

Numerical upscaling of perturbed diffusion problems

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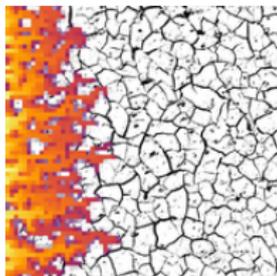
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Heterogeneous materials

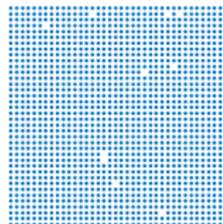
We consider heterogeneous materials with perturbations



▷ time dependency



▷ local deformation



▷ defects

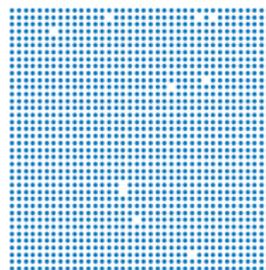
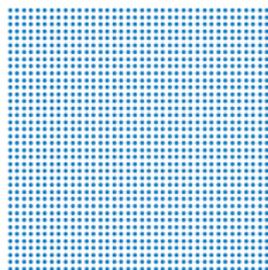
Propagating front in a porous material, large deformation in network model, and random defects in a composite.

Two issues: **changing** and **rapidly varying** data.

- 1 **Motivation and model problem**
- 2 Multiscale approach
- 3 Perturbed diffusion
- 4 Numerical examples
- 5 Final comments

Elliptic model problem

The Poisson equation with a reference \hat{A} (left) and perturbed A (right) diffusion that fulfills $0 < \alpha \leq \hat{A}, A \leq \beta$.



On weak form we have: find $\hat{u} \in V := H_0^1(\Omega)$ and $u \in V$ such that

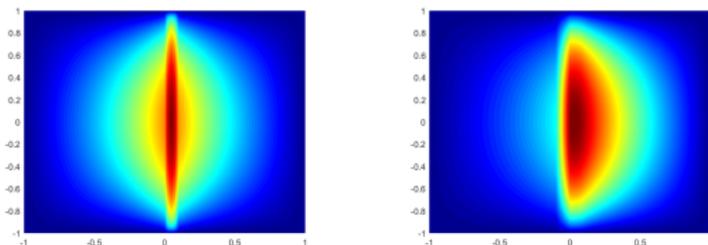
$$\hat{a}(\hat{u}, v) := \int_{\Omega} (\hat{A} \nabla \hat{u}) \cdot \nabla v \, dx = \int_{\Omega} f \cdot v \, dx \quad \text{for all } v \in V,$$

$$a(u, v) := \int_{\Omega} (A \nabla u) \cdot \nabla v \, dx = \int_{\Omega} f \cdot v \, dx \quad \text{for all } v \in V.$$

Modelling error

$$\begin{aligned}\|A^{1/2}\nabla(u-\hat{u})\|_{L^2(\Omega)}^2 &= (A\nabla(u-\hat{u}), \nabla(u-\hat{u})) \\ &= ((\hat{A}-A)\nabla\hat{u}, \nabla(u-\hat{u})) + (f-f, u-\hat{u}) \\ &\leq \alpha^{-1}\|\hat{A}-A\|_{L^\infty(\Omega)}\|\hat{A}^{1/2}\nabla\hat{u}\|_{L^2(\Omega)}\|A^{1/2}\nabla(u-\hat{u})\|_{L^2(\Omega)}.\end{aligned}$$

We conclude $\|A^{1/2}\nabla(u-\hat{u})\|_{L^2(\Omega)} \leq C\alpha^{-3/2}\|f\|_{L^2(\Omega)}\|A-\hat{A}\|_{L^\infty(\Omega)}$.

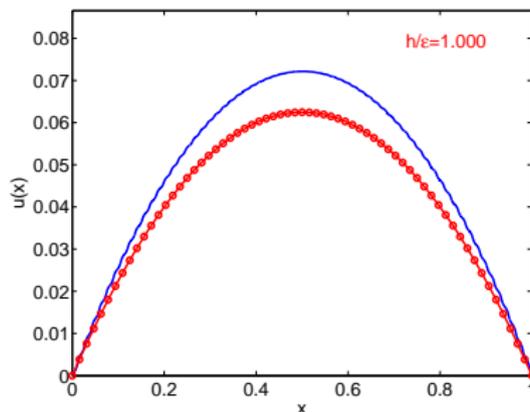


Here $\hat{A} = 1 - 0.9\chi_{\{0 < x < 0.1\}}$, $A = 1 - 0.9\chi_{\{-0.1 < x < 0\}}$, and $f = \chi_{\{0 < x < 0.1\}}$.

