

Duality-based model adaptivity in context of multiscale methods

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Prague

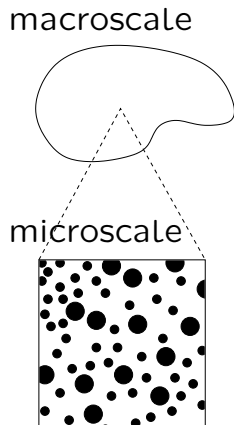
April 29, 2015

- ① An overview of multiscale methods
- ② Heterogeneous Multiscale Methods
- ③ Multiscale framework
- ④ Model adaptation
- ⑤ Conclusion

An overview of multiscale methods

What are multiscale problems?

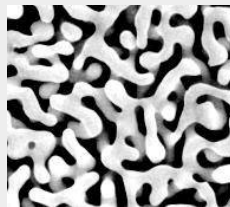
- A modeling problem is of multiscale character if relevant physical processes act on highly different length scales.
- Hard to simulate due to very high computational costs



What are multiscale problems?

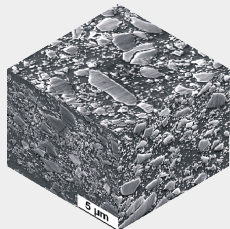
Flow in porous media

- Macroscopic flow behaviour
- Microscopic dependence of the permeability



Heterogeneous materials in structural mechanics

- Macroscopic, mechanical stress tensor
- Elastic/inelastic behaviour is highly dependent on the microstructure



A model problem

Model problem

Find $u^\varepsilon \in H_0^1(\Omega)$ s. t.

$$a^\varepsilon(u^\varepsilon, \varphi) = (A^\varepsilon(x)\nabla u^\varepsilon, \nabla \varphi) = (f, \varphi) \quad \forall \varphi \in H_0^1(\Omega), \quad (\text{I})$$

where A^ε contains *multiscale features*.

Assumptions

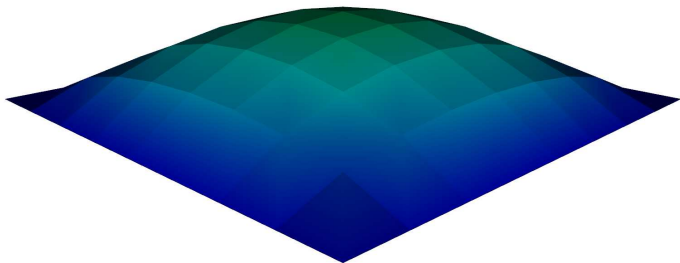
$$A^\varepsilon \in L^\infty(\Omega)^{d \times d},$$

$$A_{ij}^\varepsilon(x) = A_{ji}^\varepsilon(x) \quad \forall i, j \text{ a. e. on } \Omega,$$

$$\alpha|\xi|^2 \leq (\xi, A^\varepsilon(x)\xi) \leq \beta|\xi|^2 \quad \forall \xi \in \mathbb{R}^d \text{ a. e. on } \Omega.$$

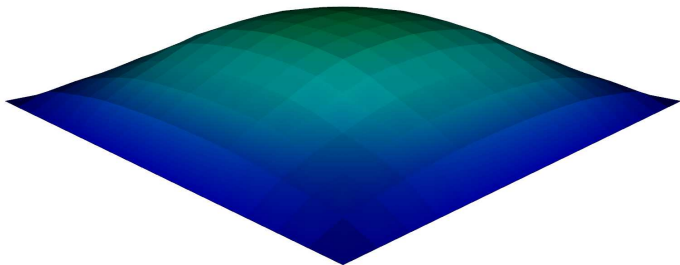
A model problem

81 degrees of freedom:



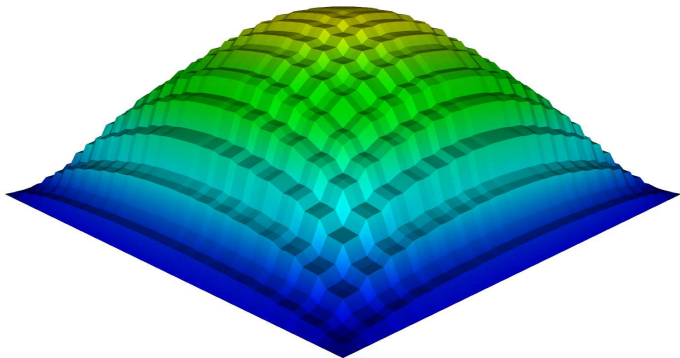
A model problem

289 degrees of freedom:



