Localization of multiscale problems

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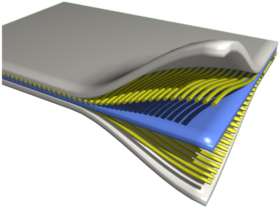
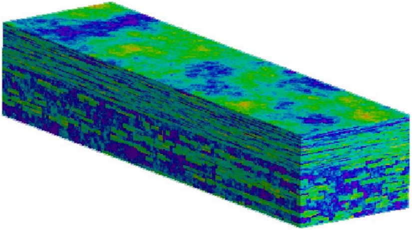
Multiscale problems

We consider applications such as





▷ composite materials ▷ flow in a porous medium

that require numerical solution of partial differential equations with rough data (module of elasticity, conductivity, or permeability).

Two topics: high contrast and parameter dependent diffusion.

Outline

1. **Elliptic model problem**
2. Introduction to LOD
3. High contrast data
4. Parameter dependent data
5. Final comments

The finite element method

The Poisson equation

$$-\nabla \cdot A \nabla u = f \quad \text{in } \Omega \qquad u = 0 \quad \text{on } \partial\Omega.$$

On weak form: find $u \in V := H_0^1(\Omega)$ such that

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

FE approximation: find $u_h \in V_h \subset V$ such that

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

Error bound if $u \in H^2(\Omega)$:

$$|||u - u_h||| := \|A^{1/2} \nabla (u - u_h)\|_{L^2(\Omega)} \sim C(A')h.$$

Multiscale methods

Objectives:

- Find a subspace $V_H^{\text{ms}} \subset V_h$ for which $u_H^{\text{ms}} \in V_H^{\text{ms}}$ solving

$$a(u_H^{\text{ms}}, v) := \int_\Omega (A \nabla u_H^{\text{ms}}) \cdot \nabla v \, dx = \int_\Omega f \cdot v \, dx \quad \text{for all } v \in V_H^{\text{ms}},$$

  fulfills

$$|||u_h - u_H^{\text{ms}}||| \leq CH,$$

  with C independent of A' and $\dim(V_H^{\text{ms}}) \ll \dim(V_h)$.
- Show that a basis for V_H^{ms} can be constructed by local parallel computations.
- Reuse the coarse representation in applications.
- Multiscale methods: VMS, MsFEM, HMM, GFEM, GMsFEM...

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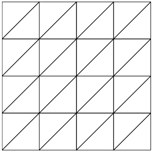
Orthogonal decompositions

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

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

Ideal multiscale representation

Given the space V_H^{ms} we construct a Galerkin approximation:

Ideal method

Find $u_H^{ms} \in V_H^{ms}$ such that

$$a(u_H^{ms}, v) = (f, v), \ \forall v \in V_H^{ms}.$$

We have that $u - u_H^{ms} = u_f \in V^f$ since u_H^{ms} is the a-orthogonal projection of u onto V_H^{ms}. Therefore

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

For V_H^{ms} to be useful we need a discrete local basis.

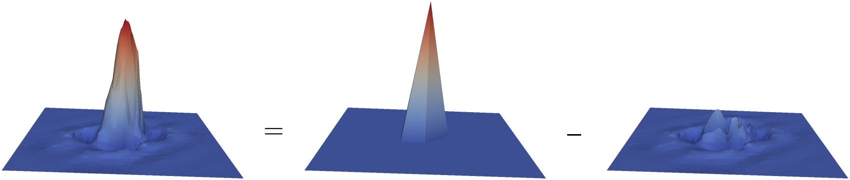
Modified nodal basis

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

Ideal multiscale FE space

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

Example



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

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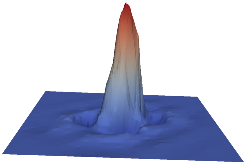

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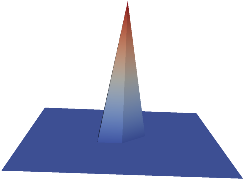

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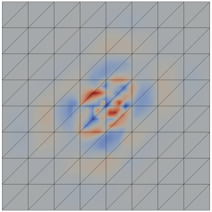
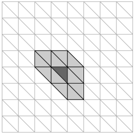


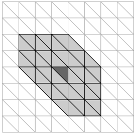
$\phi_x - Q\phi_x \in V_H^{\mathrm{ms}}$ $\qquad$ $\phi_x \in V_H$ $\qquad$ $Q\phi_x \in V^{\mathrm{f}}$

