Multiscale Model Reduction for flows in heterogeneous porous media

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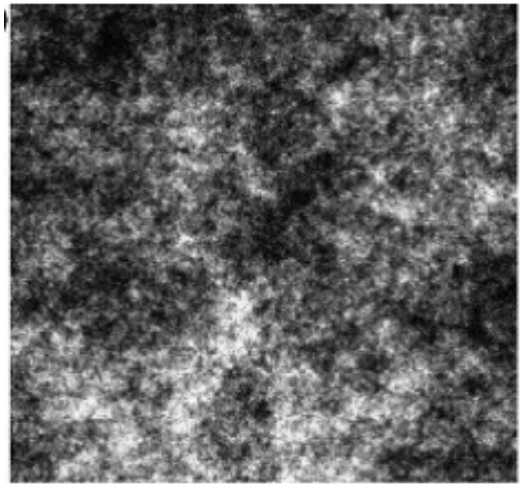
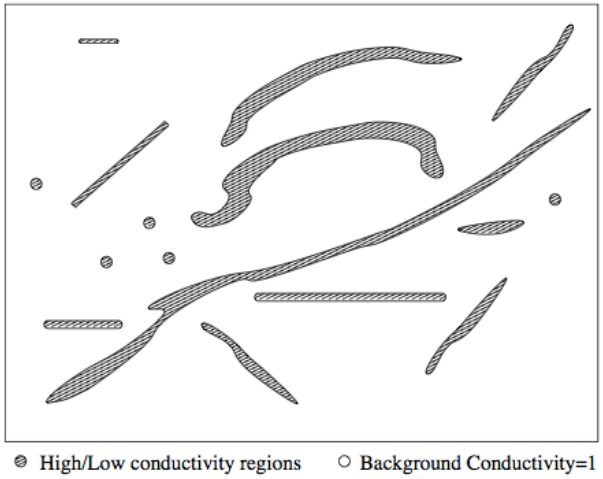
Introduction

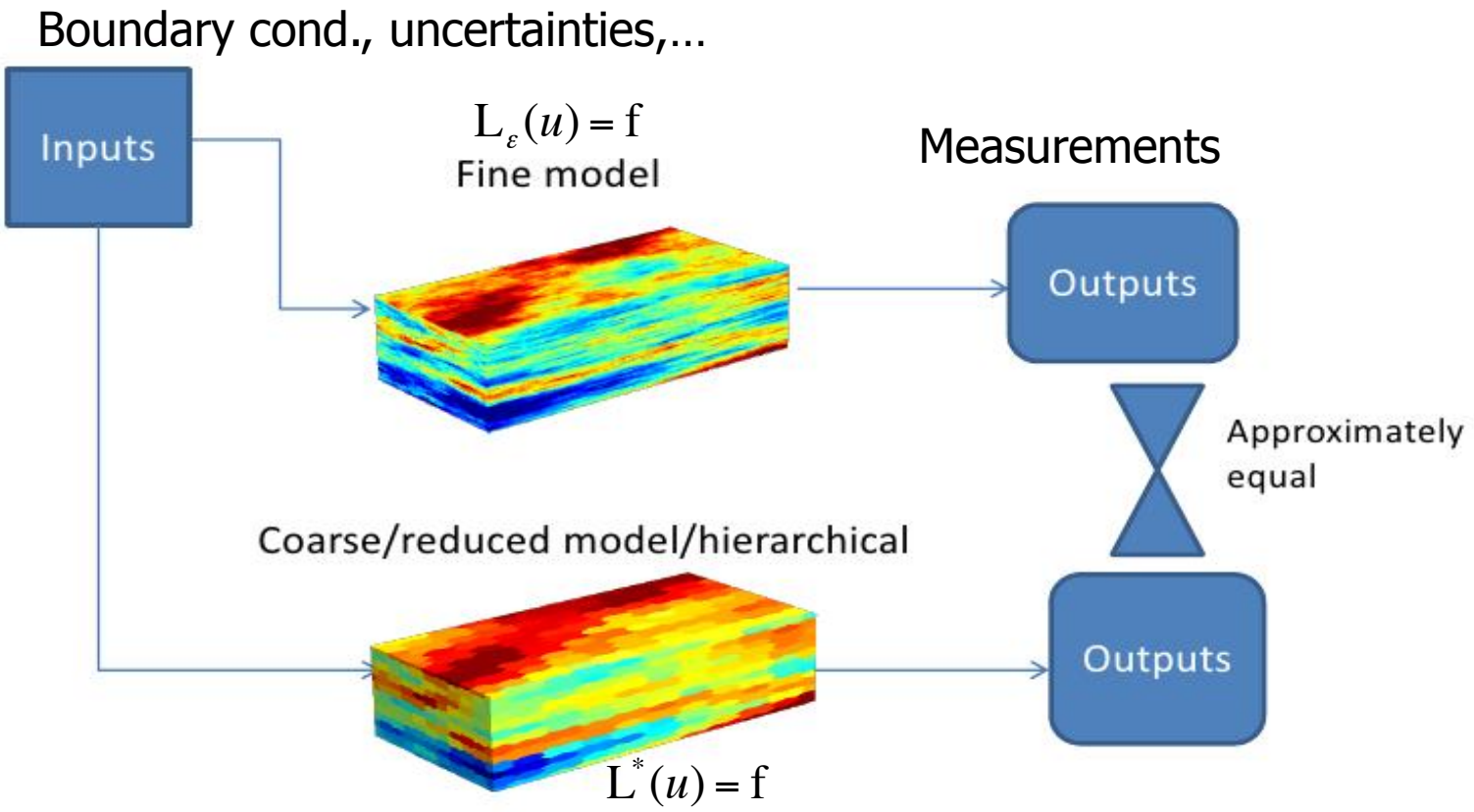
- Multiple scales, complex heterogeneities, high contrast.





- It is prohibitively expensive to resolve all scales and uncertainties. Some types of reduced models are needed.
- Our objective is the development of reduced-order models

