_c + \mathcal{T} u_c + u_{f,RH}, v_c + v_f) = (f, v_c + v_f)$$

for all $v_c \in \mathcal{V}_c$ and $v_f \in \mathcal{V}_f$.

Symmetric VMS

Since $u_{f,RH}$ is directly determined we get the following problem for u_c: find $u_c \in \mathcal{V}_c$ such that

$$a(u_c + \mathcal{T} u_c, v_c + \mathcal{T} v_c) = (f, v_c + \mathcal{T} v_c) - a(u_{f,RH}, v_c + \mathcal{T} v_c)$$

for all $v_c \in \mathcal{V}_c$.

- Here we chose $v_f = \mathcal{T} v_c$ to get a symmetric formulation
- Note that in the standard VMS procedure one basically sets $v_f = 0$ in this step and thus the resulting problem is not necessarily symmetric
- However, when the exact operator $\mathcal{T}$ is used, the methods are equivalent.

Symmetric VMS

Let

- $\tilde{\mathcal{T}}$ be a computable approximation of $\mathcal{T}$
- $U_{f,RH}$ be a computable approximation of $u_{f,RH}$

We get the method: find $U_c \in \mathcal{V}_c$ such that

$$a(U_c + \tilde{\mathcal{T}} U_c, v_c + \tilde{\mathcal{T}} v_c) = (f, v_c + \tilde{\mathcal{T}} v_c) - a(U_{f,RH}, v_c + \tilde{\mathcal{T}} v_c)$$

for all $v_c \in \mathcal{V}_c$.

On matrix form this leads to,

$$K_{\text{mod}} U_c = b_{\text{mod}}$$

Given U_c and $U_{f,RH}$, U_f can be computed.

Construction of $\tilde{\mathcal{T}}$

Recall that $u_c = \sum_i \xi_i N_{c,i}$ with $\{N_{c,i}\}$ a basis in $\mathcal{V}_c$ and let

$$a(\mathcal{T} N_{c,i}, v_f) = -a(N_{c,i}, v_f) \quad \text{for all } v_f \in \mathcal{V}_f$$

By linearity

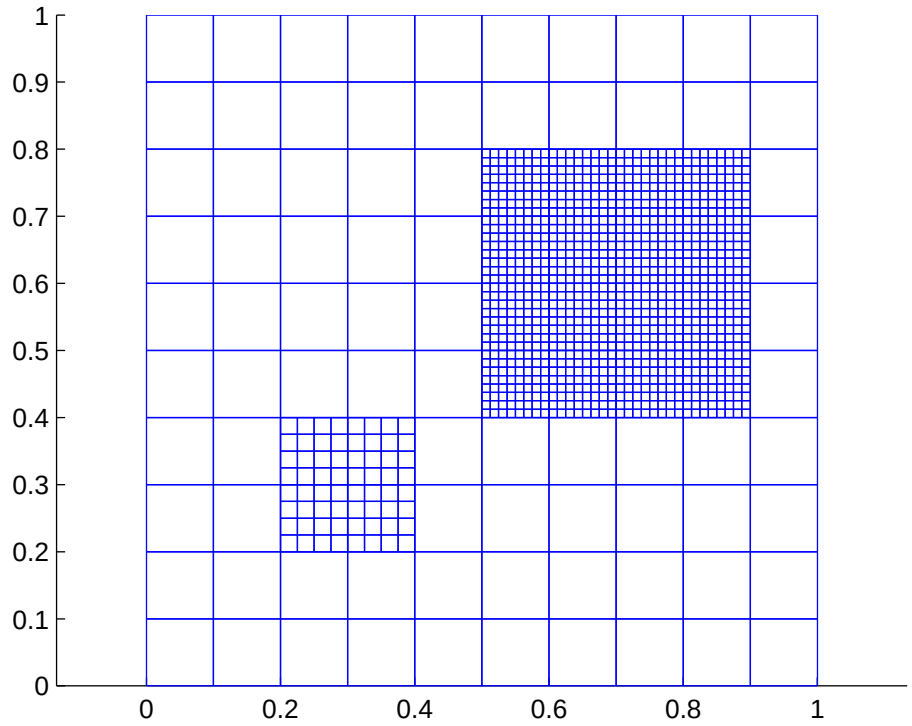
$$\mathcal{T} u_c = \sum_i \xi_i \mathcal{T} N_{c,i}$$

and thus we are led to computing $\mathcal{T} N_{c,i}$ for each coarse basis function $N_{c,i}$.