Localization

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



$\omega_{T,1}$



$\omega_{T,2}$

- 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

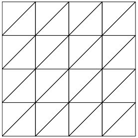
$$a(Q_\ell^T \phi_x, w) = \int_T A \nabla \phi_x \cdot \nabla w \, dx \quad \text{for all } w \in V^{\mathrm{f}}(\omega_{T,\ell})$$

Localized multiscale FE spaces

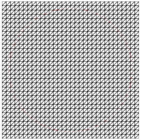
$$V_{H,\ell}^{\mathrm{ms}} = \mathrm{span}\{\phi_x - \sum_{T \in \mathcal{T}} Q_\ell^T \phi_x \mid x \in \mathcal{N}\}$$

Fine scale discretization

- Finescale mesh



mesh refinement



$\mathcal{T}$ $\quad\rightsquigarrow\quad$ $\mathcal{T}_h$ with $h \leq H$

- Reference FE space

$$V_h := \{v \in V \mid \forall T \in \mathcal{T}(\Omega), v|_T \in P_1(T)\}$$

- Reference FE solution $u_h \in V_h$ solves

$$a(u_h, v) = (f, v) \quad \text{for all } v \in V_h$$

- Fully discrete correctors $Q^T_{\ell,h}\phi_x \in V^{\mathrm{f}}_h(\omega_{T,\ell}) := V^{\mathrm{f}}(\omega_{T,\ell}) \cap V_h$:

$$a(Q^T_{\ell,h}\phi_x, w) = (A\nabla\phi_x, \nabla w)_T \;\; \text{for all } w \in V^{\mathrm{f}}_h(\omega_{T,\ell})$$

Localized Orthogonal Decomposition (LOD)

Fully discrete multiscale FE spaces

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

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

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

Remarks:

- $\dim V_{H,\ell}^{\mathrm{ms},h} = |\mathcal{N}| = \dim V_H$
- The basis functions have local support, with overlap depending on ℓ, and are independent.

Localized Orthogonal Decomposition (LOD)

Fully discrete multiscale FE spaces

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

Petrov-Galerkin version $u_{H,\ell}^{\mathrm{ms},h} \in V_{H,\ell}^{\mathrm{ms},h}$

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

Remarks:

- The inf-sup constant will depend on ℓ.
- This version of the method reduces overlap between basis functions.

A priori error analysis

Lemma (Truncation error)

$$|||Q_h v_H - Q_{\ell,h} v_H||| \leq C_1 \gamma^\ell |||Q_h v_H|||, \quad \forall v_h \in V_H$$

$C_1 < \infty$ and $\gamma < 1$ depends on β/α but not A'.

By choosing $\ell = C_2 \log(H^{-1})$ with appropriate C_2 we guarantee that the truncation leads to a higher order perturbation:

Theorem (A priori error bound)

$$|||u_h - u_{H,\ell}^{\mathrm{ms},h}||| \leq C(\alpha,\beta) H,$$

with C independent of A'.

M. & Peterseim, Localization of elliptic multiscale problems, 2014.

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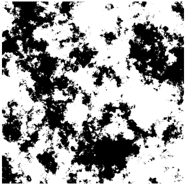
High contrast data (with Hellman)

Poisson equation:

$$-\nabla \cdot A \nabla u = f \quad \text{in } \Omega \qquad u = 0 \quad \text{on } \partial\Omega.$$

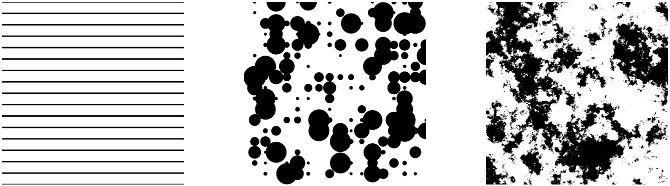
$A = 1$ in Ω_1 (black), $A = \alpha$ in Ω_α, $\alpha \ll 1$, and $f = \chi_{[1/4,3/4]^2}$.



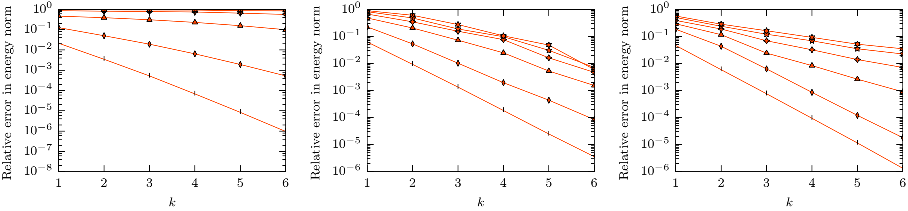
- High contrast data with channels leads to non-local behaviour.
- The decay rate of the basis functions determines the accuracy of LOD.
- The choice of interpolant $\mathfrak{I}_{\mathcal{T}} v = \sum_{x \in \mathcal{N}} \bar{v}_{\sigma_x} \phi_x$ affects the decay.