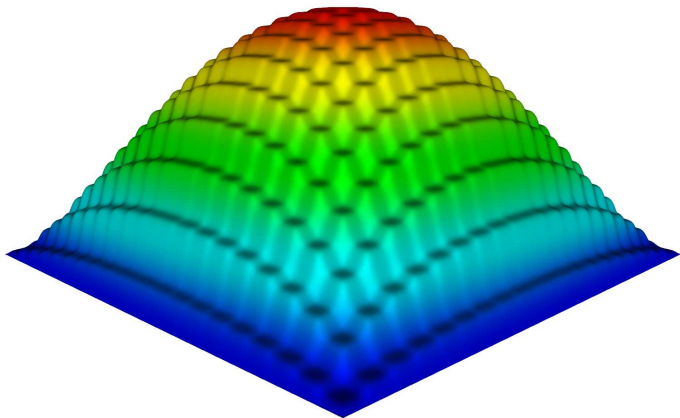
A model problem

4 225 degrees of freedom:



A model problem

263 169 degrees of freedom:



An (incomplete) overview

Multiscale modeling strategies

- Use structure of the ansatz-spaces

$$a^\varepsilon(u, \varphi) = (f, \varphi) \quad \forall \varphi \in V, \quad V = V_c \oplus V_f.$$

- Variational Multiscale Methods
(Hughes et al. '98, Brezzi '99)

- Use structure of the operator

$$A^\varepsilon(x) = A\left(x, \frac{x}{\varepsilon}\right)$$

- Homogenisation theory (e.g., Allaire '92)
- Heterogeneous Multiscale Methods (E, Engquist '03)

- Physical upscaling principles

- Computational Homogenization
(Hill '63, Geers et al. '10)
- Averaging principles (e.g., geometric mean)

Heterogeneous Multiscale Methods

Heterogeneous Multiscale Methods

$$A^\epsilon(x) = A\left(x, \frac{x}{\epsilon}\right)$$

References

- *“The heterogeneous multiscale method”*, E, Engquist '03
- *“Homogenization and Two-Scale Convergence”*, Allaire '92
- *“A posteriori error estimates for the heterogeneous multiscale finite element method for elliptic homogenization problems”*, Ohlberger '05

Heterogeneous Multiscale Methods

Model problem

$$(A^\varepsilon(x)\nabla u^\varepsilon, \nabla \varphi) = (f, \varphi) \quad \forall \varphi \in H_0^1(\Omega). \quad (\text{I})$$

- Assume a **scale separation assumption** to hold true:

$$A^\varepsilon(x) = A\left(x, \frac{x}{\varepsilon}\right), \quad \text{with } A \in C^{0,1}\left(\Omega, L_{\text{per}}^\infty(Y)^{d \times d}\right).$$

Homogenized problem

$$(A^0(x)\nabla u^0, \nabla \varphi) = (f, \varphi) \quad \forall \varphi \in H_0^1(\Omega), \quad \text{where}$$

$$A_{ij}^0(x) = \int_Y A(x, y) [\mathbf{e}_i + \nabla_y \omega_i(x, y)] \cdot [\mathbf{e}_j + \nabla_y \omega_j(x, y)] \, dy$$

and $\omega_i \in \tilde{H}_{\text{per}}^1(Y)$ are solutions of cell problems

$$\int_Y A(x, y) [\mathbf{e}_i + \nabla_y \omega_i(x, y)] \cdot \nabla \varphi \, dy = 0 \quad \forall \varphi \in \tilde{H}_{\text{per}}^1(\Omega).$$

Heterogeneous Multiscale Methods

Model problem

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$$\int_Y A(x, y) [\mathbf{e}_i + \nabla_y \omega_i(x, y)] \cdot \nabla\varphi \, dy \quad \forall \varphi \in \tilde{H}_{\text{per}}^1(\Omega).$$