We define $\tilde{\mathcal{T}}$ by solving these problems approximately by

- Restricting to a localized patch problem $\text{supp}(N_{c,i}) \subset \omega_i$
- Discretizing using a fine subgrid on ω_i

Refinement and Layers



One and two layer stars.

Construction of $U_{f,RH}$

Recall that $u_{f,RH} \in \mathcal{V}_f$ solves

$$a(u_{f,RH}, v_f) = l(v_f) \quad \text{for all } v_f \in \mathcal{V}_f$$

Using a partition of unity φ_i we can split the right hand side as follows

$$l(v_f) = \sum_i l(\varphi_i v_f)$$

and write

$$u_{f,RH} = \sum_i u_{f,RH,i}$$

where

$$a(u_{f,RH,i}, v_f) = l(\varphi_i v_f)$$

Mixed Model Problem

Poisson equation on mixed form:

$$\begin{cases} \frac{1}{a}\boldsymbol{\sigma} - \nabla u = 0 & \text{in } \Omega \\ -\nabla \cdot \boldsymbol{\sigma} = f & \text{in } \Omega \\ n \cdot \boldsymbol{\sigma} = 0 & \text{on } \Gamma \end{cases}$$

where the permeability a has multiscale features.

Typical application is the pressure equation in oil reservoir simulation

Weak Form

Find

$$\boldsymbol{\sigma} \in \boldsymbol{V} = \{\boldsymbol{v} \in H(\mathrm{div};\Omega) : \boldsymbol{n} \cdot \boldsymbol{v} = 0 \text{ on } \Gamma\}$$

$$u \in W = L^2(\Omega)/\mathbf{R}$$

such that

$$(\tfrac{1}{a}\boldsymbol{\sigma}, \boldsymbol{v}) + (u, \nabla \cdot \boldsymbol{v}) = 0$$
$$-(\nabla \cdot \boldsymbol{\sigma}, w) = (f, w)$$

for all $\boldsymbol{v} \in \boldsymbol{V}$ and $w \in W$.

Here $(\cdot, \cdot)$ denotes the $L^2(\Omega)$ scalar product for vector and scalar functions.

Coarse and Fine Scales

We introduce splittings

$$\boldsymbol{V} = \boldsymbol{V}_c \oplus \boldsymbol{V}_f$$
$$W = W_c \oplus W_f$$

where

- $\boldsymbol{V}_c$ is a finite dimensional approximation of $H(\text{div};\Omega)$. We use lowest order Raviart-Thomas basis functions.
- W_c is an approximation of $L^2(\Omega)$. We use piecewise constants.

Splitting Based on RT-elements

- The RT-elements are **normal continuous** but allow **tangential discontinuities.**
- The RT-interpolator π_c is defined by

$$\int_F n \cdot (\boldsymbol{\sigma} - \pi_c \boldsymbol{\sigma}) ds = 0$$

  for each face $F \subset \partial K$.

- We define

$$\boldsymbol{\sigma} = \pi_c \boldsymbol{\sigma} \oplus (I - \pi_c)\boldsymbol{\sigma}$$

  and thus

$$\boldsymbol{\sigma}_f = (I - \pi_c)\boldsymbol{\sigma} \quad \boldsymbol{\sigma}_c = \pi_c \boldsymbol{\sigma}$$

Conservation

Due to the splitting in coarse and fine scales we have

$$\int_F n \cdot \boldsymbol{\sigma}_f ds = 0$$

Thus the integrated total flux through a coarse scale face is represented by the coarse scale flux $\boldsymbol{\sigma}_c$!

