Numerical upscaling of perturbed diffusion problems

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Workshop on Computational multiscale methods

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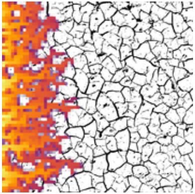
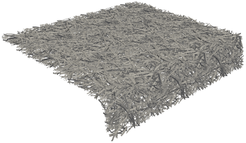
Heterogeneous materials

We consider problems with changing or perturbed diffusion.



▷ time dependency

▷ defects

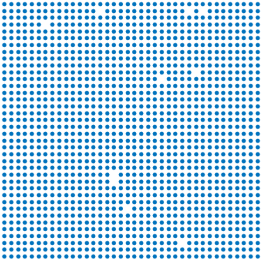


▷ local deformation

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

Two issues: rapidly varying and perturbed data.

Multiscale approach



Main objective

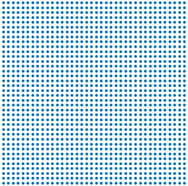
- Develop an algorithm for local recomputation of a reference multiscale basis.
- Derive corresponding error indicators.
- Take advantage of the exponential decay of the basis.

Outline

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

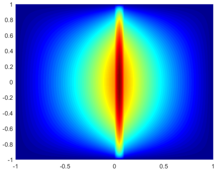
$$\hat{a}(\hat{u}, v) := \int_\Omega (\hat{A}\nabla \hat{u}) \cdot \nabla v \, dx = \int_\Omega f\, v \, dx \quad \text{for all } v \in V,$$

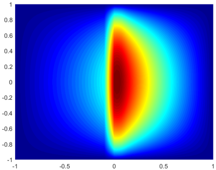
$$a(u, v) := \int_\Omega (A\nabla u) \cdot \nabla v \, dx = \int_\Omega f\, v \, dx \quad \text{for all } v \in V.$$

Modelling error

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

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



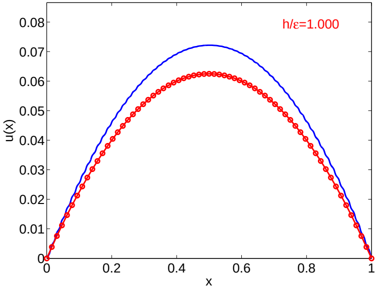


Here $\hat{A} = 1 - 0.9\chi_{\{0<x<0.1\}}$, $A = 1 - 0.9\chi_{\{-0.1<x<0\}}$, and $f = \chi_{\{0<x<0.1\}}$.

The full problem has to be resolved for each perturbation.

Resolution of fine scales

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

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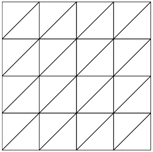
Orthogonal decomposition

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



Decomposition

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

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

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

***a*-Orthogonal Decomposition**

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

Petrov-Galerkin formulation

Given the space V_H^{ms} we define:

Petrov-Galerkin-method:
Find $u_H^{\mathrm{ms}} \in V_H^{\mathrm{ms}} \quad : \quad a(u_H^{\mathrm{ms}}, v) = (f, v), \ \forall v \in V_H.$

We have that $u = v_H^{\mathrm{ms}} + u_{\mathrm{f}}$ for some $v_H^{\mathrm{ms}} \in V_H^{\mathrm{ms}}$. Since V_H^{ms} and V^{f} are a-orthogonal:

$$|||u - u_H^{\mathrm{ms}}|||^2 := a(u - u_H^{\mathrm{ms}}, u - u_H^{\mathrm{ms}}) = |||v_H^{\mathrm{ms}} - u_H^{\mathrm{ms}}|||^2 + |||u_{\mathrm{f}}|||^2$$

$$|||u_{\mathrm{f}}|||^2 = a(u, u_{\mathrm{f}}) = (f, u_{\mathrm{f}} - \mathfrak{I}_{\mathcal{T}} u_{\mathrm{f}}) \leq \frac{C_{\mathfrak{I}_{\mathcal{T}}}}{\alpha^{1/2}} \|Hf\|_{L^2(\Omega)} |||u_{\mathrm{f}}|||.$$