Heterogeneous Multiscale Methods

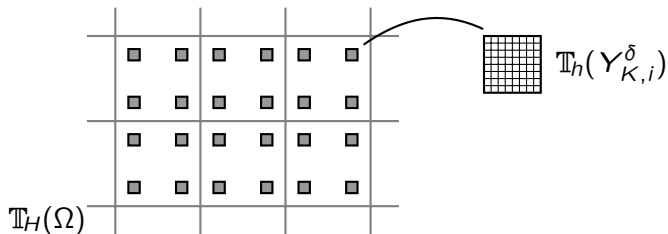
Reformulation (Allaire, Ohlberger)

$$\int_{\Omega} \int_{Y^{\delta}} A(x, \frac{y}{\delta}) [\nabla_x u^0 + \nabla_y \mathcal{R}(u^0)(x, y)] \cdot [\nabla_x \varphi^0 + \nabla_y \mathcal{R}(\varphi^0)(x, y)] dy dx = \int_{\Omega} f \varphi^0 dx,$$

with $\mathcal{R}(\varphi)(x, y)$ defined as the solution of

$$\int_{Y^{\delta}} A(x, \frac{y}{\delta}) [\nabla_x \varphi(x) + \nabla_y \mathcal{R}(\varphi)(x, y)] \cdot \nabla \psi dy = 0 \quad \forall \psi.$$

Heterogeneous Multiscale Methods

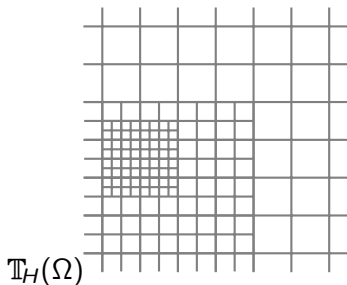


Heterogeneous Multiscale Formulation

$$\sum_{K \in \mathbb{T}_H} |K| \int_{Y_{K,i}^\delta} A^\varepsilon(x) \nabla [U + \mathcal{R}_{K,i}^h(U)(x)] \cdot \nabla [\varphi + \mathcal{R}_{K,i}^h(\varphi)(x)] dx$$
$$= \sum_{K \in \mathbb{T}_H} |K| \sum_i q_i f(x_i) \varphi(x_i) \quad \forall \varphi \in V^H(\Omega)$$

Multiscale framework

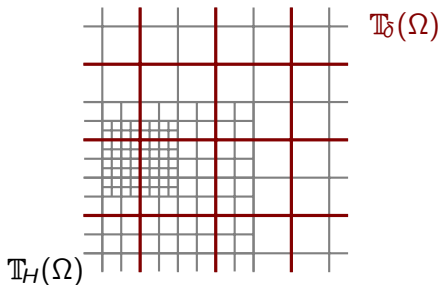
Multiscale framework



References

- “*Duality-based adaptivity in finite element discretization of heterogeneous multiscale problems*”
M., Rannacher, submitted '14

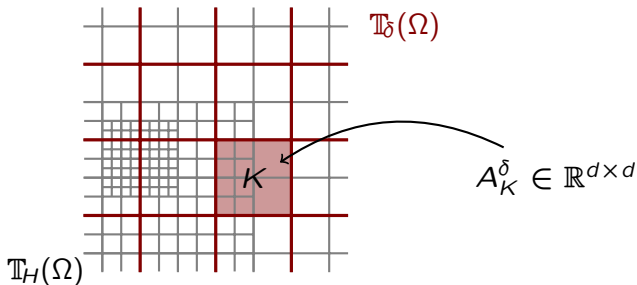
Multiscale framework



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Multiscale framework



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Multiscale framework

Numerically homogenized, continuous

Given a model $A^\delta : \mathbb{T}_\delta \rightarrow \mathbb{R}^{d \times d}$, find $u^\delta \in H_0^1(\Omega)$ s. t.

$$(A^\delta(x) \nabla u^\delta, \nabla \varphi) = (f, \varphi) \quad \forall \varphi \in H_0^1(\Omega). \quad (\text{II})$$

Multiscale framework

Numerically homogenized, continuous

Given a model $A^\delta : \mathbb{T}_\delta \rightarrow \mathbb{R}^{d \times d}$, find $u^\delta \in H_0^1(\Omega)$ s. t.

$$(A^\delta(x) \nabla u^\delta, \nabla \varphi) = (f, \varphi) \quad \forall \varphi \in H_0^1(\Omega). \quad (\text{II})$$

- Simple averaging:

$$A_{ij}^\delta|_K = \int_{Y_K^\delta} A^\varepsilon(y) dy, \quad A_{ij}^\delta|_K = \exp \left(\int_{Y_K^\delta} \log(A^\varepsilon(y)) dy \right).$$

Multiscale framework

Numerically homogenized, continuous

Given a model $A^\delta : \mathbb{T}_\delta \rightarrow \mathbb{R}^{d \times d}$, find $u^\delta \in H_0^1(\Omega)$ s. t.

$$(A^\delta(x) \nabla u^\delta, \nabla \varphi) = (f, \varphi) \quad \forall \varphi \in H_0^1(\Omega). \quad (\text{II})$$

