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Stable Multiscale Discretizations of L^2-Differential Complexes

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Collaborators

Joint work with

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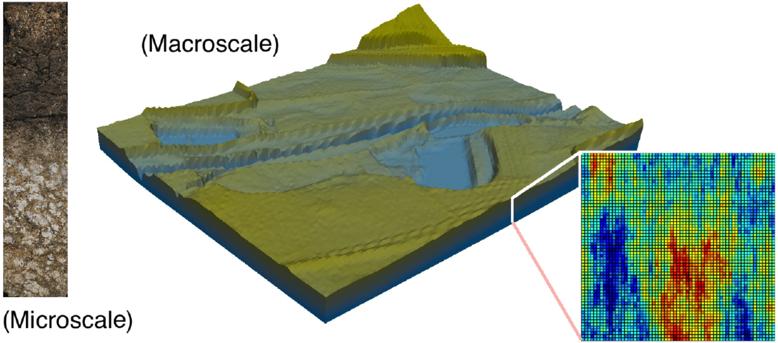
Hydrology Simulations

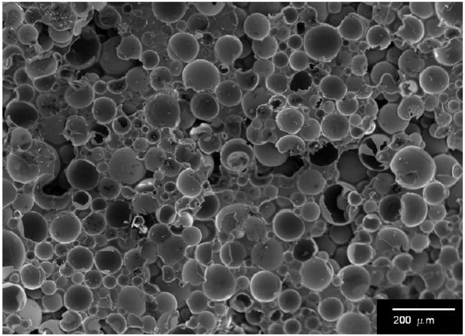
- Topography (macro scale)
- Porous soil structure (fine scale)
- Scales range from mm to km



Mechanics of Composite Materials

- Macroscopic stress is determined through microscopic structures
- Scales range from μm to m

Multiple scales and high contrast.

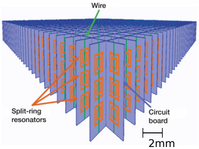


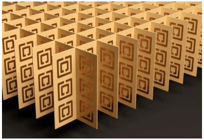
Glass fibers in a synthetic resin matrix.

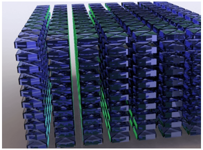
Example Applications III

Meta materials

- Materials with negative refraction index
- Ring structure made of nonmagnetic metals, interlocked cells of glass fibre circuits, vertical connecting metallic wires (metallic structure and split-ring resonators)
- Scales range from nm to m







$$\nabla \cdot D = \rho \quad \text{(Gauß law)}$$

$$\nabla \cdot B = 0 \quad \text{(Gauß law for magnetism)}$$

$$\frac{1}{c}\partial_t B + \nabla \times E = 0 \quad \text{(induction law)}$$

$$\frac{1}{c}\left(4\pi j + \partial_t D\right) = \nabla \times H \quad \text{(circuital law)}$$

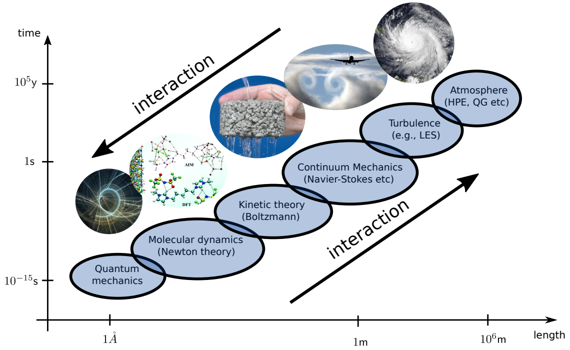
$$\underline{\underline{\varepsilon_r^{(\delta)}}}\varepsilon_0 E = D \quad \text{(material law)}$$

$$\underline{\underline{\mu_r^{(\delta)}}} H = B \quad \text{(material law)}$$

Models are derived from reasonable assumptions (scale dependent) and are valid if the interaction with other scales is not too strong.

⇒ Ideally: Use model with limited range of scales as basis for simulation!

Models on different scales



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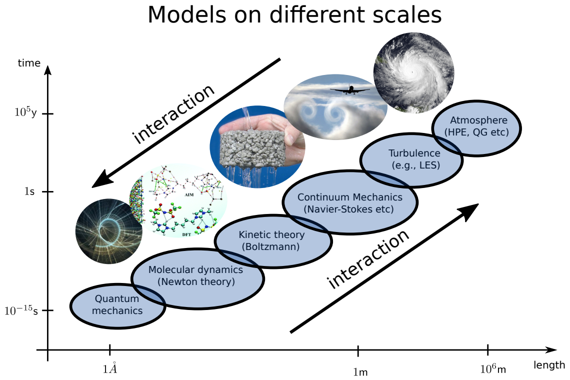


⇒ Not always possilble!
(scale interaction)

Challenge with many Scales

In order to represent a function with smallest wave $O(\varepsilon)$ in d dimensions we need at least

$$\#\ \text{unknowns} \geqslant O(\varepsilon^{-d})\ \text{[Shannon '48]} \rightarrow \text{(memory consumption)}$$

and

$$\#\ \text{flops} \geqslant O(\varepsilon^{-rd}),\ r \geqslant 1 \rightarrow \text{(time consumption)}$$

Scale Coupling
in Climate Simulations

How do the scales talk?