The full problem has to be resolved for each perturbation.

Rapid data variation

We let $A(x) = 2 + \sin(2\pi x/\epsilon)$, $\epsilon = 2^{-6}$, and $f = 1$.



- FEM on mesh $h \geq \epsilon$ leads to averaging of the diffusion and wrong effective behavior.

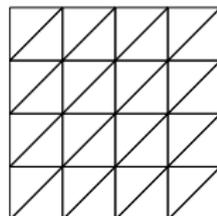
- A priori error bound:

$$\|A^{1/2}\nabla(u - u_h)\|_{L^2(\Omega)} \leq Ch\|u\|_{H^2(\Omega)} \approx Ch\epsilon^{-1}.$$

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Orthogonal decomposition

- (coarse) FE mesh \mathcal{T}_H with parameter $H > h$
- P1-FE space $V_H := \{v \in V \mid \forall T \in \mathcal{T}_H, v|_T \in P_1(T)\}$
- $\mathfrak{I}_{\mathcal{T}} : V \rightarrow V_H$ some interpolation operator



Decomposition

$$V = V_H \oplus V^f \quad \text{with } V^f := \text{kernel } \mathfrak{I}_{\mathcal{T}} = \{v \in V \mid \mathfrak{I}_{\mathcal{T}} v = 0\}$$

- For each $v \in V_H$ define finescale projection $Qv \in V^f$ by

$$a(Qv, w) = a(v, w) \quad \text{for all } w \in V^f$$

a -Orthogonal Decomposition

$$V = V_H^{\text{ms}} \oplus V^f \quad \text{with } V_H^{\text{ms}} := (V_H - QV_H)$$

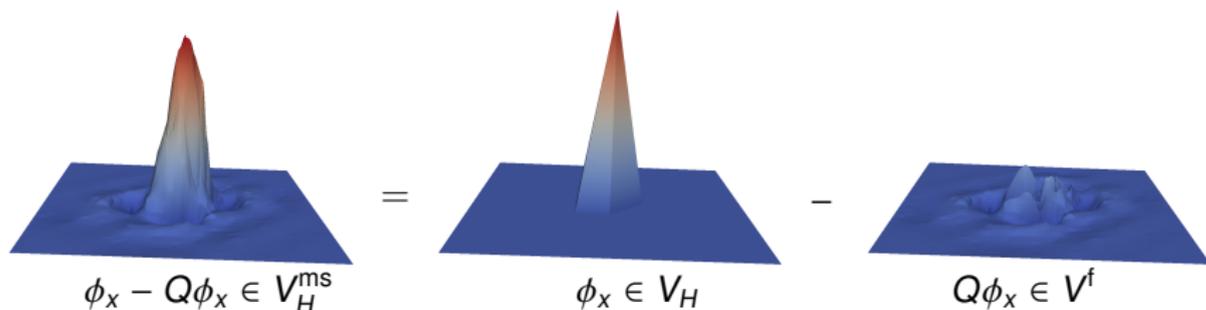
Modified nodal basis

- $\phi_x \in V_H$ denotes classical nodal basis function ($x \in \mathcal{N}$)
- $Q\phi_x \in V^f$ denotes the finescale correction of ϕ_x ($x \in \mathcal{N}$)

Multiscale FE space

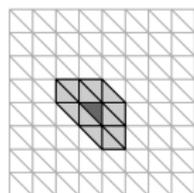
$$V_H^{\text{ms}} = \text{span} \{ \phi_x - Q\phi_x \mid x \in \mathcal{N} \}$$

Example

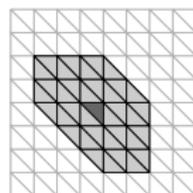


Localization

- Define nodal patches of ℓ -th order $\omega_{T,\ell}$ about $T \in \mathcal{T}_H$



$\omega_{T,1}$



$\omega_{T,2}$

- Correctors $Q_\ell^T \phi_x \in V^f(\omega_{T,\ell}) := \{v \in V^f \mid v|_{\Omega \setminus \omega_{T,\ell}} = 0\}$ solve

$$a(Q_\ell^T \phi_x, w) = \int_T A \nabla \phi_x \cdot \nabla w \, dx \quad \text{for all } w \in V^f(\omega_{T,\ell})$$