Numerical example: High contrast

High contrast data Three examples: $H = 2^{-4}$, $h = 2^{-10}$,



We let $\alpha = 10^{-1}, \ldots, 10^{-6}$ and plot $|||u_h - u_{H,k}^{\mathrm{ms},h}|||$ vs. k, with $\mathfrak{I}_{\mathcal{T}}^{SZ}$,



Heuristic motivation for lack of decay

Fine scale equation: Correctors $Q^T v_H \in V^{\mathrm{f}} = \ker(\mathfrak{I}_{\mathcal{T}})$ solve

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

Decay because localized rhs and $\mathfrak{I}_{\mathcal{T}}(Q^T v_H) = 0 \to Q^T v_H(x) \approx 0$.

If we define $g := Q^T v_H|_{\partial T}$ we note that $Q^T v_H$ minimizes

$$\frac{1}{2} \|A^{1/2} \nabla Q^T v_H\|^2_{L^2(\Omega \setminus T)} = \min_{v_f \in V^{\mathrm{f}} : v|_{\partial T = g}} \frac{1}{2} \|A^{1/2} \nabla v_f\|^2_{L^2(\Omega \setminus T)}.$$

- High derivatives in Ω_1 are penalized.
- With $\mathfrak{I}_{\mathcal{T}} v = \sum_{x \in \mathcal{N}} \bar{v}_{\sigma_x} \phi_x$ and σ_x containing both Ω_1 and Ω_α, $\mathfrak{I}_{\mathcal{T}}(Q^T v_H) = 0$ still allows large values (and small derivatives) in Ω_1 and high derivatives in Ω_α.
- To make $Q^T v_H$ decay in Ω_1 we need $\sigma_x \subset \Omega_1$.

Scott-Zhang type interpolation

Nodal variables:

Let $x \in \mathcal{N}$ be nodes of $\mathcal{T}$ and $\sigma_x \subset \Omega$ associated domains. We define a $L^2(\sigma_x)$-dual basis $\psi_x \in V_H$ fulfilling,

$$\int_{\sigma_x} \psi_x \phi_y = \delta_{xy}.$$

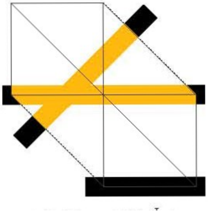
Let the nodal variable $N_x(v) = \int_{\sigma_x} \psi_x v$ and,

$$\mathfrak{I}_{\mathcal{T}}^{\sigma} v = \sum_{x \in \mathcal{N}} N_x(v) \phi_x.$$

- σ_x does not need to be full elements T or vertex patches $U_1(x)$.
- The stability of $|N_x(v)| \leq ||\psi||_{L^2(\sigma_x)} ||v||_{L^2(\sigma_x)}$ depends on the size and shape of σ_x and its distance to x.

Geometry dependent interpolation

- The interpolant $\mathfrak{I}_{\mathcal{T}} v = \sum_{x \in \mathcal{N}} \bar{v}_{\sigma_x} \phi_x$ defines V_f and V_H^{ms}.
- We need to force correctors to be small in the channels!



1. If $x \in \Omega_\alpha$ let $\sigma_x = \omega_x$, vertex patch
2. If $x \in \Omega_1$ let $\sigma_x \subset \omega_x \cap \Omega_1$, connected
3. We need sufficiently many nodes in Ω_1 (separation $\sim H$)

The we can prove decay independent of α.

Numerical example: High contrast

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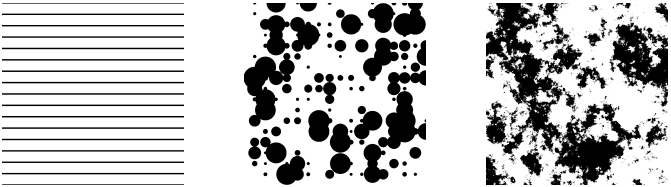
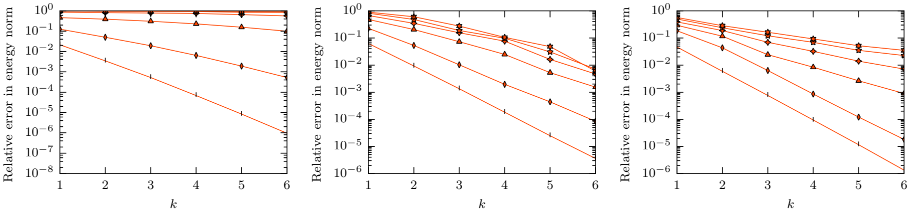


We let $\alpha = 10^{-1}, \dots, 10^{-6}$ and plot $|||u_h - u^{\mathrm{ms},h}_{H,k}|||$ vs. k with $\mathfrak{I}^{SZ}_{\mathcal{T}}$,



Hellman & M., Contrast independent localization, 2017.