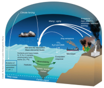
$$\begin{aligned}
\rho_t + \nabla\cdot(\rho\mathbf{v}) &= 0\\
(\rho\mathbf{v})_t + \nabla\cdot(\rho\mathbf{v}\otimes\mathbf{v} + 2\Omega\times\rho\mathbf{v}) + \nabla p &= -\nabla\cdot\boldsymbol{\tau} - \rho\mathbf{g}\\
(\rho e + \rho\boldsymbol{\Phi})_t + \nabla\cdot(\mathbf{v}[\rho e + \rho\boldsymbol{\Phi} + p]) + \nabla p &= -\nabla\cdot(\mathbf{j} + \boldsymbol{\tau}) + \rho Q\\
-\mu\left(\nabla\mathbf{v} + \nabla\mathbf{v}^T + \hat{\mu}(\nabla\cdot\mathbf{v})\mathbb{I}\right) &= \boldsymbol{\tau}\\
-\lambda\nabla T &= \mathbf{j}\\
\frac{p}{\gamma-1} + \frac{1}{2}\rho|\mathbf{v}|^2 &= \rho e
\end{aligned}$$

Dynamical Core
(resolved)

scales $\geq O(H)$

upscaling

interpolation



Parametrizations
(not resolved)

$O(H) \geq$ scales $\geq O(h)$

coarse — truncation scale — fine

$\Rightarrow$ One direction of information transfer is easy ...

Question: What fine-scale information is relevant on coarse scales?

The Problem

Many interesting systems are/have

- experimentally hardly accessible (as a whole)
- multiple scales with complex scale interactions
- transient
- dominated by advection (additional difficulty)
- large systems with algebraic/PDE constraints

State of the Arts in operational codes

- many parametrized subgrid processes (consistent scale coupling is crucial)
- Scale coupling often done only heuristically
- simulate effective behavior correctly?

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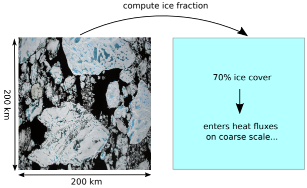
Example

Common sea ice parametrization



What's wrong with that?

Well... let's find the effective model (homogeniziation)

We have $F_\varepsilon(u_\varepsilon) = 0$ (ε represents smallest scales) so maybe we can

Find F^* and u^* so that $u_\varepsilon \to u^*$ and $F_\varepsilon \to F^*$ (in some sense) in the limit of large range of scales, scale separation with

$$F^*(u^*) = 0 \ .$$

This is called effective model.

Toy Example

What is the effective model of this PDE as $\varepsilon \to 0$?

$$\left(a(\frac{x}{\varepsilon})u^{\varepsilon}_{x}\right)_{x} = f\,, \quad x \in I = [a, b]\,, 0 < q \leqslant a \in L^{\infty}([0, 1])$$

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This?

$$m_{\mathrm{A}}(a)u_{xx}^* = f\,, \quad m_{\mathrm{A}}(a) = \int_0^1 a(y)\,\mathrm{d}y$$

→ Remember: this is sort of what is being done...

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7. But (1) and $\frac{1}{a^\varepsilon}\xi^\varepsilon = \frac{\mathrm{d}}{\mathrm{d}x}u^\varepsilon$ so that $\frac{\mathrm{d}}{\mathrm{d}x}u = m_{\mathrm{A}}(\frac{1}{a})\xi$ (uniqueness of limits)

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8. On the other hand we have $\frac{\mathrm{d}}{\mathrm{d}x}\xi = f$

... and so:

What is the effective model of this PDE as $\varepsilon \to 0$?

$$\left(a(\frac{x}{\varepsilon})u_x^\varepsilon\right)_x = f\,, \quad x \in I = [a,b]\,, a \in L^\infty([0,1])$$

Proposition

The effective model is given by

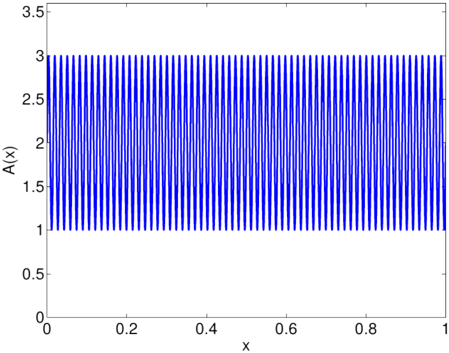
$$\frac{1}{m_H(a)} u_{xx}^* = f\,, \quad m_H(a) = \int_0^1 \frac{1}{a(y)}\,\mathrm{d}y\,.$$

In general $m_{\mathrm{A}}(a) \geqslant \frac{1}{m_{\mathrm{H}}(a)}$, i.e., averaging leads to excessive diffusion!