Splitting Based on Constants

- Let P_c be the L^2-projection onto W_c, piecewise constants on the coarse mesh
- Given v we have the splitting

$$v = P_c v \oplus (I - P_c)v$$

- Thus we are using an L^2-orthogonal splitting
- $\int_K v_f \, dx = 0$, for coarse elements K

Coarse and Fine Scales

Find $\boldsymbol{\sigma}_c \in \boldsymbol{V}_c$, $\boldsymbol{\sigma}_f \in \boldsymbol{V}_f$, $u_c \in W_c$, and $u_f \in W_f$ such that,

$$\begin{cases} (\frac{1}{a}(\boldsymbol{\sigma}_c + \boldsymbol{\sigma}_f), \boldsymbol{v}_c + \boldsymbol{v}_f) + (u_c + u_f, \nabla \cdot (\boldsymbol{v}_c + \boldsymbol{v}_f)) = 0 \\ -(\nabla \cdot (\boldsymbol{\sigma}_c + \boldsymbol{\sigma}_f), w_c + w_f) = (f, w_c + w_f) \end{cases}$$

for all $\boldsymbol{v}_c \in \boldsymbol{V}_c$, $\boldsymbol{v}_f \in \boldsymbol{V}_f$, $w_c \in W_c$, and $w_f \in W_f$.

We want to approximate the red terms by solving decoupled local problems.

Fine Scale Equations

If we let $v_c = 0$ and $w_c = 0$ we get the following relation between the fine and coarse solutions: find $\boldsymbol{\sigma}_f \in \boldsymbol{V}_f$ and $u_f \in W_f$ such that,

$$(\tfrac{1}{a}\boldsymbol{\sigma}_f, \boldsymbol{v}_f) + (u_f, \nabla \cdot \boldsymbol{v}_f) = -(\tfrac{1}{a}\boldsymbol{\sigma}_c, \boldsymbol{v}_f) - (u_c, \nabla \cdot \boldsymbol{v}_f)$$
$$-(\nabla \cdot \boldsymbol{\sigma}_f, w_f) = (f, w_f) + (\nabla \cdot \boldsymbol{\sigma}_c, w_f)$$

for all $\boldsymbol{v}_f \in \boldsymbol{V}_f$ and $w_f \in W_f$.

Using the properties of our splittings this problem can be simplified!

Orthogonality

We use a hierarchical basis of Raviart-Thomas functions for the flux and piecewise constants for the pressure.

$$(w_c, \nabla \cdot \boldsymbol{v}_f) = \sum_K (w_c, \nabla \cdot \boldsymbol{v}_f)_K = \sum_K w_c^K \int_{\partial K} \boldsymbol{n} \cdot \boldsymbol{v}_f \, dx = 0$$

where w_c^K is the constant at coarse element K.

$$(w_f, \nabla \cdot \boldsymbol{v}_c) = \sum_K (w_f, \nabla \cdot \boldsymbol{v}_c)_K = \sum_K \nabla \cdot \boldsymbol{v}_c^K \int_K w_f \, dx = 0$$

since $\nabla \cdot \boldsymbol{v}_c^K$ is constant on K.

Simplified Fine Scale Equations

- Find $\boldsymbol{\sigma}_f \in \boldsymbol{V}_f$ and $u_f \in W_f$ such that,

$$(\tfrac{1}{a}\boldsymbol{\sigma}_f, \boldsymbol{v}_f) + (u_f, \nabla \cdot \boldsymbol{v}_f) = -(\tfrac{1}{a}\boldsymbol{\sigma}_c, \boldsymbol{v}_f) - (u_c, \nabla \cdot \boldsymbol{v}_f)$$
$$-(\nabla \cdot \boldsymbol{\sigma}_f, w_f) = (f, w_f) + (\nabla \cdot \boldsymbol{\sigma}_c, w_f)$$

  for all $\boldsymbol{v}_f \in \boldsymbol{V}_f$ and $w_f \in W_f$.

- The red terms vanish and we end up with

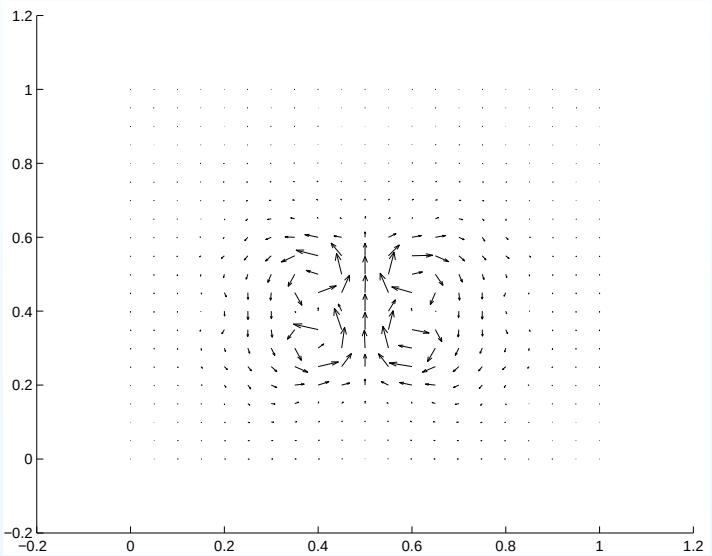
$$\begin{cases} (\tfrac{1}{a}\boldsymbol{\sigma}_f, \boldsymbol{v}_f) + (u_f, \nabla \cdot \boldsymbol{v}_f) = -(\tfrac{1}{a}\boldsymbol{\sigma}_c, \boldsymbol{v}_f) \\ -(\nabla \cdot \boldsymbol{\sigma}_f, w_f) = (f, w_f) \end{cases}$$