Localized multiscale FE spaces

$$V_{H,\ell}^{\text{ms}} = \text{span}\{\phi_x - \sum_{T \in \mathcal{T}_H} Q_\ell^T \phi_x \mid x \in \mathcal{N}\}$$

Fully discrete method (PG-LOD)

We discretize the fine scales and let

$$V_{H,\ell}^{\text{ms},h} = \text{span}\{\phi_x - \sum_{T \in \mathcal{T}} Q_{\ell,h}^T \phi_x \mid x \in \mathcal{N}\}$$

Fully discrete multiscale approximation $u_{H,\ell}^{\text{ms},h} \in V_{H,\ell}^{\text{ms},h}$

$$a(u_{H,\ell}^{\text{ms},h}, v) = (f, v) \quad \text{for all } v \in V_H$$

Theorem (A priori error bound)

$$\| \| u_h - u_{H,\ell}^{\text{ms},h} \| \| \leq C'(H + e^{-c\ell}) = CH,$$

with C independent of A' and $\ell \approx |\log(H)|$.

Elfverson, Ginting, and Henning, On multiscale methods in PG formulation, Numer. Math., 2015.

Comments on the choice of method

- 1 The multiscale representation can be reused (evolution, iteration, samples).
 - 2 Local changes in data leads to local recomputations.
 - 3 LOD allows a priori error bounds for non-periodic data.
 - 4 The PG formulation reduces communication.
- GFEM 1983-, Babuška-Osborn, Melenk, Lipton, ...
 - VMS 1995-, Hughes et.al., Larson-M., Hughes-Sangalli, ...
 - MsFEM 1996-, Hou & Wu, Efendiev et.al., ...
 - HMM 2003-, Engquist & E, ...
 - LOD 2013-, M. & Peterseim, Henning et.al., ...
 - Bayesian NH, Gamblets, 2010-, Owhadi et.al.

There are many other related methods not listed here.

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Local recomputation of basis function



We assume we have computed $\hat{Q}_\ell^T \phi_x \in V^f(\omega_{T,\ell})$ associated with \hat{A}

$$\hat{a}(\hat{Q}_\ell^T \phi_x, w) = \int_T \hat{A} \nabla \phi_x \cdot \nabla w \, dx \quad \text{for all } w \in V^f(\omega_{T,\ell})$$

We only recompute for $T \in \mathcal{T}_H \setminus \tilde{\mathcal{T}}_H$ and let

$$\tilde{Q}_\ell^T = \begin{cases} \hat{Q}_\ell^T, & T \in \tilde{\mathcal{T}}_H \\ Q_\ell^T, & T \in \mathcal{T}_H \setminus \tilde{\mathcal{T}}_H \end{cases}$$

We let $\tilde{V}_{H,\ell}^{\text{ms}} = \text{span}(\{\phi_x - \sum_{T \in \mathcal{T}_H} \tilde{Q}_\ell^T \phi_x\})$.

Local recomputation of basis function

We let $v, w \in V_H$ and define

$$\tilde{a}(v, w) = \sum_{T \in \mathcal{T}_H} (\tilde{\mathbf{A}}_T \nabla v, \nabla w)_T + (\tilde{\mathbf{A}}_T \nabla \tilde{\mathbf{Q}}_\ell^T v, \nabla w)_{\omega_\ell(T)}$$

where

$$\tilde{\mathbf{A}}_T = \begin{cases} \hat{\mathbf{A}}, & T \in \tilde{\mathcal{T}}_H \\ \mathbf{A}, & T \in \mathcal{T}_H \setminus \tilde{\mathcal{T}}_H \end{cases}$$

We let $\tilde{u} := (1 - \sum_T \tilde{\mathbf{Q}}_\ell^T) \tilde{u}_H$, where $\tilde{u} \in V_H$ solves

$$\tilde{a}(\tilde{u}_H, w) = (f, w), \quad \forall w \in V_H$$

- We note that $\hat{\mathbf{A}}|_{\omega_\ell(T)}$ on T is arbitrary in this formulation. It can e.g. refer to different time steps for different T .

A priori error analysis

Theorem (A priori error bound)

If $\ell \approx |\log(H)|$ and $\max_{T \in \tilde{\mathcal{T}}} e_T < TOL$, where

$$e_T := \max_{v|_T, v \in V_H} \frac{\|(\tilde{A} - A)A^{-1/2}\nabla(\chi_T - \tilde{Q}_\ell^T)v\|_{L^2(\omega_{T,\ell})}}{\|A^{1/2}\nabla v\|_{L^2(T)}}$$

then $\|u_h - \tilde{u}\| \leq CH + C_\ell TOL$.