Toy problem: Find solution of $u(0) = u(1) = 0$

$$-\left(a(\frac{x}{\varepsilon})u^{\varepsilon}_{x}\right)_x = 1$$

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



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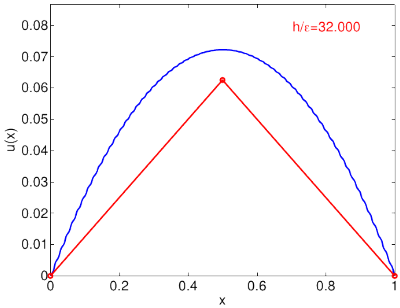

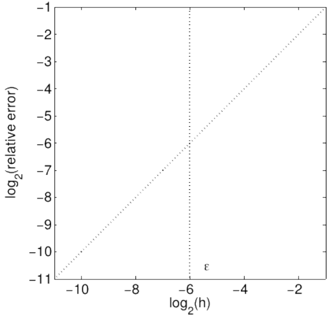

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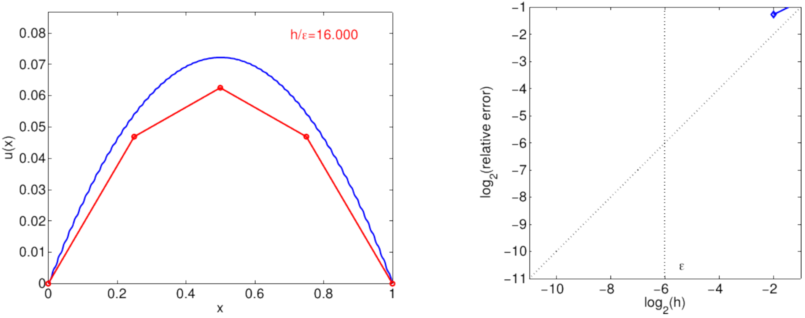

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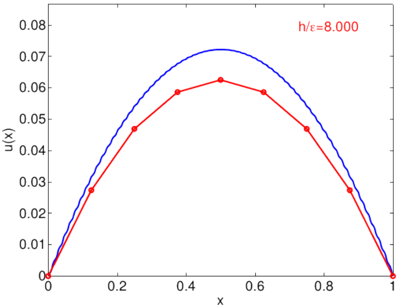

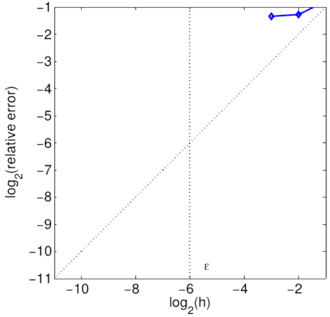

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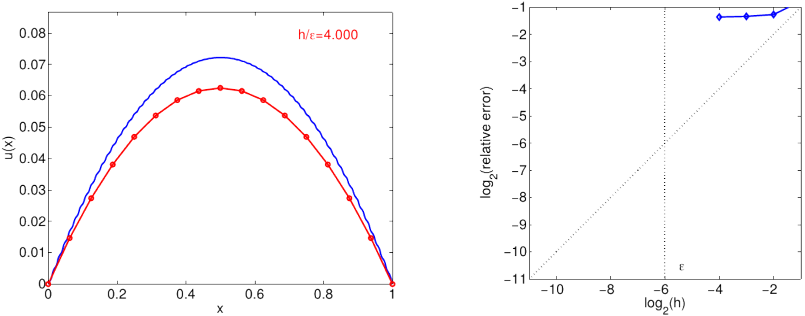

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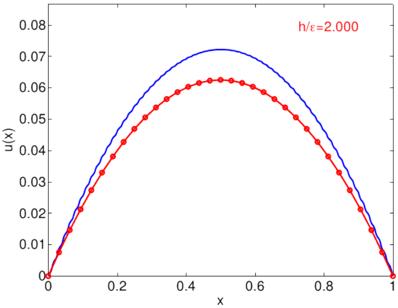

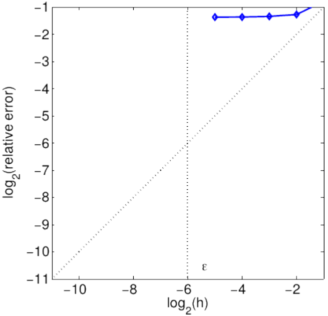

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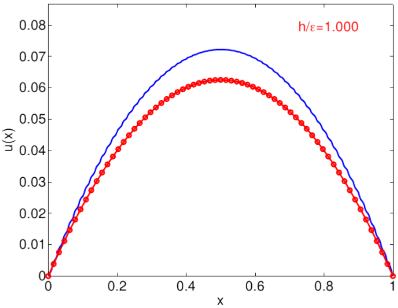

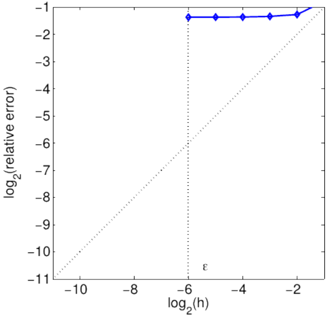

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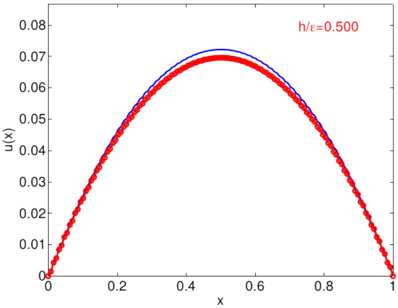