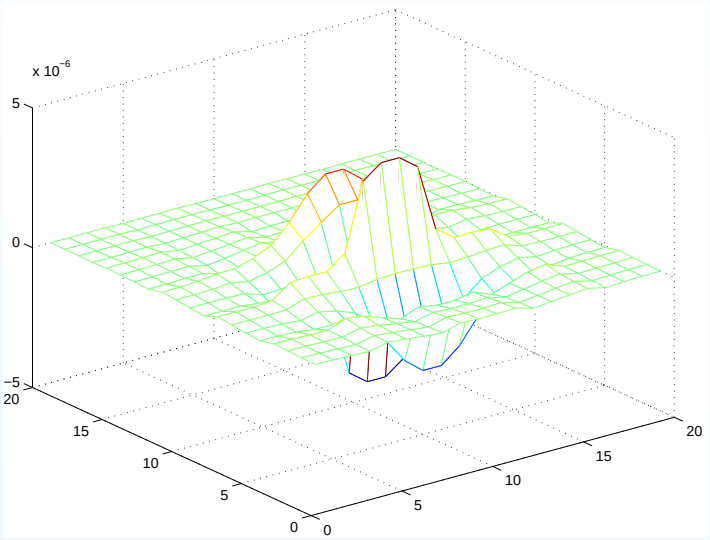
- Thus there are no couplings from the coarse scale pressure to the fine scale equations

Approximate Fine Scales

- We apply the abstract framework
- Divide the problem into contributions from the coarse scale part $\boldsymbol{\sigma}_c$ and right hand side f
- $\boldsymbol{\Sigma}_c = \sum_i \Sigma_{c,i} \boldsymbol{\phi}_i$ where $\boldsymbol{\phi}_i$ are the Raviart-Thomas basis functions. Solve the local problem driven by the basis functions (one problem for each basis function)
- Localize by restricting the problem to a patch and using homogeneous Neumann conditions
- Discretize using a suitable subgrid

Local Fine Scale Solution

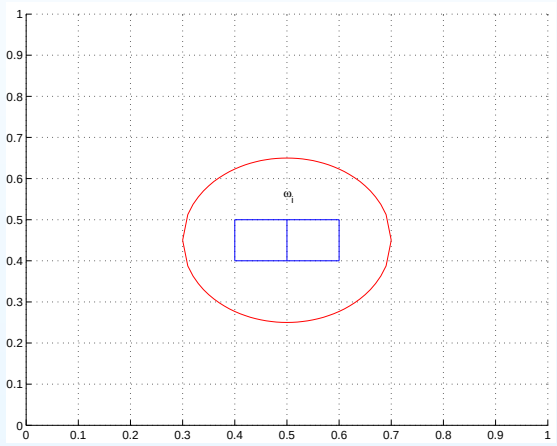




The local solutions $\boldsymbol{\sigma}_{f,i}$ and $u_{f,i}$.