Furthermore $|||v_H^{\mathrm{ms}} - u_H^{\mathrm{ms}}|||^2 = a(v_H^{\mathrm{ms}} - u_H^{\mathrm{ms}}, \mathfrak{I}_{\mathcal{T}}(v_H^{\mathrm{ms}} - u_H^{\mathrm{ms}})) = \ldots$
$= -a(u_{\mathrm{f}}, \mathfrak{I}_{\mathcal{T}}(v_H^{\mathrm{ms}} - u_H^{\mathrm{ms}})) \leq C|||u_{\mathrm{f}}|||\,|||v_H^{\mathrm{ms}} - u_H^{\mathrm{ms}}|||.$

Together we have $|||u - u_H^{\mathrm{ms}}||| \leq CH\|f\|_{L^2(\Omega)}$.

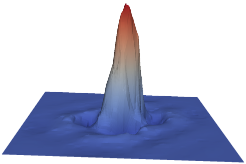
Modified nodal basis

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

Multiscale FE space

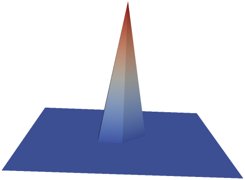
$$V_H^{\mathrm{ms}} = \operatorname{span}\{\phi_x - Q\phi_x \mid x \in \mathcal{N}\}$$

Example



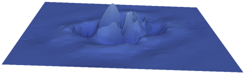
$\phi_x - Q\phi_x \in V_H^{\mathrm{ms}}$

$=$



$\phi_x \in V_H$

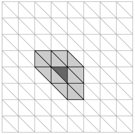
$-$



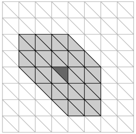
$Q\phi_x \in V^{\mathrm{f}}$

Localization

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



$\omega_{T,1}$



$\omega_{T,2}$

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

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

Localized multiscale FE space

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

Fully discrete method (PG-LOD)

We discretize the fine scales and let

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

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

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

Theorem (A priori error bound)

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

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., ...
- Baysian NH, Gamblets, 2010-, Owhadi et.al.

There are many other related methods not listed here.

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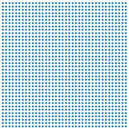
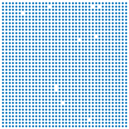
Local recomputation of basis functions





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

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

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

Local recomputation of basis functions

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

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

where

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

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

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

- One could use a instead of $\tilde{a}$ but more computations are needed.
- We note that $\tilde{A}_T$ on T is arbitrary in this formulation. It can e.g. refer to different time steps for different T.

Error indicators

Given $v \in V_H$ we have with $z = Q_\ell^T v - \tilde{Q}_\ell^T v$

$$\begin{aligned}
\|A^{1/2}\nabla(Q_\ell^T v - \tilde{Q}_\ell^T v)\|^2_{L^2(\omega_{T,\ell})} \\
&= ((\tilde{A}_T - A)\nabla\tilde{Q}_\ell^T v, \nabla z) - ((\tilde{A}_T - A)\nabla v, \nabla z)_T \\
&= \|(\tilde{A}_T - A)A^{-1/2}(\chi_T \nabla v - \nabla\tilde{Q}_\ell^T v)\|_{L^2(\omega_{T,\ell})}\|A^{1/2}\nabla z\|_{L^2(\omega_{T,\ell})} \\
&= e_T\|A^{1/2}\nabla v\|_{L^2(T)}\|A^{1/2}\nabla(Q_\ell^T v - \tilde{Q}_\ell^T v)\|_{L^2(\omega_{T,\ell})}
\end{aligned}$$

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

$$\|A^{1/2}\nabla(Q_\ell v - \tilde{Q}_\ell v)\|_{L^2(\Omega)} := \ell^{d/2} \max_{T\in\tilde{\mathcal{T}}_H} e_T\|A^{1/2}\nabla v\|_{L^2(\Omega)}.$$

- We note that e_T is only large if $\tilde{A}_T - A$ is large at T.
- The indicator e_T is independent of Q_ℓ^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*

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

then $|||u_h - \tilde{u}||| \leq CH + C\ell^{d/2}TOL$.