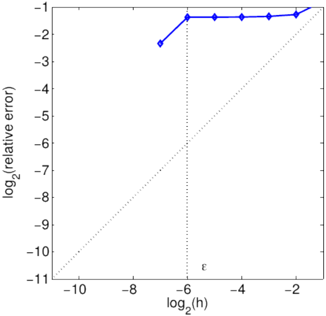

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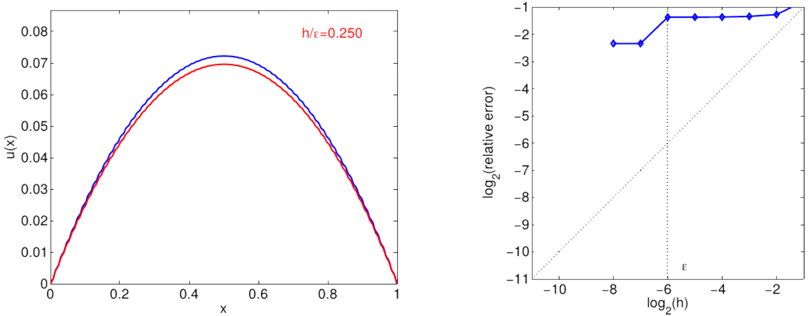

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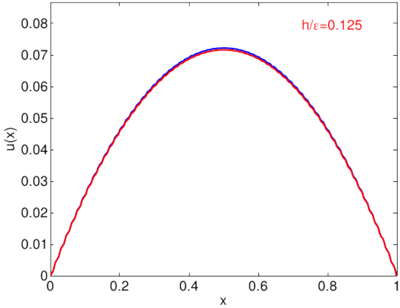

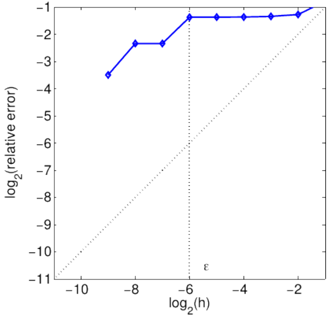

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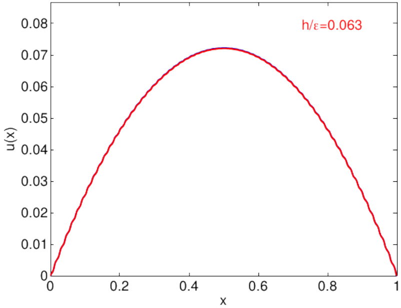

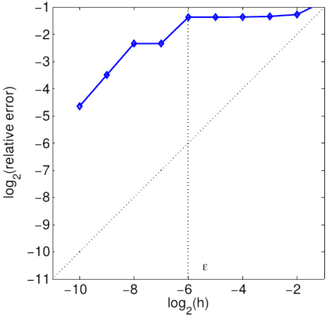

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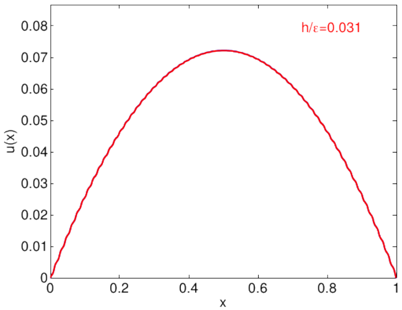

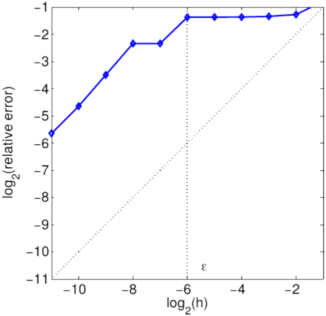

(courtesy: P.Henning, KTH, Sweden)

Galerkin orthogonality:

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A bit more intuition from FEM theory...

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Message

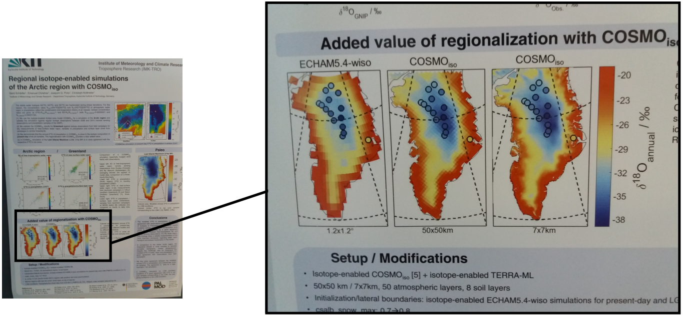
If the H^1-approximation of u is bad then the L^2-approximation is worse.
There are good L^2-projections but our Galerkin method does not find them!
But we are looking for good L^2-projections!

Homogenized models are often not available.

Without effective equation and $\varepsilon << 1$ microscale computations only in limited domains. $\Rightarrow$ We need coarse decompostion and localization.

At least: Numerical methods should reflect homogenization principles... good part is understood for elliptic problems ...

Accuracy under resoluion constraints? (courtesy: E. Christner et al., KIT, Germany)



Subgrid data represented well if resolution is prohibitively high...