Numerical example: High contrast

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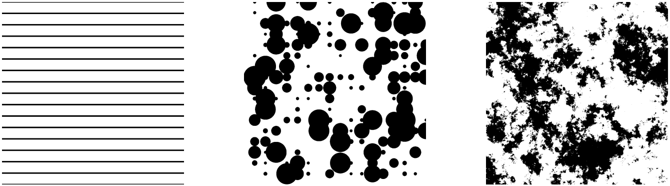

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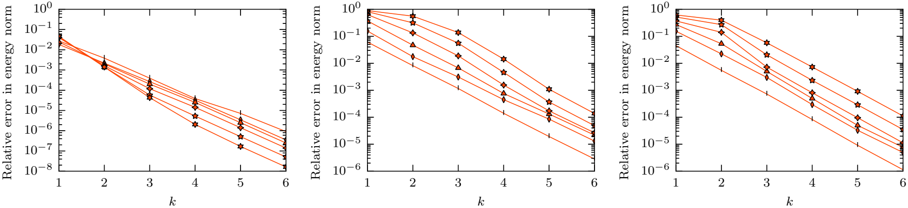

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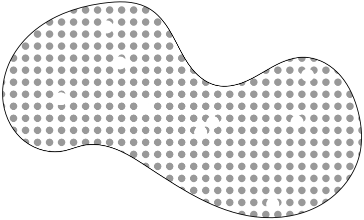
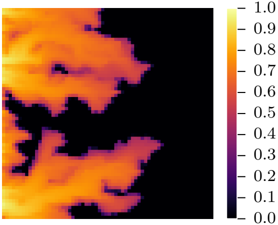
Parameter dependent data (Hellman, Keil)

The Poisson equation with a parameter

$$-\nabla \cdot A(t) \nabla u(t) = f \quad \text{in } \Omega \qquad u(t) = 0 \quad \text{on } \partial\Omega.$$





- Random defects (faults in composite material)
- Perturbations (tolerance in manufacturing)
- Time (moving front in porous media flow)

Effect of perturbed diffusion

On each patch use a perturbation $\tilde{A}_T$ of $A(t)$ in the construction of the basis: find $\tilde{Q}_\ell^T v \in V^f(\omega_{T,\ell})$ such that

$$(\tilde{A}_T \nabla \tilde{Q}_\ell^T v, \nabla w) = (\tilde{A}_T \nabla v, \nabla w)_T$$

for all $w \in V_f(\omega_{T,\ell})$. Let $\tilde{V}_\ell^{\mathrm{ms}} = V_H - \tilde{Q}_\ell V_H$ where $\tilde{Q}_\ell = \sum_{T \in \mathcal{T}} \tilde{Q}_\ell^T$. We seek $\tilde{u}_\ell^{\mathrm{ms}} \in \tilde{V}_\ell^{\mathrm{ms}}$ such that

$$\tilde{a}(\tilde{u}_\ell^{\mathrm{ms}}, v) = (f, v), \quad \forall v \in V_H,$$

(a Petrov-Galerkin formulation) where

$$\tilde{a}(u, v) = \sum_{T \in \mathcal{T}} (\tilde{A}_T \nabla \mathfrak{I}_{\mathcal{T}} u, \nabla v)_T - (\tilde{A}_T \nabla \tilde{Q}_\ell^T \mathfrak{I}_{\mathcal{T}} u, \nabla v).$$

We use the perturbed coefficient also in the assembly of the global stiffness matrix.

A priori error analysis

For any $v \in V_H$ we have with $z = Q_\ell^T v - \tilde{Q}_\ell^T v \in V^f(\omega_{T,\ell})$

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

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

Theorem (A priori error bound)

It holds

$$|||u_h - \tilde{u}_{h,\ell}^{ms}||| \leq C\Big(H + \max_{T \in \mathcal{T}} e_T\Big).$$

Local error indicators

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

- $w|_T$ has few degrees of freedom and the max can be computed by solving a small eigenvalue problem.
- Error in $\tilde{A}_T - A$ away from T gets multiplied with exponentially decaying function.
- If error is large update $\tilde{A}_T = A(t)$ leading to modified entries in a few columns of the global stiffness matrix $\tilde{a}(\phi_x, \phi_y)$.
- Only local recomputations are needed (FEM: $\|\tilde{A} - A\|_{L^\infty(\Omega)}$).