- e_T is computable and independent of Q_ℓ^T.
- We only recompute for elements T where $e_T >$ TOL.
- It is computed by solving a $(d+1)\times(d+1)$ eigenvalue problem.
- A coarse version can be computed by summing over coarse elements.

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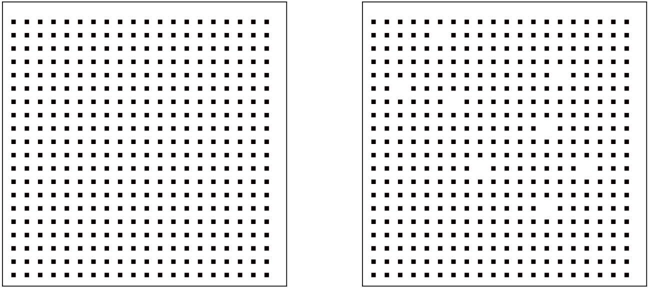
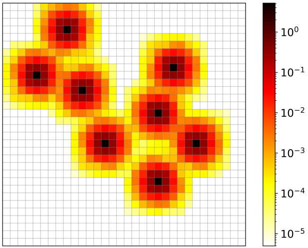
Numerical examples (defects)

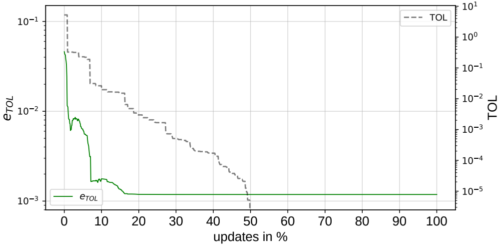
We consider an example with 2% defects with $f = \chi_{[1/8,7/8]\times[1/8,7/8]}$ and the diffusion taking values 1 (dots) and 0.01.



We let $H = 2^{-5}$, $h = 2^{-8}$, $\ell = 4$, and increase the amount of updates.

Numerical examples (defects)





Error indicator (left) and relative error in energy norm $u_h - \tilde{u}$ (right).

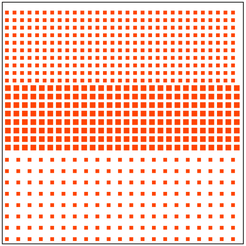
Right hand side correction eliminates H-dependency: find $u_f^T \in V^{\mathrm{f}}$ such that

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

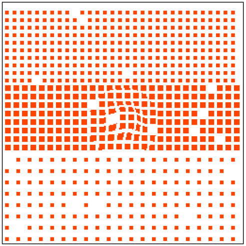
for all $v \in V^{\mathrm{f}}$. The full solution is $u^{\mathrm{full}} = u^{\mathrm{ms}} + \sum_{T \in \mathcal{T}_H} u_f^T$.

Numerical example (domain mapping)

We consider a map $\psi : \Omega \to \Omega$ that is continuous one-one and $\psi : \Gamma \to \Gamma$. We let $J = \frac{\partial \psi_i}{\partial x_j}$, $i, j = 1, ..., d$.



$$y = \psi(x)$$

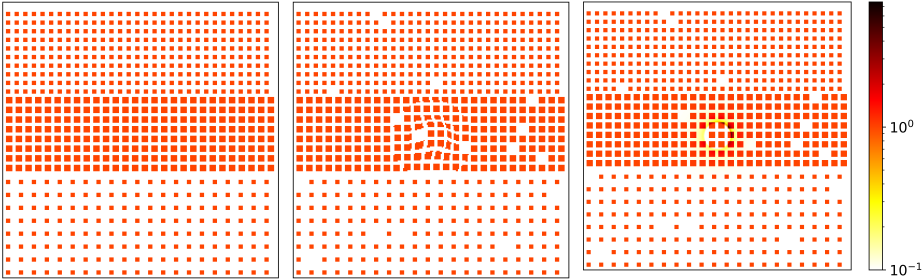


The perturbed diffusion is $(\hat{A} - D) \circ \psi^{-1}(y)$, where D account for defects, we get (in x):

$$A = det(J)J^{-1}(\hat{A} - D)J^{-T} \qquad\qquad f = det(J)f_y \circ \psi$$

Numerical examples (domain mapping)