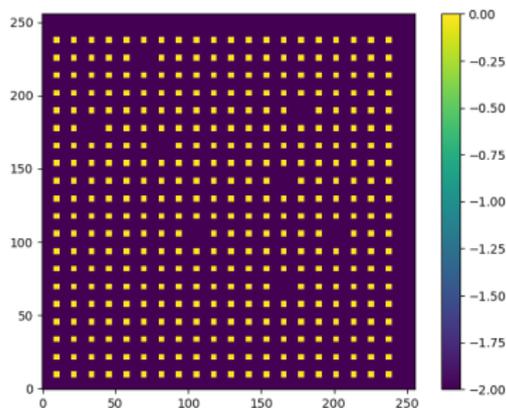
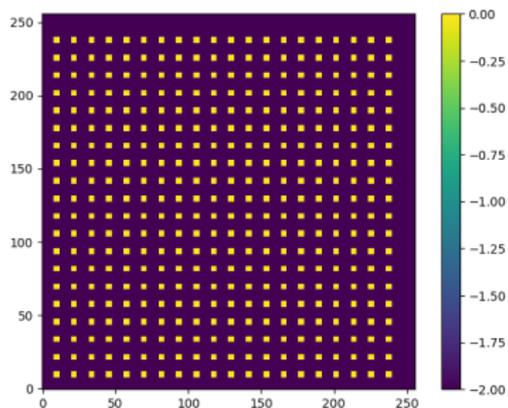
- e_T is computable and independent of Q_ℓ^T .
- e_T is large if both $A - \tilde{A}$ and $\tilde{Q}_\ell^T v$ are large.
- We only recompute for elements T where $e_T > TOL$.

Hellman and M., Numerical homogenization of elliptic PDEs with similar coefficients, MMS, 2019.

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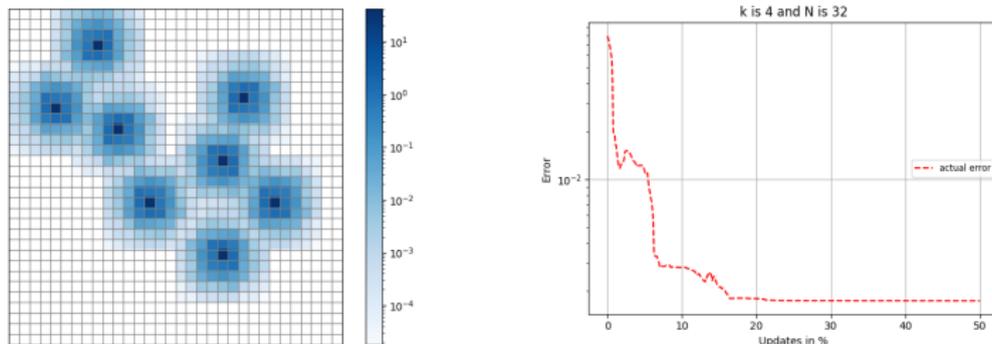
Numerical examples (defects)

We consider an example with 2% defects with $f = \chi_{[1/8,7/8] \times [1/8,7/8]}$ and the diffusion taking values 1 (dots) and 0.01.



We let $H = 2^{-5}$, $h = 2^{-9}$, $\ell = 4$, and increase the amount of updates.

Numerical examples (defects)



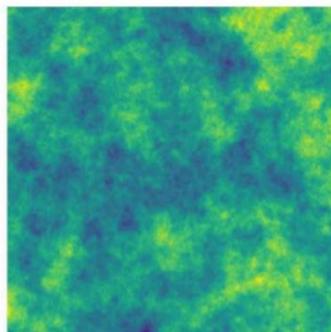
Error indicator (left) and error as a function of updates (right).

Right hand side correction eliminates H -dependency: find $u_f^T \in V^f$ such that

$$a(u_f^T, v) = (f, v)_T$$

for all $v \in V^f$. The full solution is $u^{\text{full}} = u^{\text{ms}} + \sum_{T \in \mathcal{T}_H} u_f^T$.