Idea of MsFEM [Hou & Wu, '99]

MsFEM

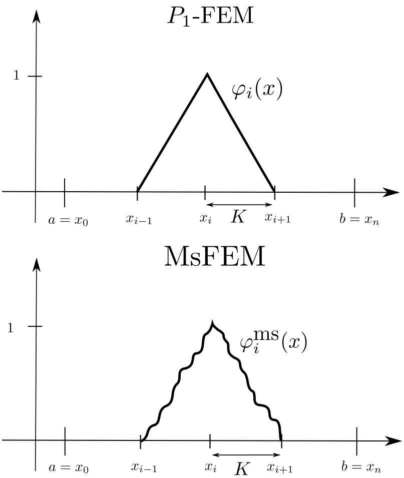
Model:

$$-\nabla \cdot (A^\varepsilon \nabla u^\varepsilon) = f$$

Idea: To capture the asymptotic structure of the solution modify the basis

$$-\nabla \cdot (A^\varepsilon \nabla \varphi_i^{\mathrm{ms}}) = 0 \quad \text{in } K$$

$$\varphi_i^{\mathrm{ms}}|_{\partial K} = \varphi_i|_{\partial K}$$



A priori estimates for model problem

Theorem (Hou & Wu, '99)

Let $u^\varepsilon \in H^2(\Omega)$ solve the model problem and $u^{\varepsilon,h} \in P^h$ be the MsFEM solution.
Then if $h < \varepsilon$

$$\left\| u^\varepsilon - u^{\varepsilon,h} \right\|_{H^1} \leqslant Ch(|u^\varepsilon|_{H^2} + \|f\|_{L^2}) \,.$$

If $h > \varepsilon$ and $u^0 \in H^2 \cap W^{1,\infty}$ is the solution to the homogenized problem then

$$\left\| u^\varepsilon - u^{\varepsilon,h} \right\|_{H^1} \leqslant C(h + \varepsilon) \|f\|_{L^2} + C \left(\frac{\varepsilon}{h} \right)^{1/2} \left\| u^0 \right\|_{W^{1,\infty}} \,.$$

Note: $|u^\varepsilon|_{H^2} = O(\varepsilon^{-1}) \to \infty$ as $\varepsilon \to 0$.

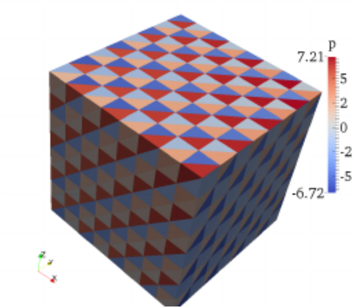
Fails if lower order terms are involved.

Observation

- Pactical problems involve systems with many unknowns (not only scalar variables)
- Different parts of the system are in different spaces (velocity u, vorticity $\nabla \times u$, divergence $\nabla \cdot u$)
- Parts are related through (differential) operators
- Parts are in different function spaces related in an exact sequence
- Still the system exhibits multiscale features
- Stability is crucial
- Violation of stability constraints causes spurious modes (numerical derivatives small, despite approximating oscillatory function)

The latter can cause large dispersion errors in dynamic models (and other instabilities).

Checkerboard Instability



$P_1 - P_0$ elements do not satisfy a stability condition!

These spaces are related in a closed (differential) complex:

$$L^2\Lambda^0(\Omega) \xrightarrow{\mathrm{d}} L^2\Lambda^1(\Omega) \xrightarrow{\mathrm{d}} L^2\Lambda^2(\Omega) \xrightarrow{\mathrm{d}} L^2\Lambda^3(\Omega)$$

- exterior differentials d are vieved as closed unbounded operators
- Note that this is a complex, i.e. $\mathrm{d}^2 = 0$ and $\mathcal{R}(\mathrm{d}) \subset \mathcal{N}(\mathrm{d})$

We look at a multiscale version of this complex:

$$L^2\Lambda^0(\Omega, A_\varepsilon^0) \xrightarrow{\mathrm{d}} L^2\Lambda^1(\Omega, A_\varepsilon^1) \xrightarrow{\mathrm{d}} L^2\Lambda^2(\Omega, A_\varepsilon^2) \xrightarrow{\mathrm{d}} L^2\Lambda^3(\Omega, A_\varepsilon^3)$$

with norms

$$\|u\|_{L^2\Lambda^k(\Omega, A_\varepsilon^k)} = \left\|\sqrt{A_\varepsilon^k}u\right\|_{L^2\Lambda^k(\Omega)}$$

for uniformly positive $A_\varepsilon^k : L^2\Lambda^k \to L^2\Lambda^k$

The domain complex is the complex of the domains of
$\mathrm{d} : L^2\Lambda^k(\Omega, A_\varepsilon^k) \to L^2\Lambda^{k+1}(\Omega, A_\varepsilon^{k+1})$.

$$H\Lambda^0(\mathrm{d}, A_\varepsilon^0) \xrightarrow{\mathrm{d}} H\Lambda^1(\mathrm{d}, A_\varepsilon^1) \xrightarrow{\mathrm{d}} H\Lambda^2(\mathrm{d}, A_\varepsilon^2) \xrightarrow{\mathrm{d}} H\Lambda^3(\mathrm{d}, A_\varepsilon^3)$$

which are endowed with the graph norms

$$\|u\|^2_{H\Lambda^k(\mathrm{d}, A_\varepsilon^k)} = \|u\|^2_{L^2\Lambda^k(\Omega)} + \left\| \sqrt{A_\varepsilon^{k+1}}\, \mathrm{d}u \right\|^2_{L^2\Lambda^{k+1}}$$

and are therefore Hilbert spaces.