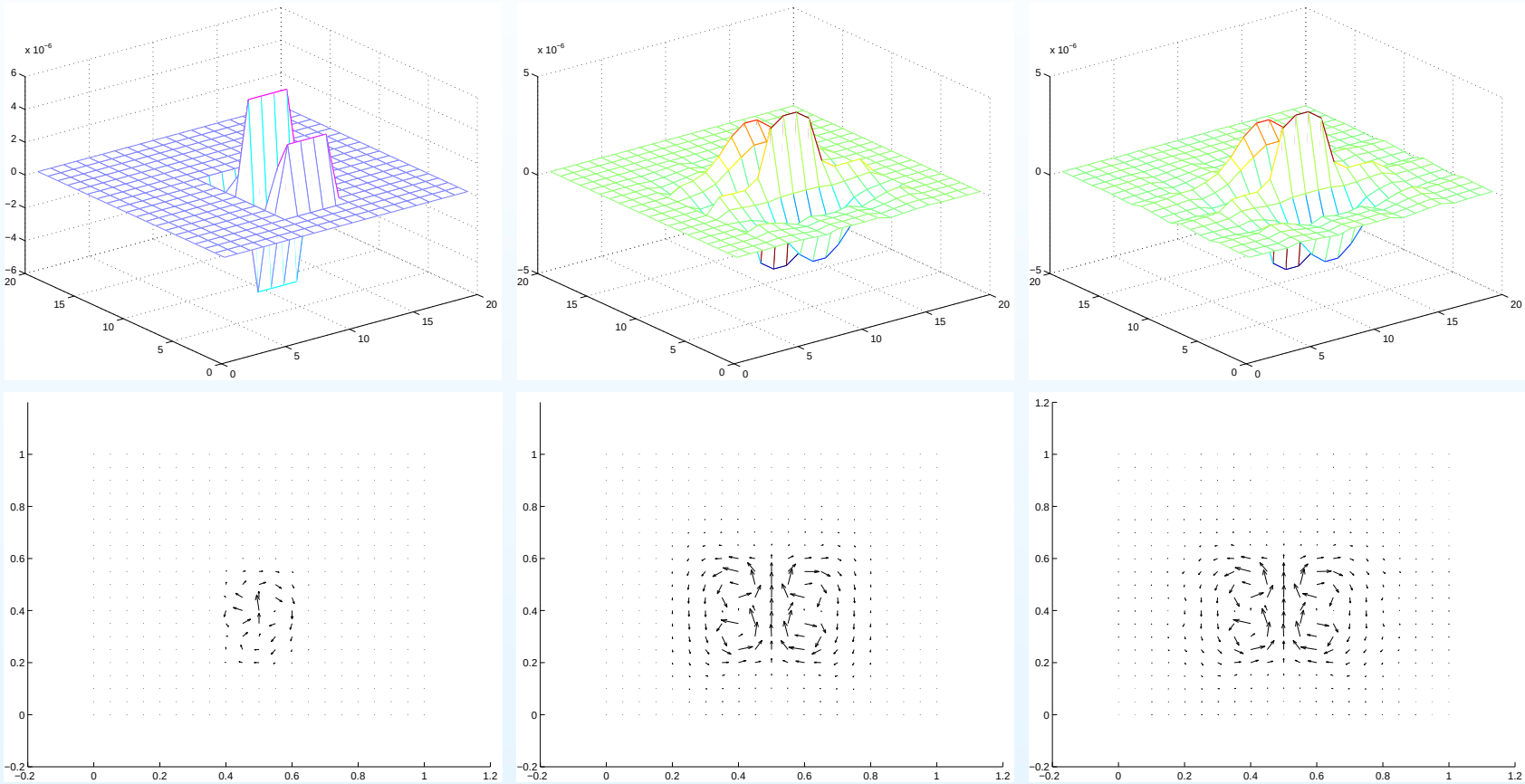
Restriction to Patches

The equations are solved in a slice space where solutions decay rapidly, $\int_E \boldsymbol{n} \cdot \boldsymbol{\sigma}_{f,i}\, dx = 0$ and $\int_K u_{f,i}\, dx = 0$.



The patch ω_i typically consists of coarse elements but could have any geometry.

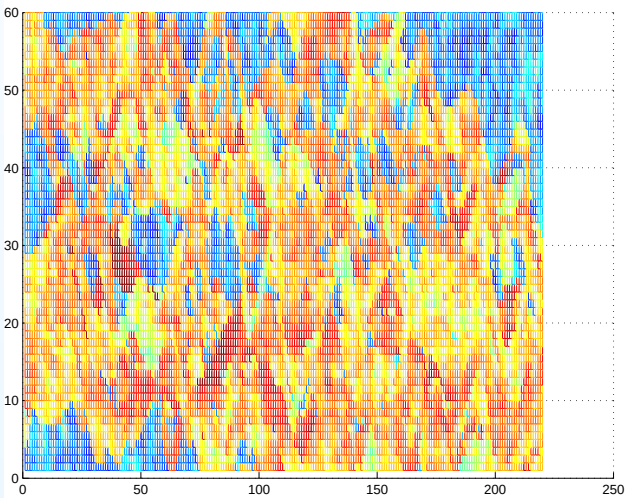
Local Solutions on Patches



1, 2, and 3 layer patches. Above $U_{f,i}$ below $\mathbf{\Sigma}_{f,i}$.