Numerical examples (two phase flow)



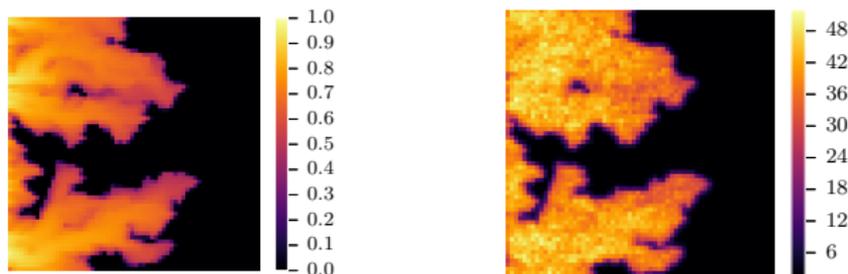
$$-\nabla \cdot \lambda(s)K\nabla u = 0 \quad \dot{s} - \nabla \cdot \lambda_w(s)\nabla u = 0$$

- K piecewise constant, log-normal, correlation length 0.05.
- The total mobility $\lambda(s) = s^3 + (1 - s)^3$ and $\lambda_w(s) = s^3$.
- Pressure u has Dirichlet 1 (left) and 0 (right).
- Initial condition $s(0) = 0$.
- $s = 1$ on the inflow for the saturation.

Numerical examples (two phase flow)

Let $0 < t_1 < t_2 < \dots < t_n < \dots < t_N$ and use a dG0 upwind forward Euler type scheme¹ for the saturation with the pressure and saturation solved sequentially i.e. diffusion $A_n(x) = \lambda(s_{n-1})K(x)$.

- We let $h = 2^{-9}$, $H = 2^{-6}$, $N = 2000$, and $\tau = 1/N$.
- We allow $\{\tilde{A}_T\}_{T \in \mathcal{T}_H}$ to be evaluated at different times.

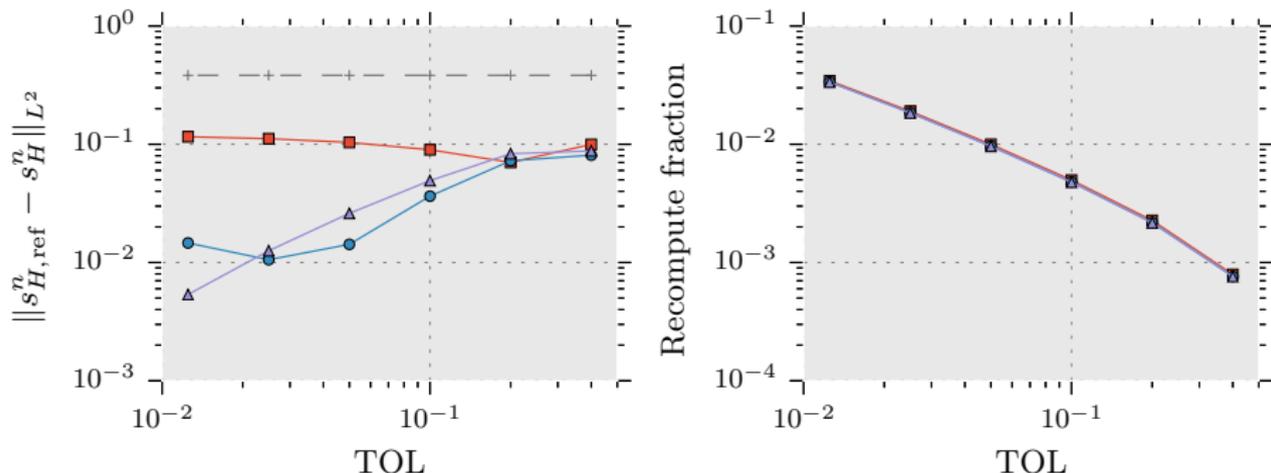


With $\ell = 2$, TOL = 0.05 we get below 2% L^2 -error in s_H^{2000} and on average 20.3 recomputations per coarse element i.e. 1%.

¹Odsæter et. al. Postprocessing of non-conservative fluxes, CMAME 2017

Numerical examples (two phase flow)

We let $\ell = 1, 2, 3$ and vary TOL in the example.



Dashed is standard Galerkin on coarse mesh. Solution improves with $\ell = 1$ (squares) $\ell = 2$ (circles) $\ell = 3$ (diamonds). More recomputations with decreasing TOL (right).

Only coarse scale saturations are computed to minimize storage.

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Comments and future work

- We derive error indicators driving local recomputation of multiscale basis functions.
- We prove a priori error bounds for the proposed method.
- We show that multiscale methods can be useful also for problems with locally varying diffusion.
- Future work: application to random diffusion problems. Sample diffusion locally and recompute basis when needed.

Thank you for your attention!