- Mathematical homogenization:

$$A_{ij}^\delta|_K = \int_{Y_K^\delta} A^\varepsilon(x) (\mathbf{e}_i + \nabla w_i(x)) \cdot (\mathbf{e}_j + \nabla w_j(x)) dx,$$

with $w_i \in H_{\text{per}}^1(Y_K^\delta)$ solving a cell/sampling problem:

$$\int_{Y_K^\delta} A^\varepsilon(x) (\mathbf{e}_i + \nabla w_i(x)) \cdot \nabla \varphi dx = 0 \quad \forall \varphi \in H_{\text{per}}^1(Y_K^\delta).$$

Multiscale framework

Numerically homogenized, semi discretized

Find $u^{\delta,h} \in H_0^1(\Omega)$ s. t.

$$\left(A^{\delta,h}(x) \nabla u^{\delta,h}, \nabla \varphi \right) = (f, \varphi) \quad \forall \varphi \in H_0^1(\Omega), \quad (\text{III})$$

where $A^{\delta,h} : \Omega \rightarrow \mathbb{R}^{d \times d}$ is an approximation on A^δ .

Multiscale framework

Numerically homogenized, semi discretized

Find $u^{\delta,h} \in H_0^1(\Omega)$ s. t.

$$\left(A^{\delta,h}(x) \nabla u^{\delta,h}, \nabla \varphi \right) = (f, \varphi) \quad \forall \varphi \in H_0^1(\Omega), \quad (\text{III})$$

where $A^{\delta,h} : \Omega \rightarrow \mathbb{R}^{d \times d}$ is an approximation on A^δ .

- Simple averaging:

$$A_{ij}^{\delta,h} \Big|_K = Q_{Y_K^\delta}^h(A^\varepsilon), \quad \dots$$

Multiscale framework

Numerically homogenized, semi discretized

Find $u^{\delta,h} \in H_0^1(\Omega)$ s. t.

$$\left(A^{\delta,h}(x) \nabla u^{\delta,h}, \nabla \varphi \right) = (f, \varphi) \quad \forall \varphi \in H_0^1(\Omega), \quad (\text{III})$$

where $A^{\delta,h} : \Omega \rightarrow \mathbb{R}^{d \times d}$ is an approximation on A^δ .

- Homogenization: Discretize with meshes $\mathbb{T}_h(Y_K^\delta)$:

$$A_{ij}^{\delta,h} \Big|_K = \int_{Y_K^\delta} A^\varepsilon(x) (\mathbf{e}_i + \nabla w_i^h(x)) \cdot (\mathbf{e}_j + \nabla w_j^h(x)) dx,$$

with $w_i^h \in V^h(Y_K^\delta)$ solving a cell/sampling problem:

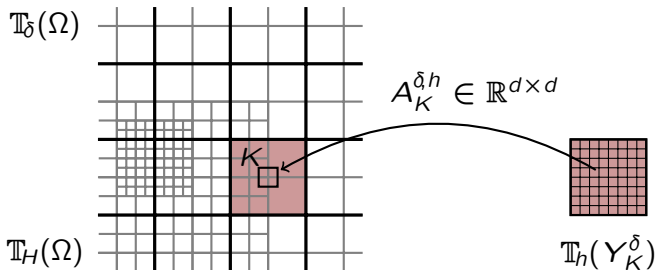
$$\int_K A^\varepsilon(x) (\mathbf{e}_i + \nabla w_i^h(x)) \cdot \nabla \varphi dx = 0 \quad \forall \varphi \in V^h(K).$$

Multiscale framework

Numerically homogenized, fully discretized

Find $U \in V^H(\Omega)$ s. t.

$$(A^{\delta,h}(x)\nabla U, \nabla\varphi) = (f, \varphi) \quad \forall \varphi \in V^h(\Omega). \quad (\text{IV})$$



Model: $A^\delta : \mathbb{T}_\delta \rightarrow \mathbb{R}^{d \times d}$ Discretization: $\mathbb{T}_H, \{\mathbb{T}_h(Y_K^\delta)\}$

Multiscale framework

Dual problem

Let $j : H_0^1(\Omega) \rightarrow \mathbb{R}$ be a functional; define a dual problem:
Find $z^\varepsilon \in H_0^1(\Omega)$ s. t.

$$(A^\varepsilon(x)\nabla\varphi, \nabla z^\varepsilon) = \langle j, \varphi \rangle \quad \forall \varphi \in H_0^1(\Omega). \quad (\text{V})$$