Theorem (Poincaré Inequality and Hodge decomposition)

With $\mathfrak{B}^k = \mathrm{d}H\Lambda^{k-1}(\mathrm{d}, A_\varepsilon^{k-1})$, $\mathfrak{Z}^k = \mathcal{N}(\mathrm{d}) \subset H\Lambda^k(\mathrm{d}, A_\varepsilon^k)$ *and* $\mathfrak{H}^k = \mathfrak{Z}^k \cap \mathfrak{B}^{k,\perp}$ *we have*

$$\|u\|_{H\Lambda^k(\mathrm{d}, A_\varepsilon^k)} \leqslant C \, \|\mathrm{d}u\|_{H\Lambda^k(\mathrm{d}, A_\varepsilon^k)}, \quad u \in \mathfrak{Z}^{k,\perp_V} \quad \text{(Poincaré)}$$

and the decompositions

$$L^2\Lambda^k(\mathrm{d}, A_\varepsilon^k) = \mathfrak{B}^k \oplus \mathfrak{H}^k \oplus \mathfrak{B}^*_k$$

and

$$H\Lambda^k(\mathrm{d}, A_\varepsilon^k) = \mathfrak{B}^k \oplus \mathfrak{H}^k \oplus \mathfrak{Z}^{k,\perp_V}$$

from the closed range theorem.

→ Finding Helmholtz decompositions in weighted spaces helps to understand and design stable multiscale methods.

How to find such decompositions?

→ Finding Helmholtz decompositions in weighted spaces helps to understand and design stable multiscale methods.

How to find such decompositions?

Solve the weighted Hodge-Laplace euqation in each segement of the domain complex:

$$H(\mathrm{grad}, A_\varepsilon^0) \xrightarrow{\nabla} H(\mathrm{curl}, A_\varepsilon^1) \xrightarrow{\nabla\times} H(\mathrm{div}, A_\varepsilon^2) \xrightarrow{\nabla\cdot} L^2(\Omega, A_\varepsilon^3)$$

which seeks for $f \in L^2\Lambda^k$

$$u \in \mathcal{D}(L^k) = \left\{ u \in H\Lambda^k \cap H\Lambda^{k,*} \mid \mathrm{d}u \in H\Lambda^{k+1,*} \text{ and } \mathrm{d}^* u \in H\Lambda^{k-1} \right\}$$

such that $u \perp \mathfrak{H}^k$ and ($\mathfrak{H}^k$ harmonic forms)

$$L^k u = \mathrm{d}^* A_\varepsilon^{k+1}\, \mathrm{d}u + \mathrm{d}A_\varepsilon^{k-1}\, \mathrm{d}^* u = f - P_{\mathfrak{H}^k} f$$

Note: Solutions are differential forms!

The Weighted Hodge-Laplace Problem

- In each segment of the complex this equation takes a different form
- The problem is well posed
- There is a strong, a primal weak form and a mixed weak form

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It turns out that only the mixed weak form is suitable for discretiztaion!!!

This is the ordinary diffusion equation in weak form as a Neumann problem with

$$\mathcal{D}(L) = \left\{u \in H(\text{grad}) \mid \nabla \cdot A_\varepsilon \nabla u \in L^2 \,, \partial_n u = 0\right\}$$

such that

$$\int \nabla v \cdot A_\varepsilon \nabla u = \int v(f - P_{\mathfrak{H}^0}) \quad v \in H(\text{grad})$$

$$\int u = 0$$

Boundary conditions are natural!

$\rightarrow$ Neumann boundary conditions:

$$\partial_n u = 0 \text{ on } \partial\Omega$$

The Weighted Hodge-Laplace Problem
$k = 1$

This is the weighted vector Laplace equation in weak form with

$$u \in H(\text{curl}) \cap H_0(\text{div}) \,, \nabla \times u \in H_0(\text{curl}) \,, B_\varepsilon \nabla \cdot u \in H(\text{grad})$$

such that

$$\int \tau B_\varepsilon^{-1} \sigma - \int \nabla \tau \cdot u = 0 \,, \quad \tau \in H(\text{grad})$$
$$\int v \cdot \nabla \sigma + \int \nabla \times v \cdot A_\varepsilon \nabla \times u = \int v \cdot f \,, \quad v \in H(\text{curl})$$

with $\sigma = B_\varepsilon \nabla u$.

Boundary conditions are natural!

$\rightarrow$ magnetic boundary conditions:

$$u \cdot n = 0 \quad \text{and} \quad \nabla \times u \times n = 0 \text{ on } \partial\Omega$$

This is the weighted vector Laplace equation in weak form with

$$u \in H_0(\mathrm{curl}) \cap H(\mathrm{div})\,, A_\varepsilon \nabla \times u \in H(\mathrm{curl})\,, \nabla \cdot u \in H_0(\mathrm{grad})$$

such that

$$\int \tau A_\varepsilon^{-1} \sigma - \int \nabla \times \tau \cdot u = 0\,, \quad \tau \in H(\mathrm{curl})$$

$$\int v \cdot \nabla \times \sigma + \int \nabla \cdot v B_\varepsilon \nabla \cdot u = \int v \cdot f\,, \quad v \in H(\mathrm{div})$$

with $\sigma = A_\varepsilon \nabla \times u$.

Boundary conditions are natural!

$\rightarrow$ electric boundary conditions:

$$u \times n = 0 \quad \text{and} \quad \nabla \cdot u = 0 \text{ on } \partial\Omega$$

This is the weighted Diffusion equation in mixed weak form with

$$\mathcal{D}(L) = \{u \in H_0(\text{grad}) \mid \nabla \cdot A_\varepsilon \nabla u \in L^2\}$$

such that

$$\int \tau A_\varepsilon^{-1} \sigma - \int \nabla \cdot \tau \cdot u = 0\,, \quad \tau \in H(\text{div})$$

$$\int v \cdot \nabla \cdot \sigma = \int v \cdot f\,, \quad v \in L^2$$

with $\sigma = A_\varepsilon \nabla \times u$.