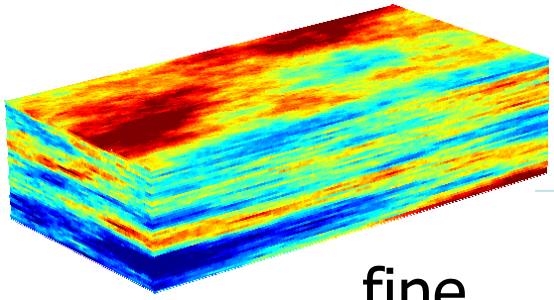
Reduced-Order Modeling Concept



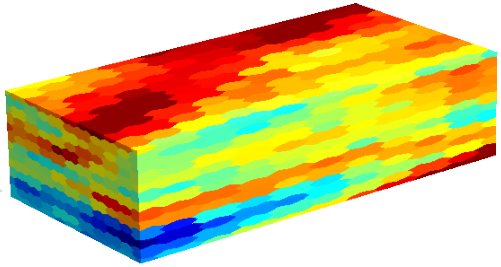
Reduced/coarse models

LOCAL

- Numerical homogenization

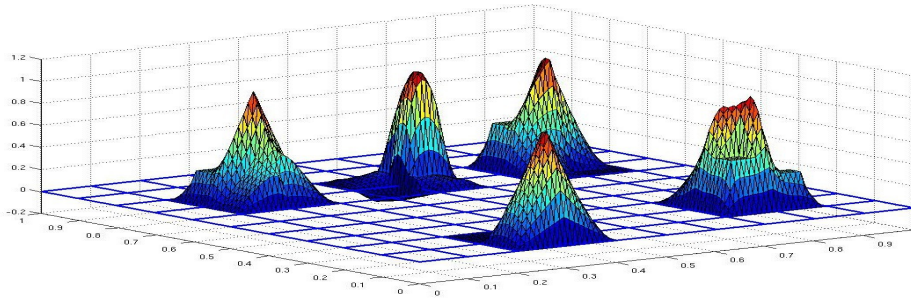


fine



coarse

- Multiscale (on a coarse grid) methods



GLOBAL

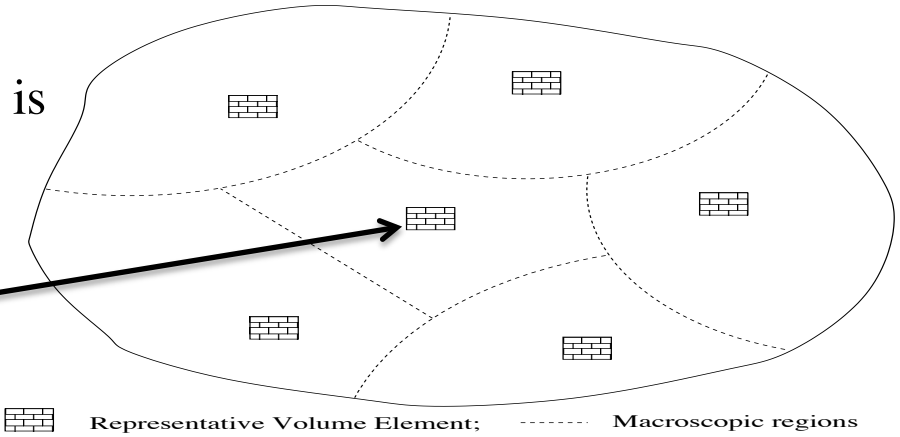
- Uses global snapshots and find best n-dimensional subspace based on, e.g., POD, BT,…

Reduced-order model in a scale-separation case.

$$-\mathrm{div}\left(\mathrm{k}\left(\mathrm{x},\frac{x}{\varepsilon}\right)\nabla \mathrm{u}\right)=\mathrm{f(x)},\ \text{where k(x,y) is periodic in y, y} = \frac{\mathrm{x}}{\varepsilon}.$$

$\hat{u}(\mathrm{x},\mathrm{x}/\varepsilon) = u_0(x) + \varepsilon N(\mathrm{x},\mathrm{y})\cdot \nabla_{\mathrm{x}} u_0,$ where $N(\mathrm{x},\mathrm{y})$ is periodic in y and solves

$$\boxed{\mathrm{div}_{\mathrm{y}}(\mathrm{k}(\mathrm{x},\mathrm{y})(\nabla_{\mathrm{y}}\mathrm{N}+\mathrm{I}))=0 \text{ in Y}}$$



$$-\mathrm{div}(\mathrm{k}^{*}(\mathrm{x})\nabla \mathrm{u}_0)=\mathrm{f(x)}$$

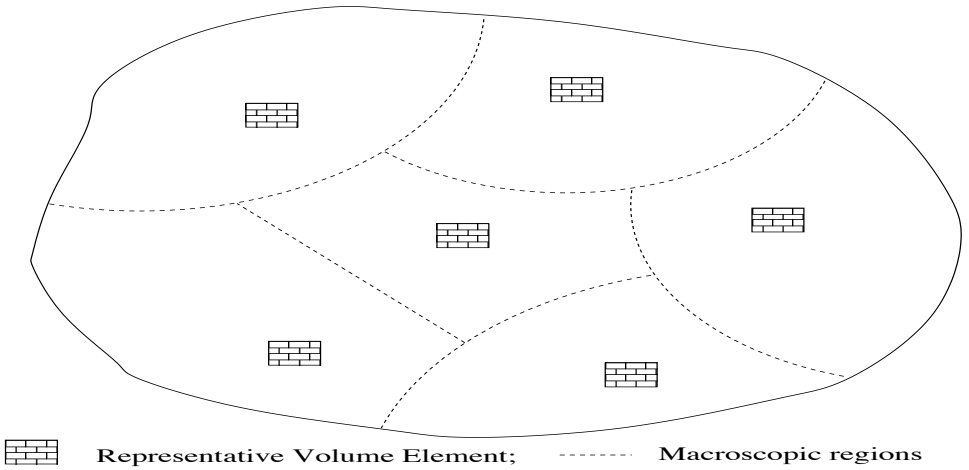
$$\mathrm{k}^{*}(\mathrm{x})=\frac{1}{|Y|}\int_{Y}\mathrm{k}(\mathrm{x},\mathrm{y})(\nabla_{\mathrm{y}}\mathrm{N}+\mathrm{I})\ \mathrm{dy}$$

$$\| u(\mathrm{x}) - \hat{u}(\mathrm{x},\mathrm{x}/\varepsilon)\|_{H^1(D)} \le C\sqrt{\varepsilon}$$

Reduced-order model in a scale-separation case. Homogenization

$-\mathrm{div}(k(x,\frac{x}{\varepsilon})\nabla u)=f(x)$. Define $y=\frac{x}{\varepsilon}$.

$$\hat{u}_\varepsilon(x)=u_0(x)+\varepsilon N\left(x,\frac{x}{\varepsilon}\right)\cdot\nabla u_0$$



In each coarse region,

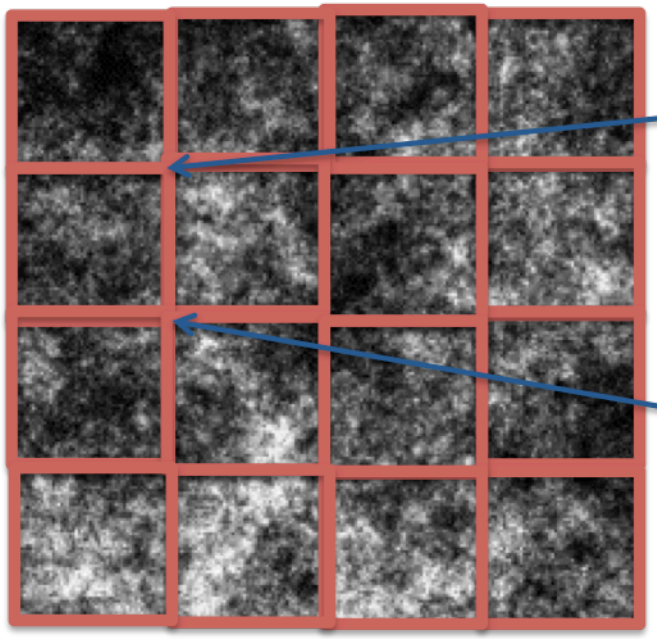
$$\nabla_x\hat{u}_\varepsilon(x)\approx\nabla_x u_0(x)+\nabla_y N(x,y)\cdot\nabla_x u_0\approx\left(\mathrm{I}+\nabla_y N(x,y)\right)\cdot\xi$$

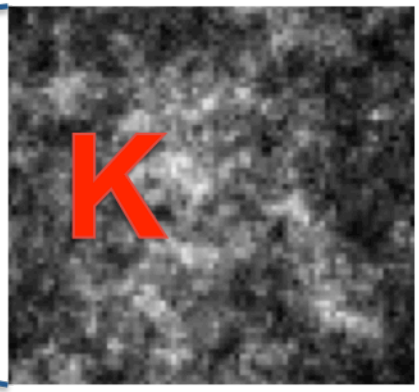
where $\xi=\nabla_x u_0(x)\approx\mathrm{const}$.

This shows that the solution can be approximated in each coarse region using very few (in 2D) "degrees of freedom".

For some non-periodic cases, e.g., when $k = k(x/\varepsilon,\omega)$ is homogeneous and ergodic, large Representative Volumes are needed (and periodic boundary conditions can be replaced by Dirichlet or Neumann, e.g., Bourgeat and Piatnitski, 2003).