This leads to the error identity:

$$\begin{aligned} \langle j, e \rangle &= \langle j, u^\varepsilon \rangle - \langle j, U \rangle = \underbrace{(f, z^\varepsilon) - (A^{\delta,h}\nabla U, \nabla z^\varepsilon)}_{\text{I}} \\ &+ \underbrace{((A^{\delta,h} - A^\delta)\nabla U, \nabla z^\varepsilon)}_{\text{II}} + \underbrace{((A^\delta - A^\varepsilon)\nabla U, \nabla z^\varepsilon)}_{\text{III}}. \end{aligned}$$

Multiscale framework

Residual on the macroscale:

$$(I) = \sum_{K \in \Pi_H} (f, z^\varepsilon - \psi^H)_K - (A^{\delta, h} \nabla U, \nabla z^\varepsilon - \nabla \psi^H)_K$$

Residual on the microscale:

$$(II) = \sum_{K \in \Pi_\delta} ((A^{\delta, h} - A^\delta) \nabla U, \nabla z^\varepsilon)_K$$

In case of homogenization:

$$(II) = \sum_{K \in \Pi_\delta} \sum_{Q \in \Pi_h(Y_K^\delta)} \sum_{i, j} \left(\int_K f \partial_i U \partial_j z^\varepsilon dx \right) \left\{ - \int_Q A^\varepsilon (\mathbf{e}_j + \nabla w_j^h) \cdot (\nabla w_i - \nabla \psi_{w_i}^h) dy \right\}$$

Multiscale framework

Remark: Approximating the dual solution

- It is computationally infeasible to resolve z^ε completely.
- It is crucial to get a good (local) approximation of z^ε for a *quantitative* estimate of the *model error*
 - (I), (II) correspond to *moments of first order*:

$$(II) = \sum_{K \in \Pi_\delta} \left((A^{\delta,h} - A^\delta) \nabla U, \underbrace{\nabla z^\varepsilon}_{\text{fluct.}} \right)_K$$

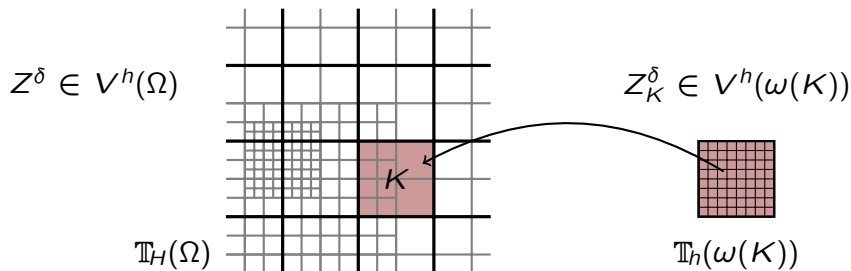
- (III) corresponds to a *moment of second order*:

$$(III) = \sum_{K \in \Pi_\delta} \left(\underbrace{(A^\delta - A^\varepsilon)}_{\text{fluct.}} \nabla U, \underbrace{\nabla z^\varepsilon}_{\text{fluct.}} \right)_K$$

Multiscale framework

Remark: Approximating the dual solution

- Solve a reduced dual problem: Find $Z^\delta \in V^H(\Omega)$ s. t.
$$(A^\delta(x)\nabla\varphi, \nabla Z^\delta) = \langle j, \varphi \rangle \quad \forall \varphi \in V^H(\Omega).$$
- Additional local enhancement $Z^\delta + Z_K^\delta$ on K :
$$(A^\epsilon(x)\nabla\varphi, \nabla(Z^\delta + Z_K^\delta))_{\omega(K)} = \langle j, \varphi \rangle \quad \forall \varphi \in V^h(\omega(K)).$$



Model adaptation

Model adaptation

Model and model error indicator

$$\text{Model: } A^\delta : \mathbb{T}_\delta \rightarrow \mathbb{R}^{d \times d},$$

$$\theta^\delta = \sum_{K \in \Pi_\delta} \eta_K^\delta, \quad \eta_K^\delta = ((A^\delta - A^\varepsilon) \nabla U, \nabla z^\varepsilon)_K.$$

Model adaptation strategies:

- Adapt $\{Y_K^\delta : K \in \mathbb{T}_\delta(\Omega)\}, \mathbb{T}_\delta(\Omega)$
- Adapt A^δ (for fixed $\mathbb{T}_\delta(\Omega)$)
 - switch model
 - model optimization