Hellman & M., Numerical homogenization of PDE similar coeff., 2018.

Reuse of LOD basis in parameter space

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

Simple approach: Given $A = A(t)$, $t \in \mathcal{S}$, and TOL. For $T \in \mathcal{T}$:

- Pick $t_0 \in \mathcal{S}$, let $\tilde{A}_T = A(t_0)$ compute $\tilde{a}_{T,0}(\phi_x,\phi_y) = (\tilde{A}_T\nabla\phi_y,\nabla\phi_x)_T - (\tilde{A}_T\nabla\tilde{Q}_\ell\phi_y,\nabla\phi_x)$.
- Find parameter set $S_0 = \{t \in S : e_T(A(t),A(t_0)) \leq TOL\}$.
- Let $\tilde{A}_T = A(t_n)$, $t_n \notin \cup_{k=0}^{n-1} S_k$, compute entries $\tilde{a}_{T,n}(\phi_x,\phi_y)$ and find $S_n = \{t \in S : e_T(A(t),A(t_n)) \leq TOL\}$.
- Works for a discrete set of parameters $\mathcal{S}$.

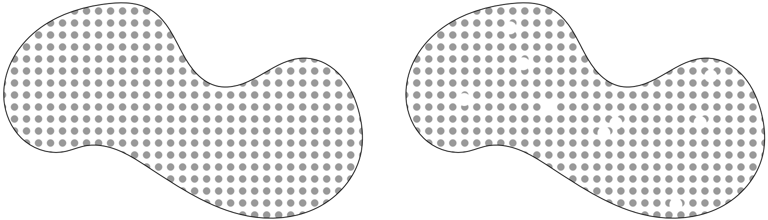
For T and t_k we store matrix entries $\{\tilde{a}_{T,k}(\phi_x,\phi_y)\}_{k=0}^n$. To add new parameters, more details needs to be stored.

Example: random diffusion

Poisson equation:

$$-\nabla \cdot A(\omega)\nabla u(\omega) = f \quad \text{in } D \quad u(\omega) = 0 \quad \text{on } \partial D, \quad \omega \in \Omega.$$

On each element T find $\{\omega_i\}_{i=1}^n$ such that $S \subset \cup_{i=1}^n S_i$ off-line. On-line assemble global LOD matrix by picking right entries from each T and solve coarse problem for each sample.



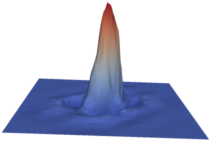
A few configurations need to be stored for each $T \in \mathcal{T}$. Periodicity can be exploited.

In FEM the full problem is solved for each sample.

Comments and issues

- The possibility to apply $\tilde{A}_T$ independently on each T should be exploited. No communication with other elements.
- Parametrized rep. of the LOD matrix entries from each element is the output, not the full parametrized LOD basis.
- Few parameters may be active on each patch (exponential decay).
- Periodicity can be exploited.
- Storage is reasonable, not even LOD basis have to be stored simultaneously.
- How to find good ω_k and regions $S_k = \{\omega : e_T(A(\omega) - A(\omega_k)) < TOL\}$ is open. Note that e_T is computable, only local information is needed and it is off-line.
- Techniques from the RBM community should be useful.

Connection to RBM-LOD



- The goal is to reduce solves for the training set in RBM.
- $Q_\ell(t)\phi_x$ is parametrized and reduced basis computed.
- Error analysis bounds $|||Q_\ell(t)\phi_x - \tilde{Q}_\ell(t)\phi_x|||$ leading to H^{-1} term in global error and therefore larger patches.
- PG formulation is *not* used: multiplication of parametrized basis is needed. Affects communication and storage.
- The assumption $A(t) = \sum_{k=1}^{K} \theta_k(t) A_k(x)$ is crucial and performance depends on K.

Abdulle & Henning, A reduced basis LOD, JCP 2015.

Outline

1. Elliptic model problem
2. Introduction to LOD
3. High contrast data
4. Parameter dependent data
5. **Final comments**

Comments and conclusion

- Thin high conductivity channels are challenging and important.
- Global fine scale connections are equally problematic for iterative methods (Multigrid, DD).
- The choice of interpolant is crucial.
- LOD can be tuned to handle modeling error in the diffusion.
- PG formulation, elementwise localization and error indicators allows us to attack parametrized problems.
- Possibility to collaborate on RBM-LOD.

Thank you for your attention!