Numerical homogenization





$$div(k\nabla\phi_1) = 0 \text{ in K}$$
$$\phi_1 = x_1 \text{ on } \partial K$$

$$div(k\nabla\phi_2) = 0 \text{ in K}$$
$$\phi_2 = x_2 \text{ on } \partial K$$

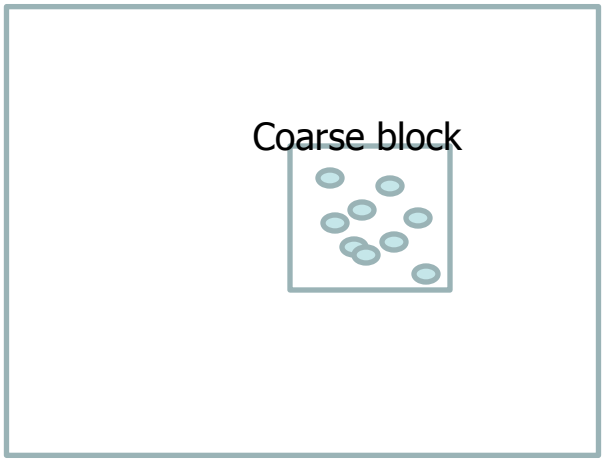
$$k^* = \left[\left\langle k\nabla\phi_1 \right\rangle \left\langle k\nabla\phi_2 \right\rangle\right]$$

In general, k^* can be computed by: (1) $L_k(\phi_i) = 0$ in K, $\phi_i = b_i$ on ∂K;

(2) $L_{k^*}(\phi_i^*) = 0$ in K, $\phi_i^* = b_i$ on ∂K; (3) Min. $k^* = \arg\min \sum_i |E_i(\phi_i) - E_i^*(\phi_i^*)|$

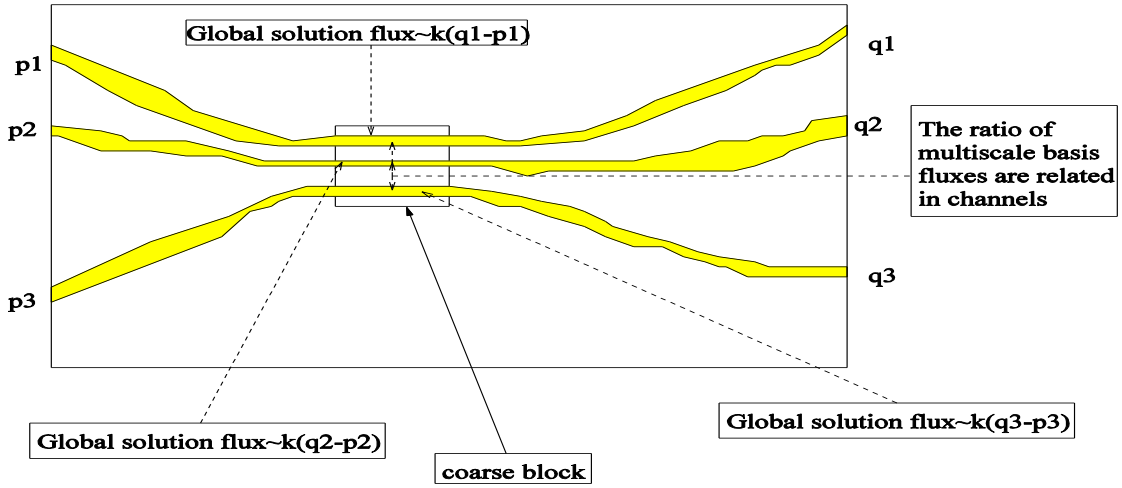
Scale separation issues

- Many applications don't have scale separation and distinct features need to be modeled separately
- We want to find a reduced dimensional representation of the solution space on a coarse grid
- We use multiscale finite element concepts.
- "Optimal dimensional" coarse spaces are studied in preconditioners (joint work with Galvis, 2009, 2010)



Localizable features

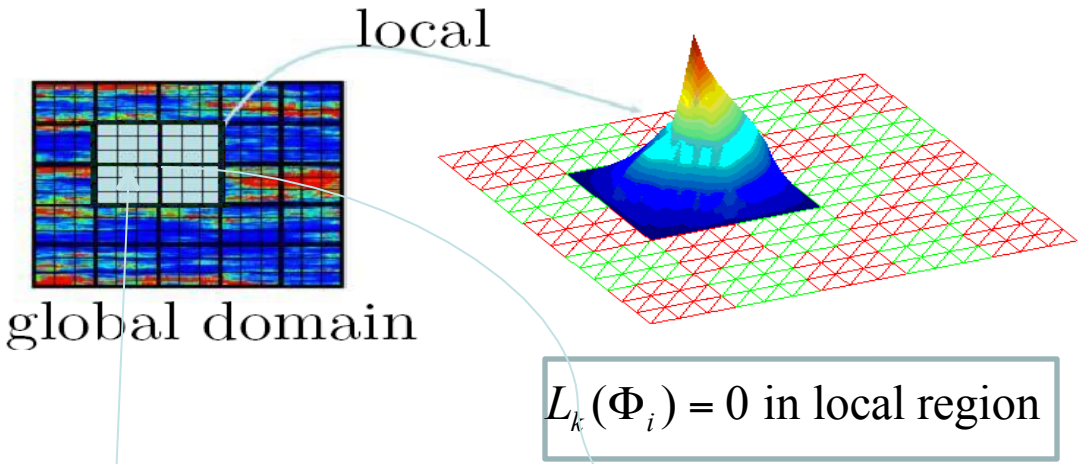
Non-localizable features



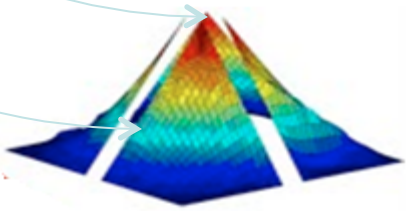
Multiscale FE methods*.

- We look for a reduced approximation of fine-scale solution $u = \sum_{i=1}^{fine} u_i \phi_i$

as $u^* = \sum_{i=1}^{coarse} u_i^* \Phi_i$, such that $\|u - u^*\|$ is small. Goal is to find Φ_i.



- $L_k(\Phi_i) = 0$ in ω_i, $\Phi_i = \Phi_i^0$ on $\partial\omega_i$.
- $L(u) = -div(k\nabla u)$

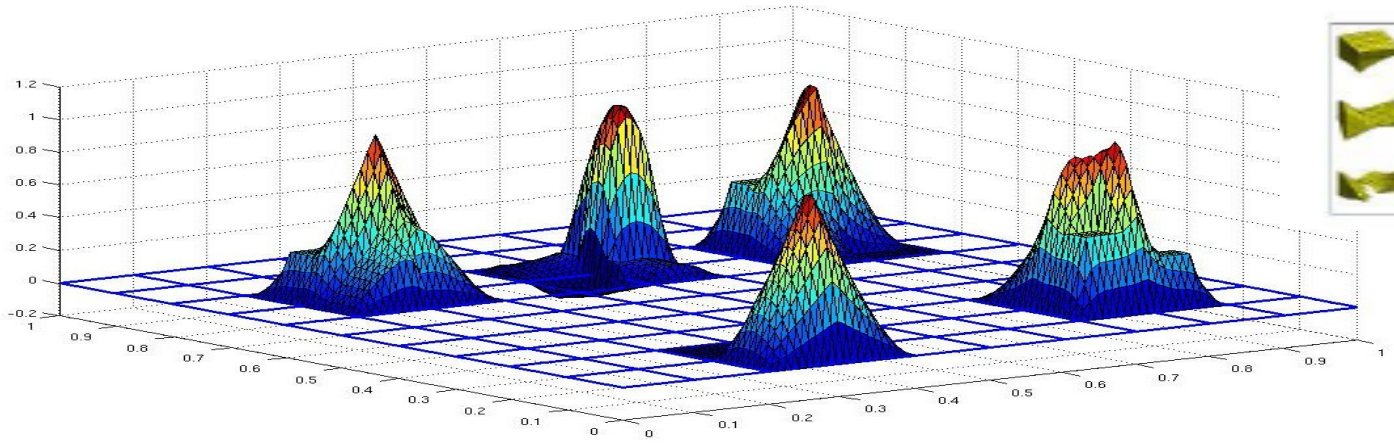


*. Babuska and Osborn, 1983; Hou and Wu, 1997

Multiscale FE methods.