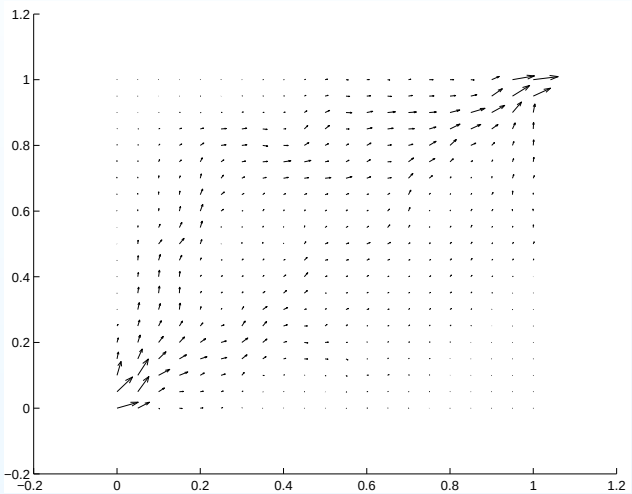
Example

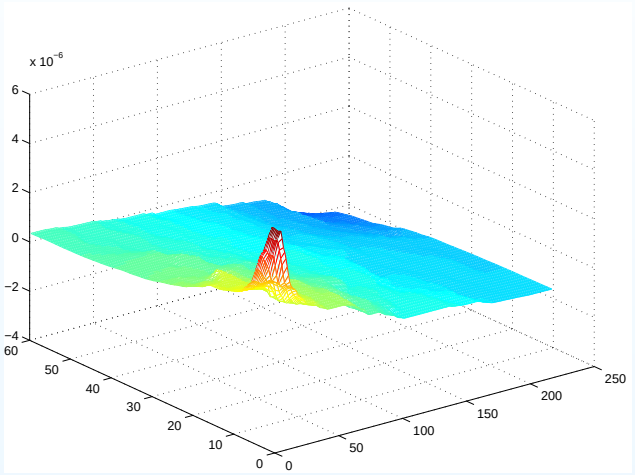
In the figure we display the bottom layer of the Upper Ness formation



We let $f = 1$ in the lower left corner and $f = -1$ in the upper right corner. $\max a / \min a = 8.8e6$.

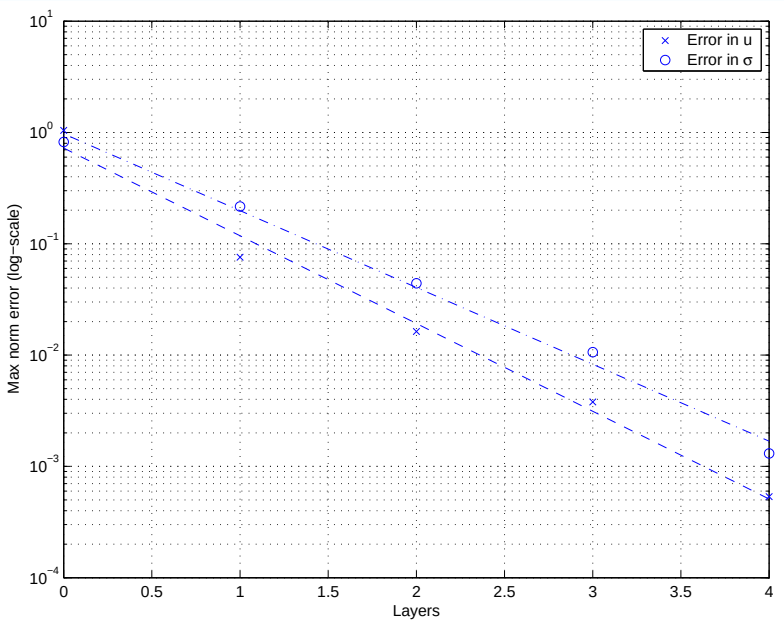
Example





To the left we see the flux and to the right the pressure. We use 220×60 elements for the reference solution.