Model adaptation

Strategy I (M., Rannacher '14)

- use simple averaging strategy (e. g. geometric average)
 - adapt $\mathbb{T}_\delta(\Omega)$ locally with the error indicator η_K^δ .
-
- Adapt $\mathbb{T}_H(\Omega)$ and $\{h_K : K \in \mathbb{T}_\delta(\Omega)\}$ with η_K^H , or η_K^h .
 - If η_K^δ is large for some $K \in \mathbb{T}_\delta(\Omega)$
 - split K into 2^d sampling regions K_i ,
 - shrink sampling region Y_K^δ by a factor of 2^{-d} , set $h_{K_i} = h_K$
 - This also only requires a reduced dual problem z^δ .

Model adaptation

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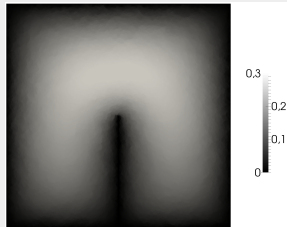
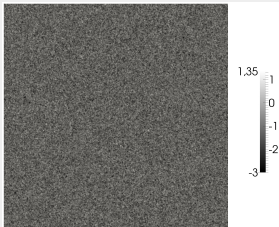
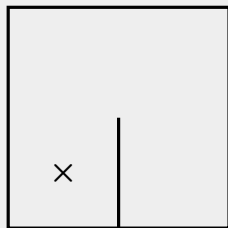
Model adaptation

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 - This also only requires a reduced dual problem z^δ .

Model adaptation

Numerical example



Microstructure (a log-normally distributed random field with Gaussian correlation):

$$A^\varepsilon(x) = I_d \times \gamma \times \exp(10 \times g(x)/255)$$

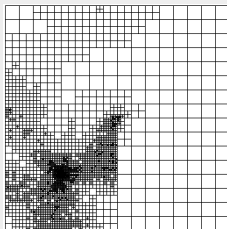
Quantity of interest:

$$\langle j, \varphi \rangle := \partial_{x_2} \varphi(\hat{x}), \quad \hat{x} = (0.25, 0.25).$$

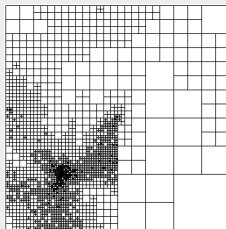
Model adaptation

strategy	L^2 error	$ \langle j, u^\varepsilon - U \rangle $
arithmetic	6.85e-2 (40%)	9.40e-1
geometric	3.66e-3 (2.2%)	7.93e-1
HMM	2.87e-3 (1.7%)	7.93e-1

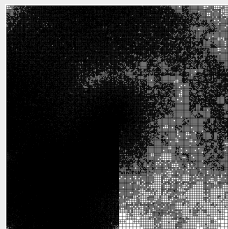
(a) \mathbb{T}_H



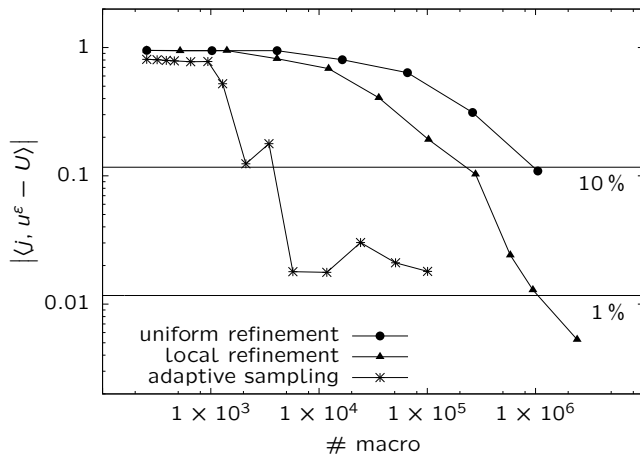
(b) \mathbb{T}_δ



(c) \mathbb{T}_H



Model adaptation



- Main mechanism for saving: Approximation property of geometric average

Model adaptation

Strategy II: Optimization problem (M. '15)