Boundary conditions are natural!

→ Dirichlet boundary conditions:

$$u = 0 \text{ on } \partial\Omega$$

Finite element exterior calculus (FEEC) says stable discretizations can be obtained if the diagram

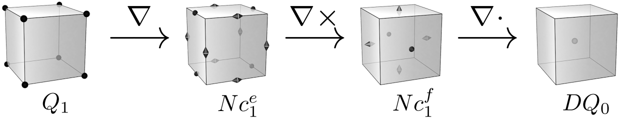
$$\begin{array}{ccccccc} H(\text{grad}) & \xrightarrow{\nabla} & H(\text{curl}) & \xrightarrow{\nabla\times} & H(\text{div}) & \xrightarrow{\nabla\cdot} & L^2 \\ \downarrow \Pi_{\mathsf{ms}}^{(\text{grad})} & & \downarrow \Pi_{\mathsf{ms}}^{(\text{curl})} & & \downarrow \Pi_{\mathsf{ms}}^{(\text{div})} & & \downarrow \Pi_{L^2} \\ \mathsf{Q}_1^{\mathsf{ms}} & \xrightarrow{\nabla} & \mathsf{Ned}_0^{\mathsf{ms}} & \xrightarrow{\nabla\times} & \mathsf{RT}_0^{\mathsf{ms}} & \xrightarrow{\nabla\cdot} & \mathsf{DQ}_0 \end{array}$$

commutes, i.e. we must seek bounded co-chain projections.

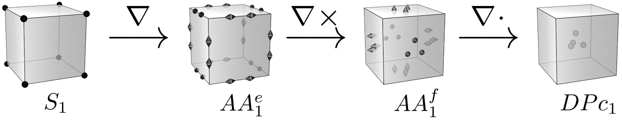
Can we mimic a rigorous construction of stable elements in this framework for multiscale discretizations?

Examples of Stable Discretizations

$Q_r^- \Lambda^k$-family



$S_r \Lambda^k$-family



Look at one coarse cell K and denote Ned_k and RT_k the $k-th$ standard lowest order Nédélec basis (Raviart-Thomas resp.):

$H(\mathrm{curl}, K)$-basis

Find $\sigma_k \in \mathsf{Ned}_k + H_0(\mathrm{curl}, K)$ and $u_k \in \nabla \times \mathsf{Ned}_k + H_0(\mathrm{div}, K)$ s.th.

$$A_\varepsilon^{-1}\sigma_k - \nabla \times u_k = 0$$
$$\nabla \times \sigma_k + \nabla B_\varepsilon \nabla \cdot u_k = \nabla \times \mathsf{Ned}_k + u_{k1}^* - u_{k2}^*$$

for $\tau \in H_0(\mathrm{curl}, K)$ and $v \in H_0(\mathrm{div}, K)$.

$H(\mathrm{div}, K)$-basis

Find $\sigma_j \in H_0(\mathrm{curl}, K)$ and $u_j \in \mathsf{RT}_j + H_0(\mathrm{div}, K)$ s.th.

$$A_\varepsilon^{-1}\sigma_j - \nabla \times u_j = 0$$
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$\longrightarrow$ Guaranteed stability! Why?

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- Note that $u_{k_2}^* - u_{k_2}^* = 0$ (geometric argument)
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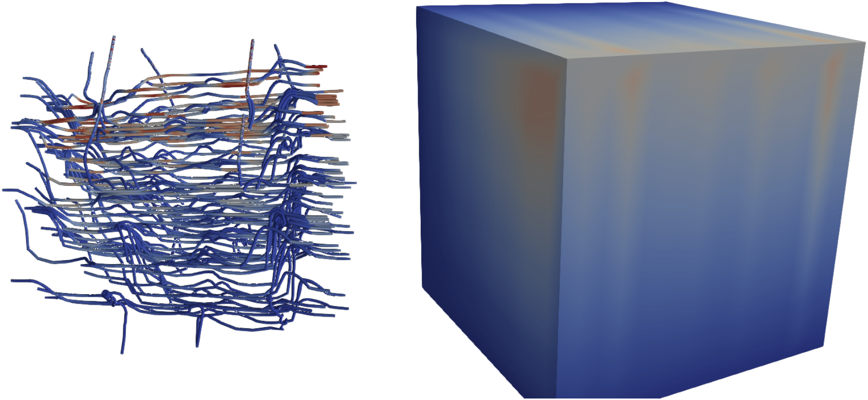
→ Therefore, we have $\nabla \times \mathsf{Ned}_0^{\mathsf{ms}} \subset \mathsf{RT}_0^{\mathsf{ms}}$.
→ Now using the definition of the DOFs (face moments) and by means of Stokes theorem

$$\nabla \times \Pi_{\mathsf{ms}}^{(\text{curl})} g = \Pi_{\mathsf{ms}}^{(\text{div})} \nabla \times g \,, \quad g \in H(\text{curl})$$

The Projections are $H(\text{curl})$- and $H(\text{div})$-bounded due to well-posedness of the Hodge-Laplace (here with essential boundary conditions).