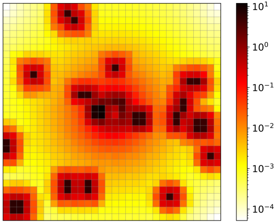
We again have 2% defects with $f = \chi_{[1/8,7/8]\times[1/8,7/8]}$ and the diffusion taking values 1 (dots) and 0.01.

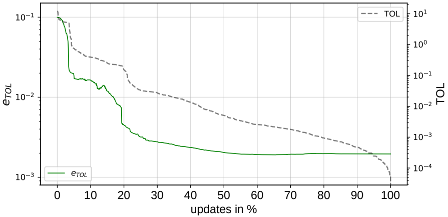


Domain mapping becomes change in value perturbation in x.

We let $H = 2^{-5}$, $h = 2^{-8}$, $\ell = 4$, and increase the amount of updates.

Numerical examples (domain mapping)

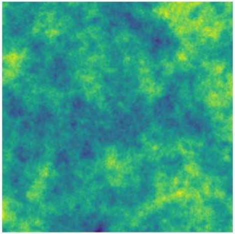




Error indicator (left) and relative error in energy norm $u_h - \tilde{u}$ as a function of updates (right).

- The domain mapping leads to smaller errors.
- Again right hand side correction eliminates H-dependency.

Numerical examples (two phase flow)



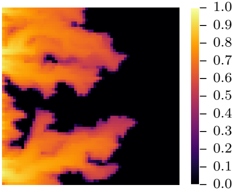
$$-\nabla \cdot \lambda(s) K \nabla u = 0 \qquad \dot{s} - \nabla \cdot \lambda_w(s) K \nabla u = 0$$

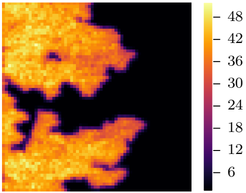
- K piecewise constant, log-normal, correlation length 0.05.
- The total mobility $\lambda(s) = s^3 + (1-s)^3$ and $\lambda_w(s) = s^3$.
- Pressure u has Dirichlet 1 (left) and 0 (right).
- Initial condition $s(0) = 0$.
- $s = 1$ on the inflow for the saturation.

Numerical examples (two phase flow)

Let $0 < t_1 < t_2 < \cdots < t_n < \ldots t_N$ and use a dG0 upwind forward Euler type scheme[1] 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.



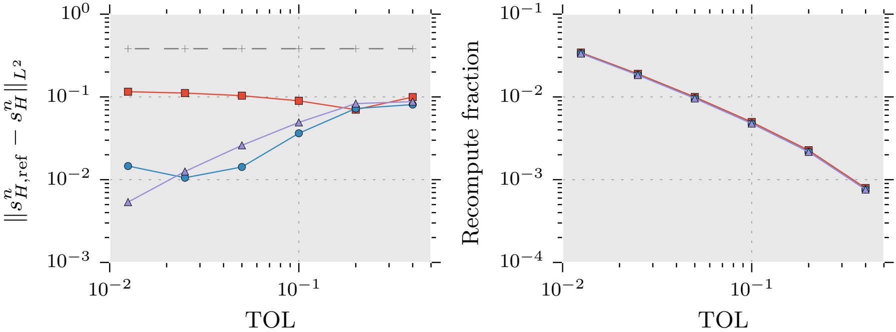


With $\ell = 2$, $\mathrm{TOL} = 0.05$ we get below 2% L^2-error in s_H^{2000} and on average 20.3 recomputations per coarse element i.e. 1%.

[1] Odsæter et. al. Postprocessing of non-conservative flux ..., 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.

Outline

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 necessary.

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

Thank you for your attention!