For a given Π_δ and initial $A^{\delta,0}$ define an *optimal model*,

$$\tilde{A}^\delta : \Pi_\delta \rightarrow \mathbb{R}^{d \times d},$$

to be a solution of

$$\operatorname{argmin}_{A^\delta : \Pi_\delta \rightarrow \mathbb{R}^{d \times d}} \sum_{K \in \Pi_\delta} \left(\underbrace{(A^\delta - A^\varepsilon) \nabla U(A^\delta), \nabla z^\varepsilon}_{=\eta_K} \right)_K^2 + \kappa |A_K^\delta - A_K^{\delta,0}|^2$$

subject to

$$(\xi A^\delta(x), \xi) \geq \alpha^* |\xi|^2 \quad \forall \xi \in \mathbb{R}^d, \forall x \in \Omega,$$

$$(A^\delta \nabla U(A^\delta), \nabla \varphi) = (f, \varphi) \quad \forall \varphi \in V_H.$$

Model adaptation

Algorithm (pure model adaption)

- 1 Compute $A^{\delta,0}, A^\delta \leftarrow A^{\delta,0}$
- 2 Solve primal and (reduced) dual problem $U(A^\delta), Z^\delta(A^\delta)$
- 3 Compute estimators

$$\eta_K = ((A^\delta - A^\varepsilon) \nabla U(A^\delta), \nabla Z^\delta + \nabla Z_K^\delta)$$

and solve

$$(JJ^T + \lambda I) \delta A^\delta = -J^T \eta.$$

- 4 $A^\delta \leftarrow A^\delta + \delta A^\delta$
- 5 If stopping criterion not reached continue at (2)

Numerical results

Example: Advection-diffusion problem

$$\gamma(\nabla u^\varepsilon, \nabla \varphi) + (\mathbf{b}^\varepsilon \cdot \nabla u^\varepsilon, \varphi) = (f, \varphi),$$

with dominant, microscopic transport \mathbf{b}^ε .

Effective Model

$$(A^\delta \nabla u^\delta, \nabla \varphi) + (\mathbf{b}^\delta \cdot \nabla u^\delta, \varphi) = (f, \varphi),$$

with $\mathbf{b}^\delta(K) := \int_K \mathbf{b}^\varepsilon \, dx$.

Modified model-error indicator

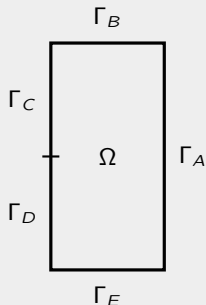
$$\eta_K^\delta = ((\gamma \text{Id} - A^\delta) \nabla u^\delta, \nabla z^\varepsilon)_K - ((\mathbf{b}^\varepsilon - \mathbf{b}^\delta) \cdot \nabla u^\delta, z^\varepsilon)_K.$$

Numerical results

Quantity of interest:

$$\langle j, \varphi \rangle = \int_{\Gamma_B} \varphi \, d\sigma_x$$

Domain:



Two different choices for adv. field \mathbf{b}^ε :

- Periodic coefficient:

$$\mathbf{b}^\varepsilon(\mathbf{x}) = (-1)^{\lfloor x/\varepsilon \rfloor + \lfloor y/\varepsilon \rfloor} \mathbf{b}(\hat{\mathbf{x}}.)$$

- Random coefficient:

$$\mathbf{b}^\varepsilon(\mathbf{x}) = \text{curl } \Psi^\varepsilon,$$

with random scalar $\Psi^\varepsilon \in C^2(\Omega)$.

Numerical results

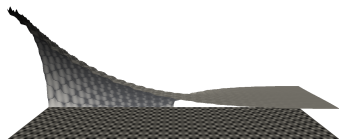
	$L^2(\Omega)$	$ \langle j, U \rangle $	$ \langle j, u^\varepsilon - U \rangle $	$ \tilde{\theta}^\delta $	I_{eff}	I_{loc}
1	5.77	4.31	-2.6e+0 (142 %)	-2.6e+0	1.01	1.67
7	1.34	1.79	-1.02e-2 (0.57 %)	-1.77e-2	1.61	7.86
15	1.33	1.78	5.40e-3 (0.31 %)	-2.00e-3	-0.14	21.81

(a) Fully resolved dual solution, periodic coefficients

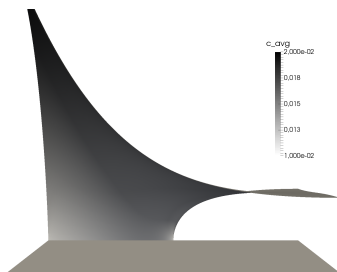
	$L^2(\Omega)$	$ \langle j, U \rangle $	$ \langle j, u^\varepsilon - U \rangle $	$ \tilde{\theta}^\delta $	I_{eff}	I_{loc}
1	5.77	4.31	-2.6e+0 (142 %)	-6.2e+0	2.44	1.66
6	1.33	1.76	2.31e-2 (1.30 %)	-3.37e-2	-1.46	5.04
15	1.32	1.74	4.34e-2 (2.44 %)	-3.31e-3	-0.08	10.1