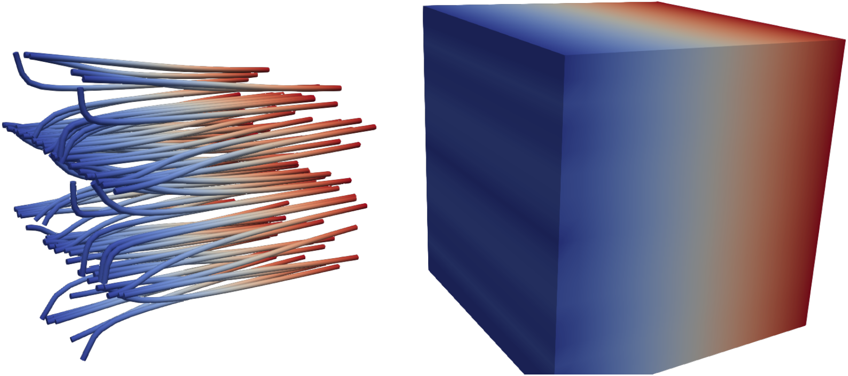
Q.E.D.

Modified Nédélec Basis



Basis on a coarse cell K, left: streamlines

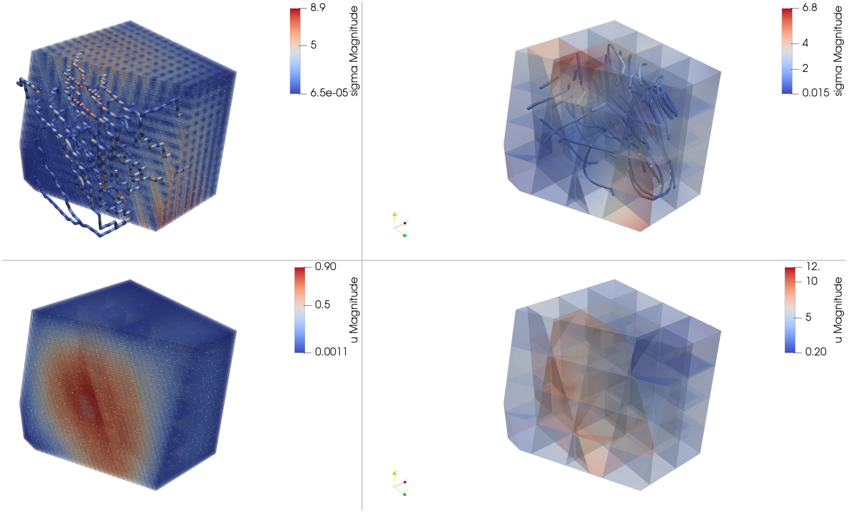
Modified Raviart-Thomas Basis



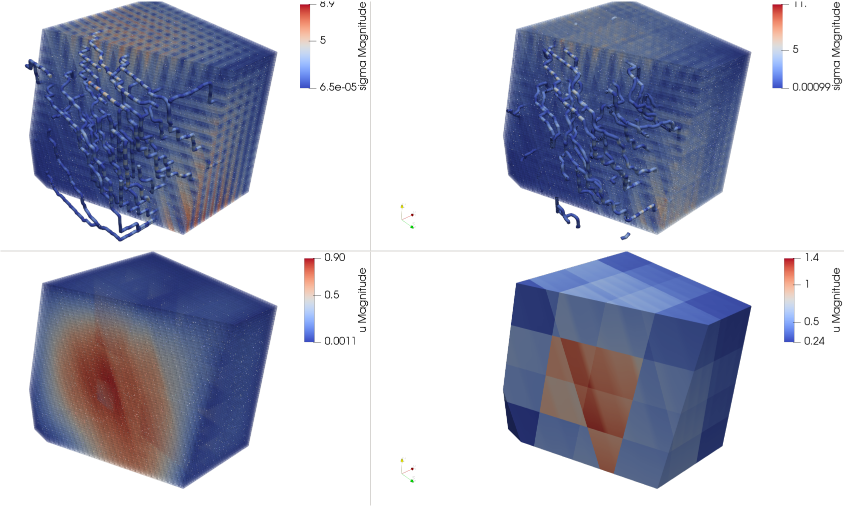
Basis on a coarse cell K, left: streamlines

Multiscale Discretization of Hodge-Laplace

Standard Problem $k = 2$



left: high resolution standard solution; right: low resolution solution with standard basis (wrong magnitudes and/or directions)



left: high resolution standard solution; right: low resolution solution with multiscale basis (almost correct magnitudes and directions)

- Proof can be extended to the whole complex
- Basis has information of fine scale structure
- We can show that classical multiscale FEMs are special cases of out construction ($k = 0, 3$)
- oversampling is possible (to reduce resonance errors)
- Accuracy proof through homogenization
- Many applications possible (Climate, Mechanics, Maxwell, MHD ...)
- Embedd into semi-Lagrangian reconstruction framework (data-driven setting)
- Code is C++ and parallel (documented, uses Deal.ii, p4est, MPI, Trilinos, TBB, VTK)
- Using or C++ code we computed up to 200 million DoFs on a 12 nodes cluster (scales better with number of nodes)

Again: This Framework defines a rigorous way to add multiscale correctors to elements constructed by FEEC – not only the ones shown.

→ Paper to come but Code is already on Github
`https://github.com/konsim83/MPI-MSFEC`!

Questions? Comments?