Example



55×15 coarse elements and $h = H/4$. We get exponential decay in max norm error compared with reference solution when increasing the number of layers!

A Posteriori Error Estimate

The following energy norm bound holds

$$\|\boldsymbol{v}\|_a^2 \leq C_a^2 \sum_i R_{\omega_i}^2 + R_{\partial\omega_i}^2$$

where

$$R_{\omega_i} = \|\frac{1}{a}(\Sigma_c^i \boldsymbol{\phi}_i + \boldsymbol{\Sigma}_{f,i}) - \nabla U_{f,i}^*\|_{\omega_i}^2 + \|\frac{h}{a}(f\psi_i + \nabla \cdot (\Sigma_c^i \boldsymbol{\phi}_i + \boldsymbol{\Sigma}_{f,i}))\|_{\omega_i}^2$$

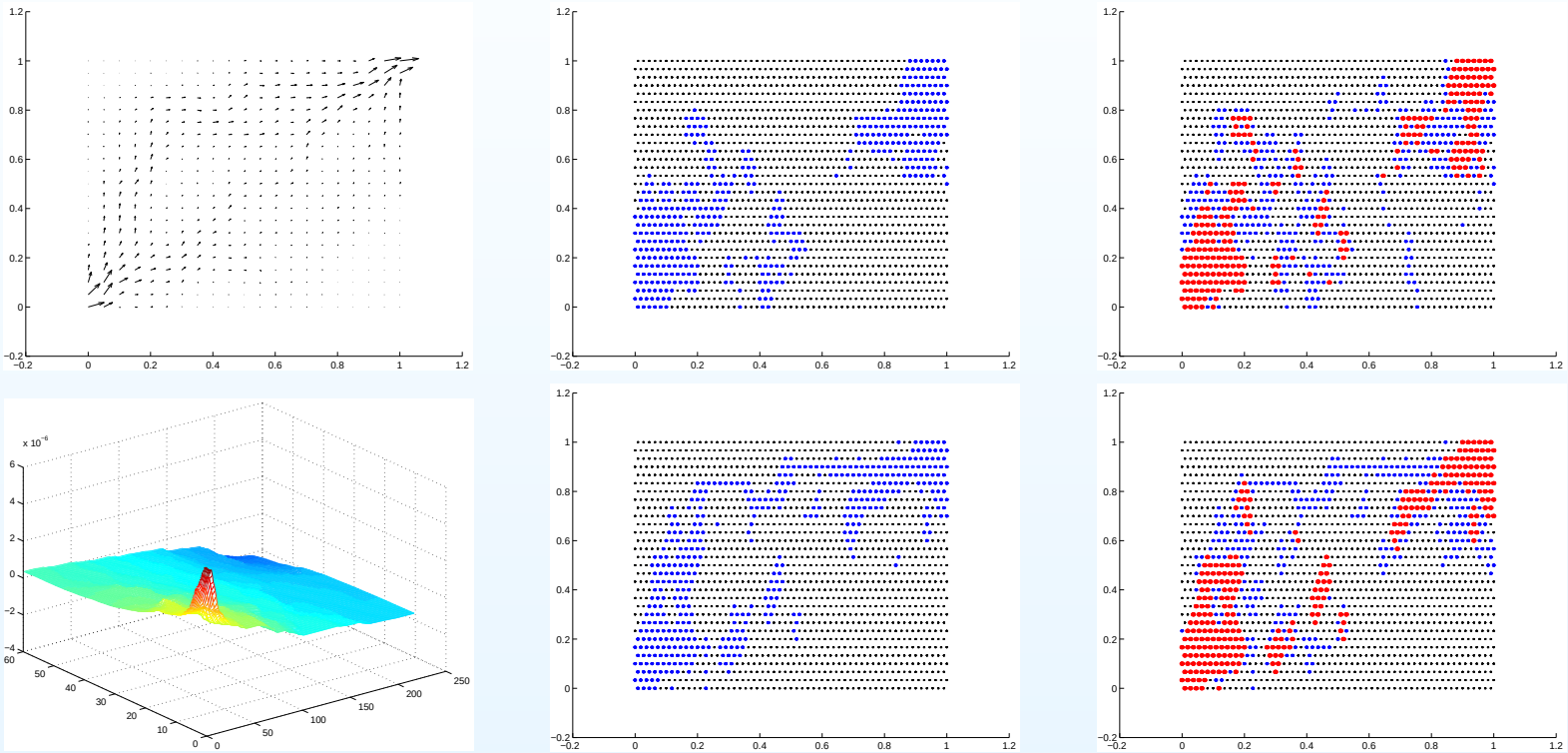
$$R_{\partial\omega_i} = \|\frac{1}{2\sqrt{h}} U_{f,i}^*\|_{\partial\omega_i \setminus \Gamma}^2$$

U^* is a post proc version of U, $C_a \sim \|\sqrt{a}\|_{L^\infty(\omega_i)}$.