- $u = \sum_i u_i \Phi_i$, where u_i are found by a "Galerkin substitution" (Babuska et al. 1984, Hou and Wu, 1997),

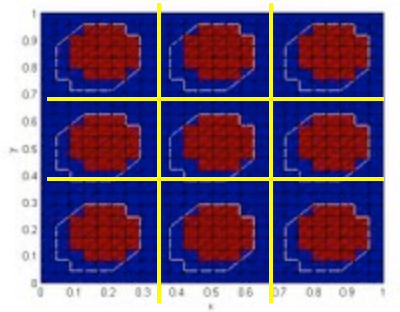
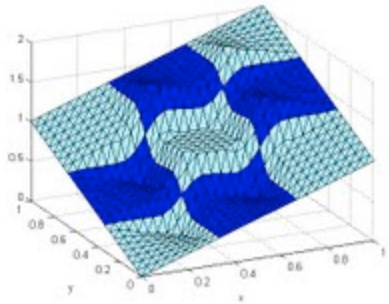
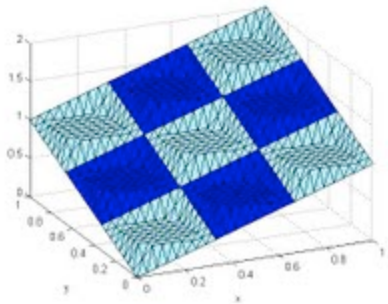
$$\left\langle L\left(\sum_i u_i \Phi_i\right), \Phi_j \right\rangle = \left\langle f, \Phi_j \right\rangle$$. Integrals can be approximated for scale separation case.



From Aarnes et al.,

Scale separation. Boundary conditions

- Numerical homogenization is similar to MsFEM with one basis per coarse node
- Local boundary conditions need to contain "correct" structure of small-scale heterogeneities.

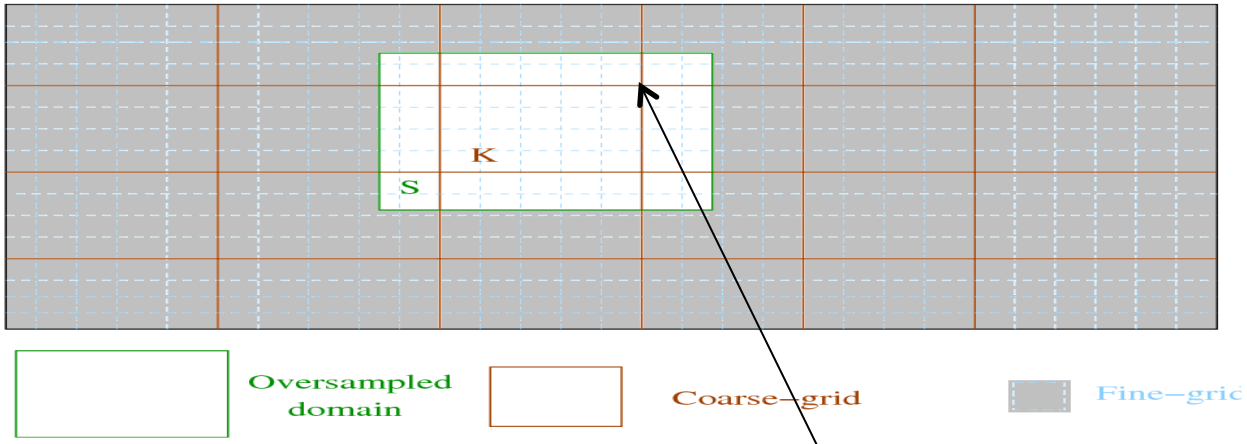




- Piecewise linear boundary conditions result to large discrepancies near the edges of coarse blocks

$$\text{Error} \propto (\frac{\varepsilon}{H})^{\beta}, \text{ where } \varepsilon \text{ is a physical scale and } H \text{ is the coarse mesh size, } H >> \varepsilon.$$

Oversampling

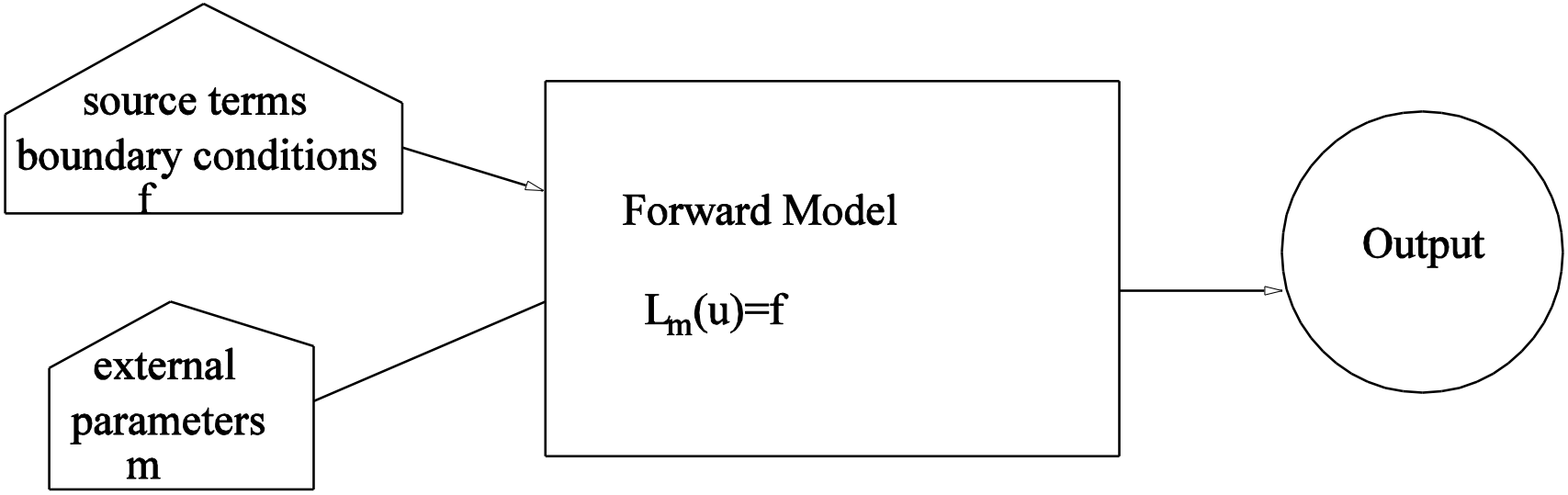
- To reduce the effects of artificial local boundary conditions, oversampling techniques are developed and analyzed (Hou and Wu 1997, Efendiev, Hou, and Wu 1999, Gloria 2010,…)



- $\Phi_i = \sum c_{ij} \Phi_j^{ovs}$ with some constraints on Φ_j, e.g., $\Phi_j(x_i) = \delta_{ij}$. Here Φ_i^{ovs} are oversampling basis functions defined on S.

- These methods can have large errors. How can we enrich spaces in a systematic way?