(b) Reduced, locally enhanced dual solution, periodic coefficients

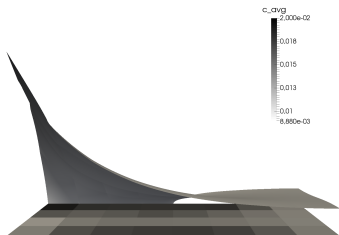
Numerical results



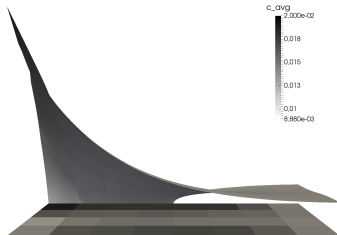
(a) Reference solution



(b) Initial solution



(c) Fully resolved dual solution



(d) Locally enhanced dual solution

Numerical results

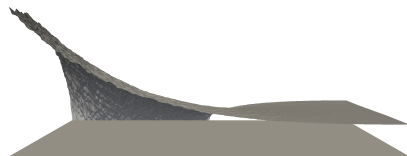
	$L^2(\Omega)$	$ \langle j, U \rangle $	$ \langle j, u^\varepsilon - U \rangle $	$ \tilde{\theta}^\delta $	I_{eff}	I_{loc}
1	4.43e-1	3.86e-1	-1.69e-1 (77.9 %)	-1.69e-1	1.00	2.21
11	1.39e-1	2.26e-1	-9.14e-3 (4.21 %)	-9.35e-3	1.00	13.2
15	1.13e-1	2.23e-1	-6.28e-3 (2.89 %)	-6.51e-3	0.99	17.3

(c) Fully resolved dual solution, random coefficients

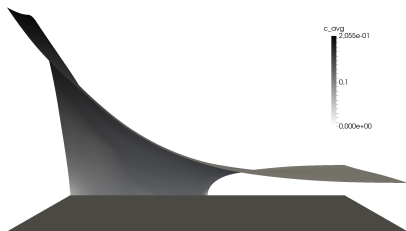
	$L^2(\Omega)$	$ \langle j, U \rangle $	$ \langle j, u^\varepsilon - U \rangle $	$ \tilde{\theta}^\delta $	I_{eff}	I_{loc}
1	4.43e-1	3.86e-1	-1.69e-1 (77.9 %)	-2.96e-1	1.76	2.15
10	7.99e-2	2.20e-1	-3.02e-3 (1.39 %)	-1.27e-2	4.18	4.91
15	9.70e-2	2.14e-1	3.07e-3 (1.41 %)	7.00e-3	2.28	10.4

(d) Reduced, locally enhanced dual solution, random coefficients

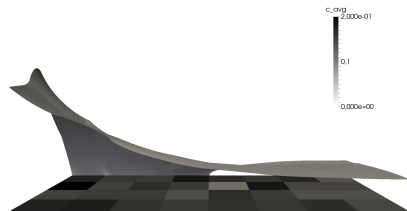
Numerical results



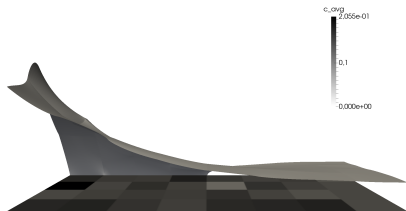
(e) Reference solution



(f) Initial solution



(g) Fully resolved dual solution



(h) Locally enhanced dual solution

Conclusion

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Conclusion

- Multiscale formulations are based on structure in ansatz spaces (VMM) or in the operator (HMM).
- Error estimation with Dual-Weighted Residual method.
- A modified heterogeneous multiscale scheme was presented, suitable for error splitting.
- Adjustment of an effective model $A^\delta : \Pi_\delta \rightarrow \mathbb{R}^{d \times d}$ by
 - Adaptation of discretization $\{Y_K^\delta : K \in \mathbb{T}_\delta(\Omega)\}, \mathbb{T}_\delta(\Omega)$
 - Model adaptation A^δ (for fixed $\mathbb{T}_\delta(\Omega)$)

Thank you for your attention!

Special thanks to:

Heidelberg Graduate School of Mathematical and
Computational Methods for the Sciences



<http://www.mathcomp.uni-heidelberg.de/>

The community of



<http://www.dealii.org/>