Adaptive Strategy

- Start with one layer patches with one refinement in all local problems
- Solve the problem
- Calculate the error indicators R_{ω_i} and $R_{\partial\omega_i}$ on each patch
- If $R_{\omega_i}(h)$ large refine h (25%)
- If $R_{\partial\omega_i}(L)$ increase L (25%)
- Repeat

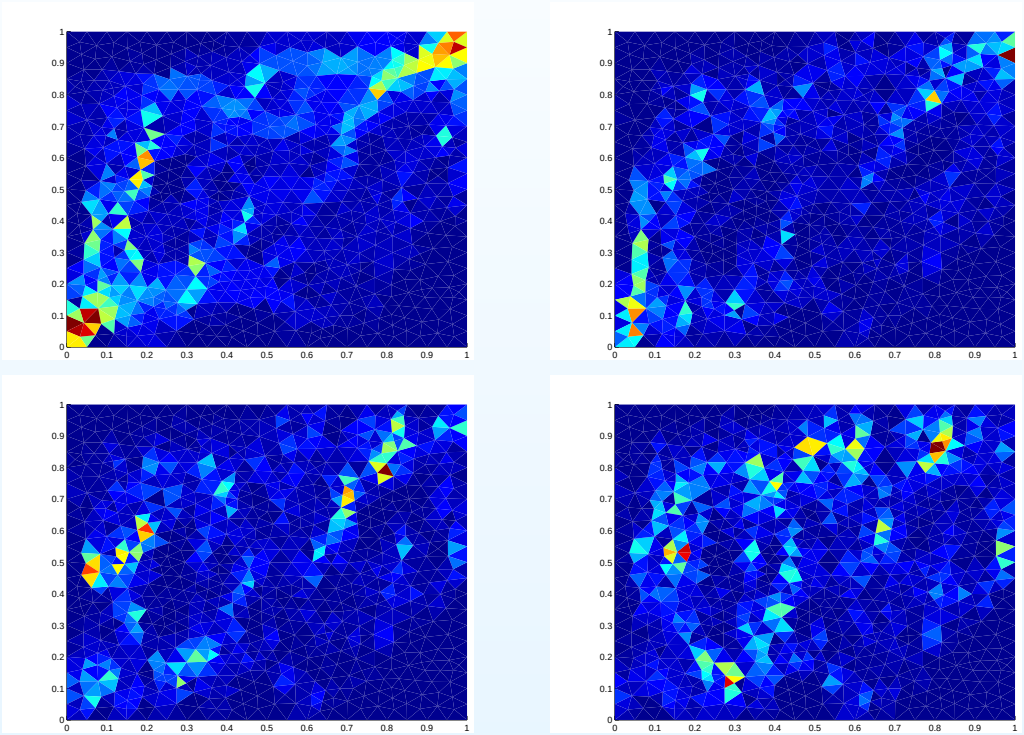
Layers and Refinements



Black circle is one, blue is two and red is three layers/refinements (layers top, refs bottom).

Relative Error in Energy Norm

Galerkin 105.6% and one iteration 15.8%.



Two iterations 10.1% and three iterations 7.6%.

Conclusions from Example

- The error indicators finds critical areas
- More computational effort in these areas decreases the global error quickly
- To get an equally good approximation without adaptivity we need to use three refinements on two layer patches
- In the example above we still have 70% of the patches using one layer and one refinement

Summary

The AVMS provides:

- Systematic technique for construction of a computable approximation of the fine scale part of the solution using decoupled localized subgrid problems.
- A posteriori error estimation framework in both norms and goal functionals
- Adaptive algorithms for automatic tuning of critical discretization parameters

Current Work and Outlook

- Implementation in 3D and more extensive numerical tests
- More scales and different types of physics
- Multiscale approach for transport problems
- DG would lead to a nicer splitting for the problem on standard form