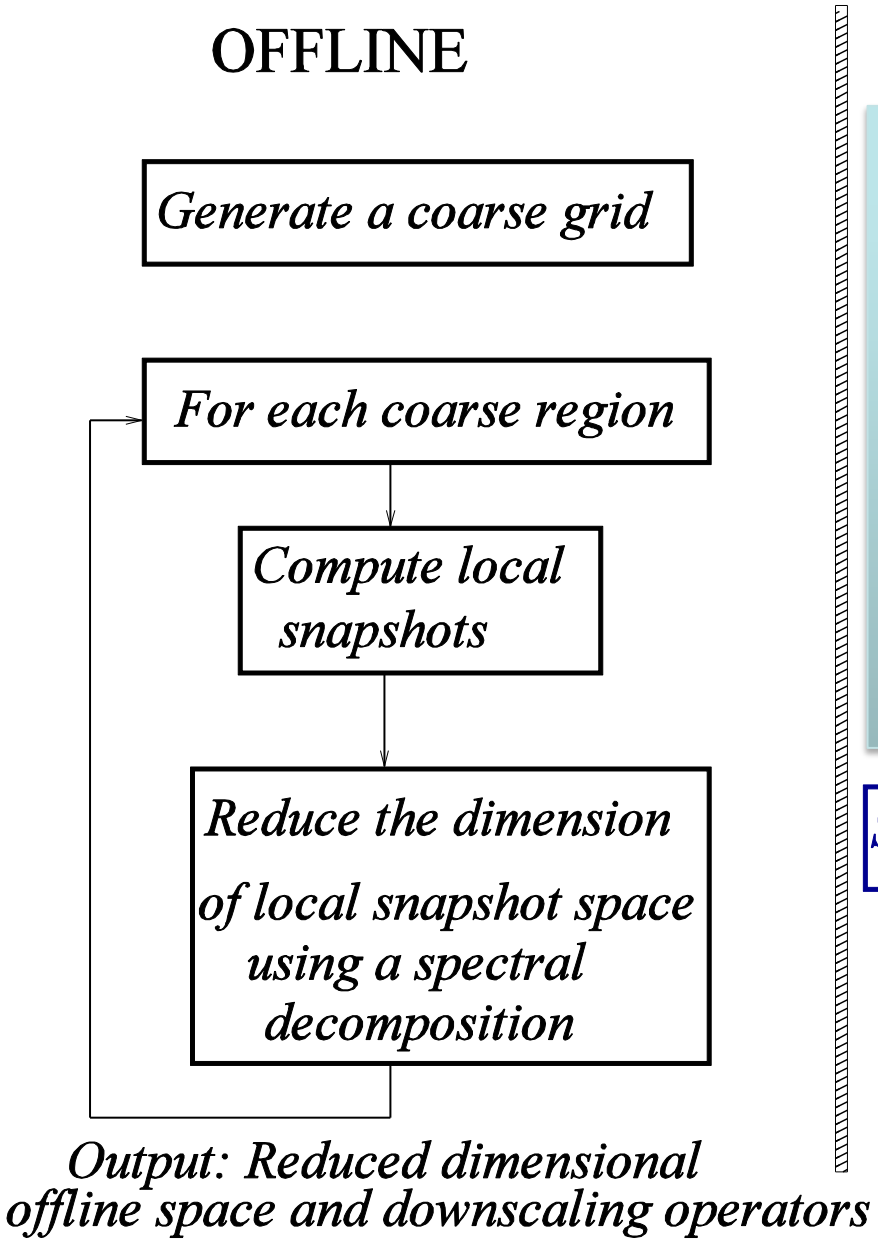
General Multiscale Model Reduction Framework (GMsFEM)*



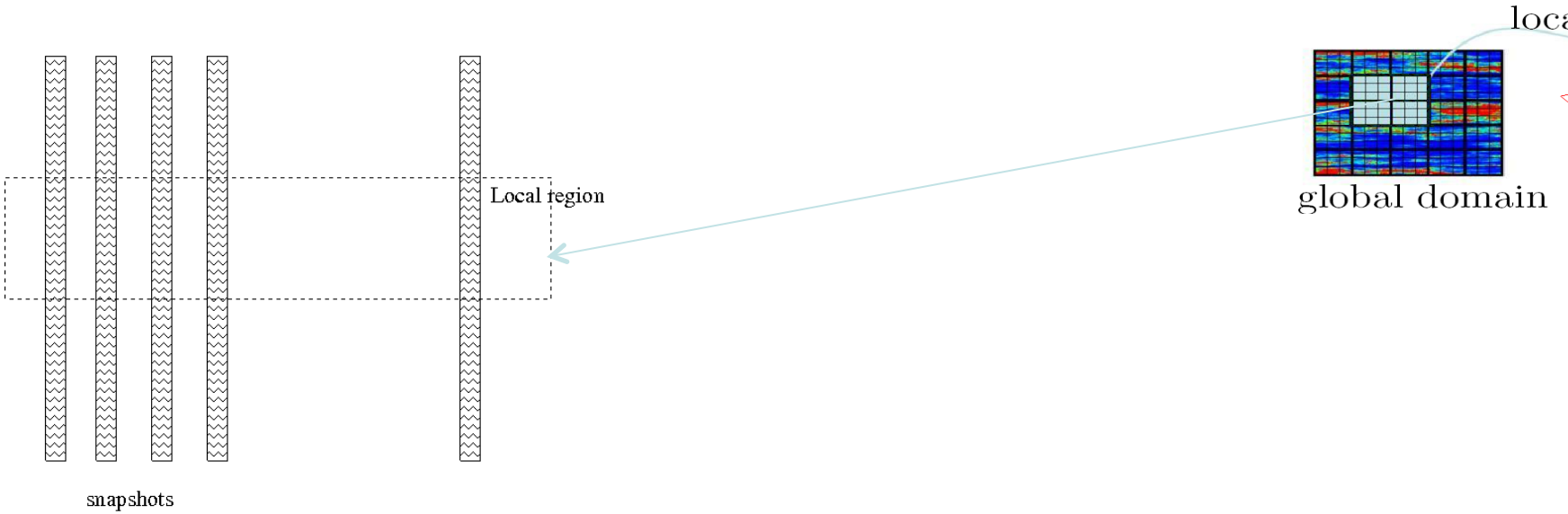
$$\text{Example. } -\operatorname{div}(k(x;\mu)\nabla p) = f, \quad \mu \in \Lambda, \quad k(x;\mu) = \sum_i k_q(x)\Theta_q(\mu)$$

*Efendiev, Galvis, and Wu, JCP 2011 and Efendiev, Galvis, Hou, Generalized Multiscale Finite Element Method, JCP 2013

GMsFEM


OFFLINE
Generate a coarse grid
For each coarse region
Compute local snapshots
Reduce the dimension of local snapshot space using a spectral decomposition
Output: Reduced dimensional offline space and downscaling operators
ONLINE
Not needed for parameter-independent problems
Solve a coarse-scale problem
Iterative process (if needed)

(Local) Multiscale model reduction.

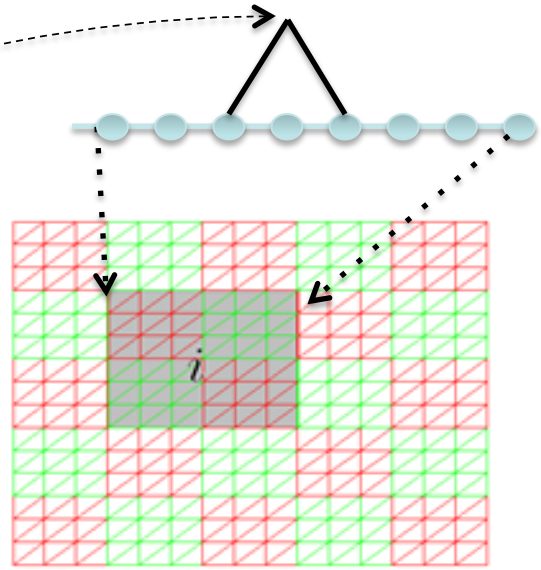


Snapshot space

- The snapshot space consists of unit vectors.
  Limitations: no oversampling, difficult to impose special properties

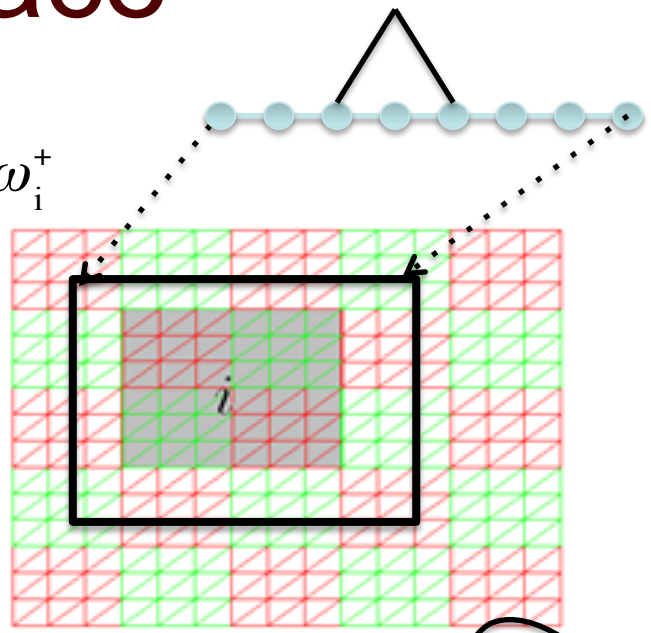
- No parameter case: $L(\psi_j^{\omega_i})=0$ in ω_i

$$\psi_j^{\omega_i} = \delta_j \text{ in } \partial\omega_i$$



Snapshot space

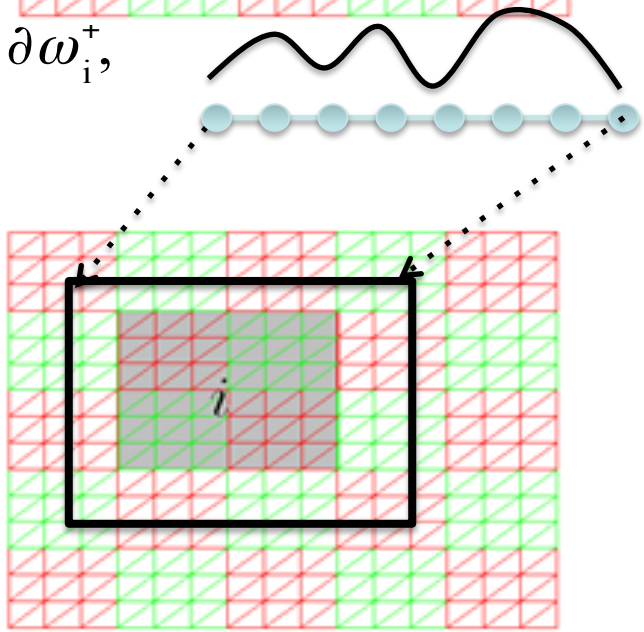
- Oversampling: $L(\psi_j^{\omega_i^+})=0$ in ω_i^+, $\psi_j^{\omega_i^+} = \delta_j$ in $\partial\omega_i^+$



- Oversampling: $L(\psi_j^{\omega_i^+})=0$ in ω_i^+, $\psi_j^{\omega_i^+} = R_j$ in $\partial\omega_i^+$,

where R_j is i.i.d. Gaussians.

Fewer snapshots are computed.



$$V_{\text{snap}}^{\omega_i} = \text{Span}\{\psi_j^{\omega_i}\}$$

Offline space

We would like to find a subspace of $\Psi^{\text{snap}}_{\omega_i} = \text{span}\{\psi_1^{\omega_i},...,\psi_{M_{\text{snap}}}^{\omega_i}\}$ such that

$m_{\omega_i}(u\text{-}u_0) \le \delta\, a_{\omega_i}(u\text{-}u_0)$ for bilinear forms m(•) and a(•) and small δ.

Local spectral problems are motivated by analysis and depends on global discretization, smoothness of the solution (ε), snapshots...

Define $R_{\text{snap}} = [\psi_1^{\text{snap}},...,\psi_{M_{\text{snap}}}^{\text{snap}}]$ (e.g., $R_{\text{snap}} = I$ for Choice 1) and

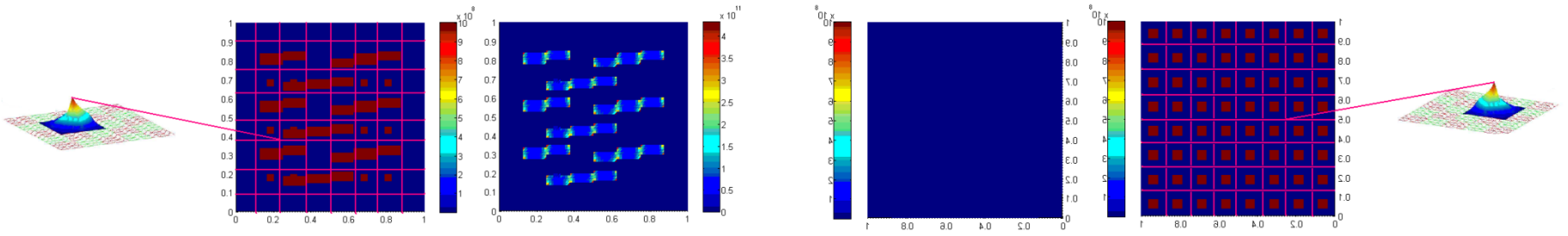
$$A^{\text{off}} = (R_{\text{snap}})^T A\, R_{\text{snap}}, \quad M^{\text{off}} = (R_{\text{snap}})^T M\, R_{\text{snap}}$$

Example: $\psi^T M^{\text{off}} \phi := "\int_{\omega_i} \tilde{k}(x)\psi\, \phi", \quad \psi^T A^{\text{off}} \phi := "\int_{\omega_i} k(x)\nabla\psi\cdot\nabla\phi"$

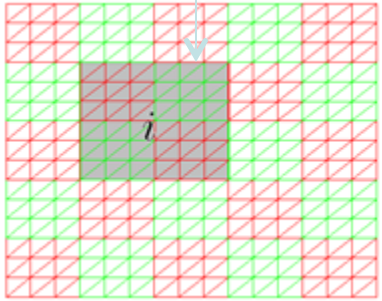
Offline space construction is based using "dominant" eigenvectors of:

$$A^{\text{off}}\Psi^{\text{off}}_k = \lambda_k M^{\text{off}}\Psi^{\text{off}}_k$$

A coarse space construction. Example.

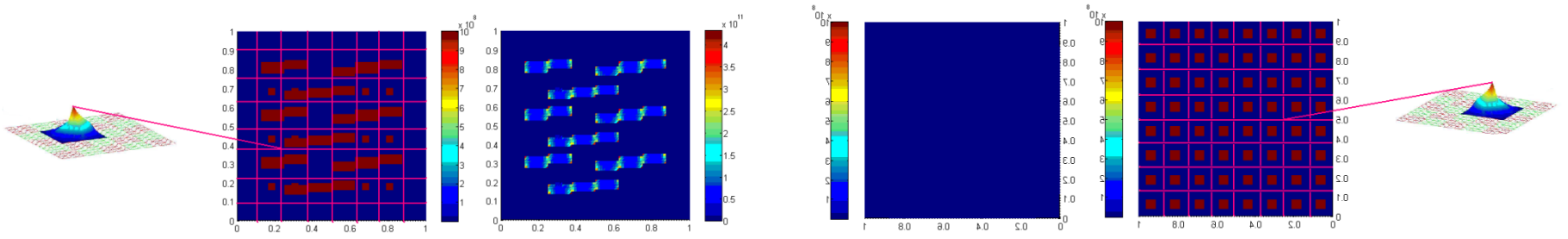


- Start with initial basis functions Φ_i and compute $\tilde{k} = \sum_i k\nabla\Phi_i \cdot \nabla\Phi_i$.
- For each ω_i, solve local spectral problem $-\mathrm{div}(k\nabla\psi_i) = \lambda_i \tilde{k}\psi_i$ (motivated by analysis) and choose "small" eigenvalues and corresponding eigenvectors.

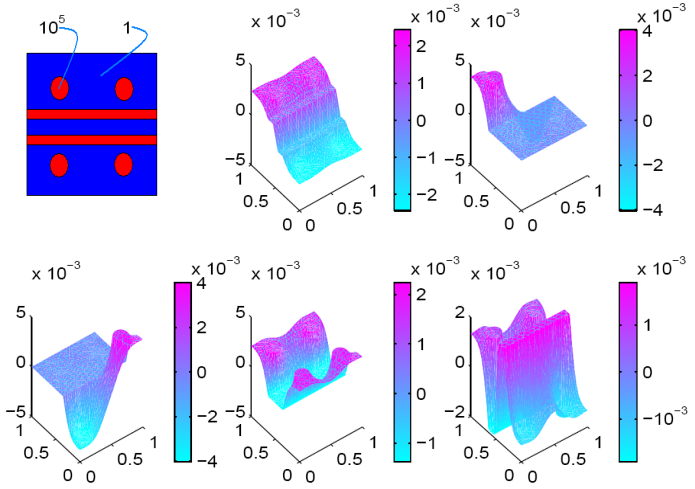


Note that “special” eigenvalue problems are used.

A coarse space construction. Example



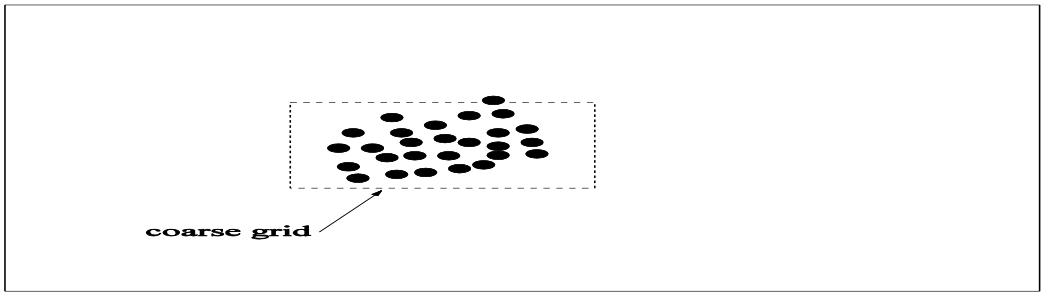
- Φ_i are multiscale FEM functions - $\tilde{k} = \sum_i k \,|\nabla \Phi_i|^2$ (choice of init. basis is important)
- $-\mathrm{div}(k\nabla\psi_i) = \lambda_i \tilde{k}\psi_i$
- Identify $\lambda_1 = 0 \le \lambda_2 \le \ldots \le \lambda_n$.
- There are 2 small (inversely $\propto$ to high-contrast) eigs for multiscale Φ_i and 6 for bilinear Φ_i
- "Gap" in the spectrum --- $\dfrac{\int k\,|\nabla\psi|^2}{\int \tilde{k}\psi^2}$.



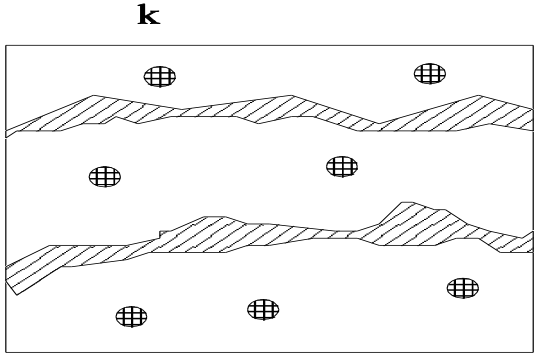
- For harmonic snapshots, the fast decay can be achieved by using oversampling in the space of harmonic snapshots (Babuska and Lipton, MMS 2011)

A coarse space construction. Example

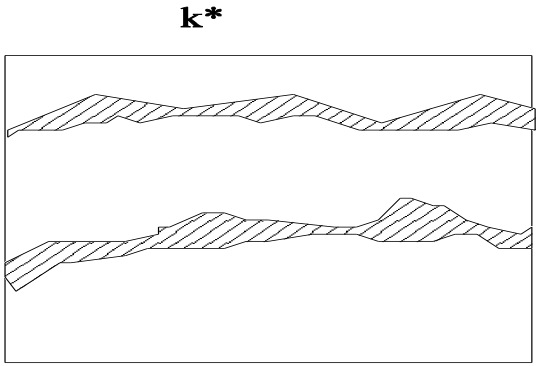
- If there are many inclusions, we may have many basis functions. We know "many isolated inclusion domain" can be homogenized (one basis per node).



- Channels vs. inclusions.



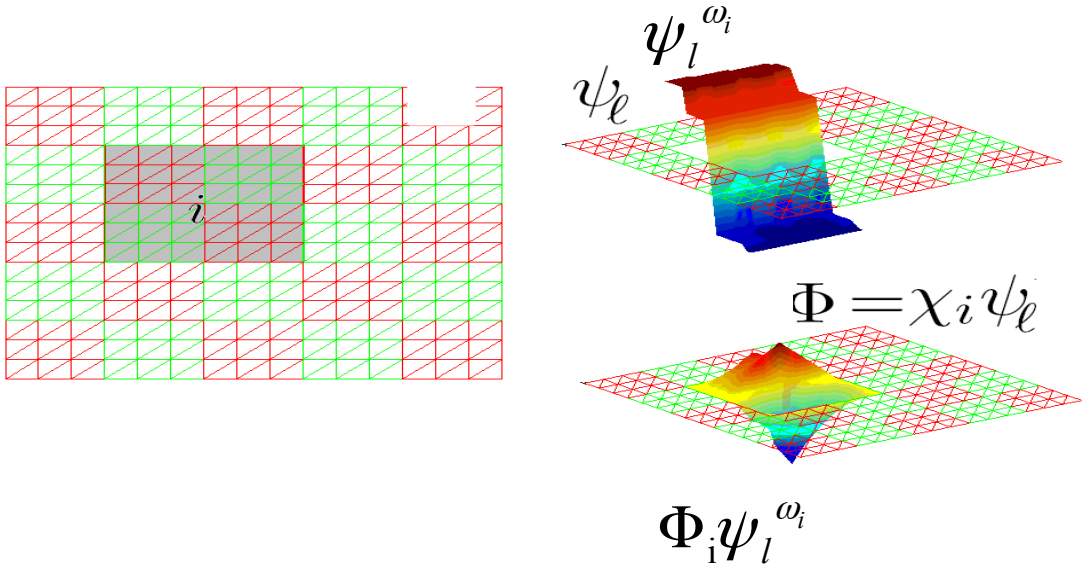
Coarse grid with isolated inclusions and channels



Coarse grid without isolated inclusions

Coarse space construction

- Coarse space: $V_0 = Span\left\{\Phi_i \psi_l^{\omega_i}\right\}$



- Condition number of two-level (optimal) preconditioners - $1/\Lambda_*$ (with Galvis, SIAM MMS 2010)
- Coarse-grid approximation (under some assumptions) - H^γ / Λ_* (with Galvis and Wu, JCP, 2010)
- Multilevel preconditioners (optimal for high-contrast problems) (with Galvis and Vassilevski, 2010

Online space

- For parameter-dependent problems, the offline space is constructed using some selected values of μ_i.
- In the online stage, for each new μ, the local spectral problem is solved to define multiscale basis functions.

Mixed GMsFEM

- Mixed formulation is needed for the mass conservation

$$k^{-1}\, v + \nabla p = 0, \quad \mathrm{div}(v) = f$$

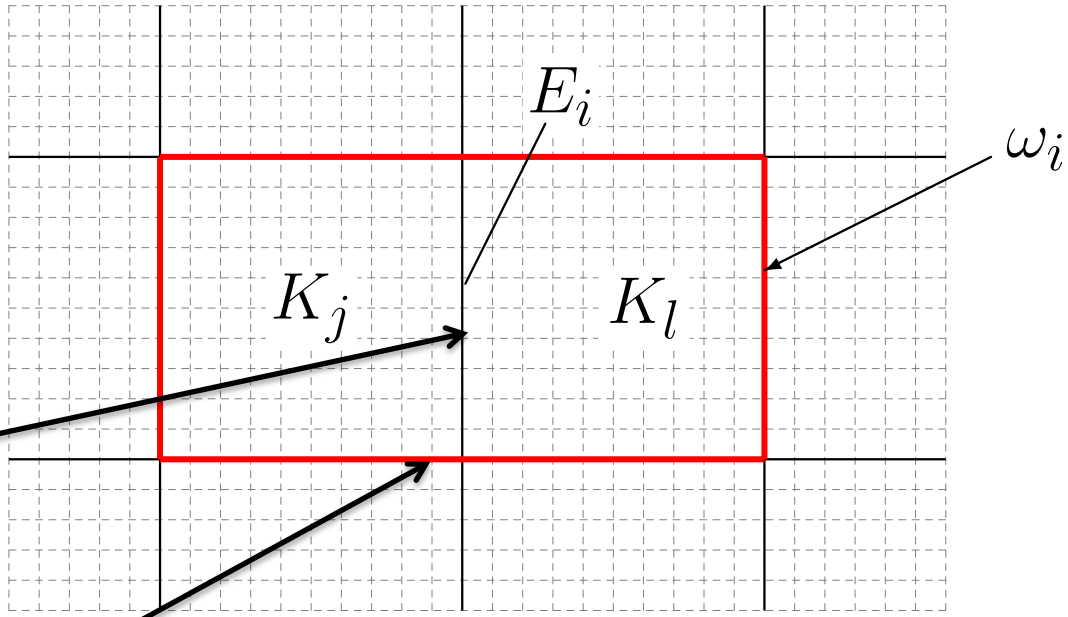
$k^{-1}\, v_j^{(i)} + \nabla p_j^{(i)} = 0$ in ω_i

$\mathrm{div}(v_j^{(i)}) = \alpha_j^{(i)}$ in ω_i

$v_j^{(i)} \cdot m_i = \delta_j^{(i)}$ on E_j

$\delta_j^{(i)} = 1$ on j-th fine edge

$v_j^{(i)} \cdot n_i = 0$ in $\partial\omega_i$



Mixed GMsFEM

Take $\Psi_j^{i,snap} := v_j^{(i)}$ and form $V_{snap}^{(i)} = \text{span}_j\{\Psi_j^{i,snap}\}$

For each edge, the local spectral problem is

$$a_i(v,w)=\lambda m_i(v,w),\ \forall w \in V_{snap}^{(i)}$$

$$m_i(v,w)=\int_{\omega_i} k^{-1} v \cdot w, \qquad a_i(v,w)=\int_{E_i} [p_v][p_w]$$

By selecting dominant eigenvectors, we form the offline space for the velocity

$$V_{off} = \text{span}\{\Psi_j^{i,off}\}.$$

The offline space for pressure is piecewise constant functions.

Mixed GMsFEM

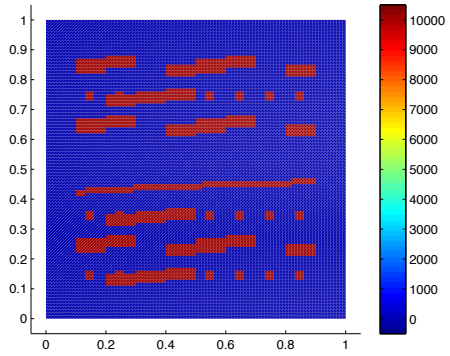
Theorem.

$$\int_D k^{-1} |v_h - v_{ms}|^2 \prec \Lambda^{-1} \sum_i a_i(\hat{v},\hat{v}) + O(H)$$

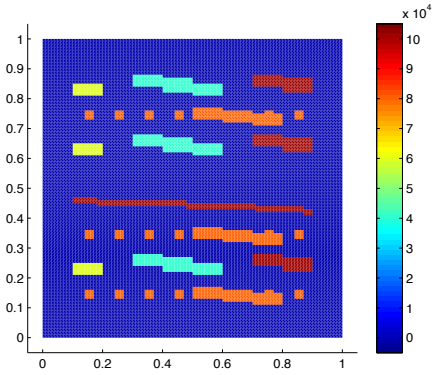
$$\Lambda = \min_{1 \le i \le N_0} \lambda_{l_i+1}^{(i)}$$

Remark. The eigenvalue problem can be considered via an optimization point.

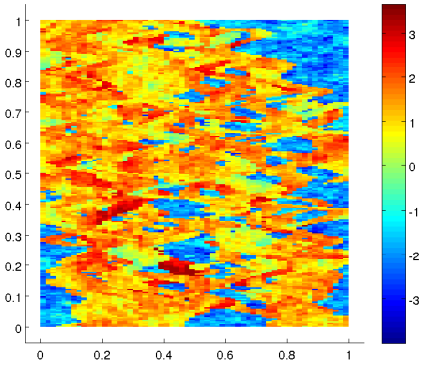
Numerical Results



(a) κ_1



(b) κ_2



(c) κ_3 in $\log_{10}$ scale

Basis per edge	Error(v)
2	0.06
3	0.03
4	0.013
5	0.054

Convergence is correlated to $1/\Lambda$

Applications to two-phase flow and transport

- Multi-phase flow and transport. E.g., two-phase - $\nabla \cdot \left(\lambda(\mathrm{S})\mathrm{k}\nabla \mathrm{p}\right) = q,\ \mathrm{S}_t + \mathbf{v} \cdot \nabla \mathrm{f}(S) = 0,$

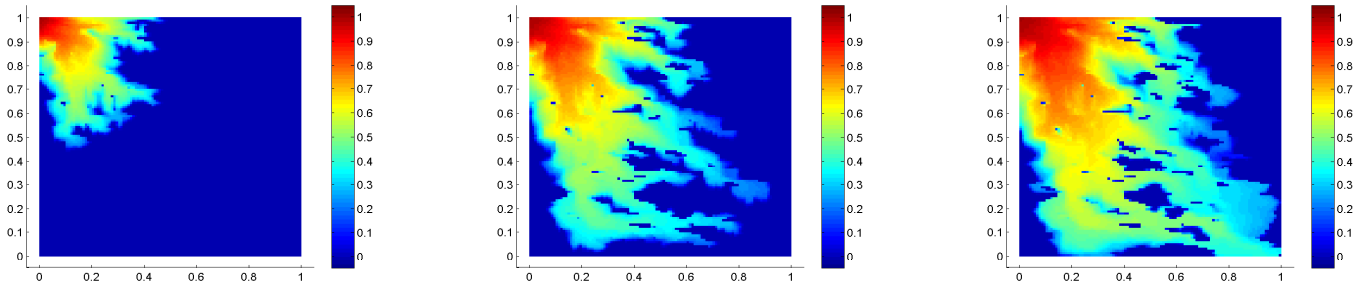
  where $\mathbf{v}=-\lambda(\mathrm{S})\mathrm{k}\nabla \mathrm{p}$.

- A workflow: offline - construct multiscale basis functions. (1) solve pressure equation (with mass conservative discretization) on a coarse grid, compute fine-scale velocity (adaptively); (2) solve the saturation equation on a fine.

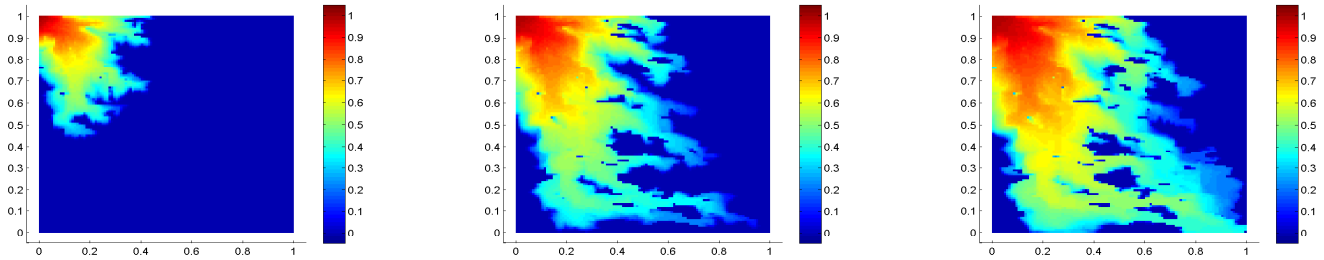
- Multiscale basis functions are not updated throughout simulations

Numerical results

reference

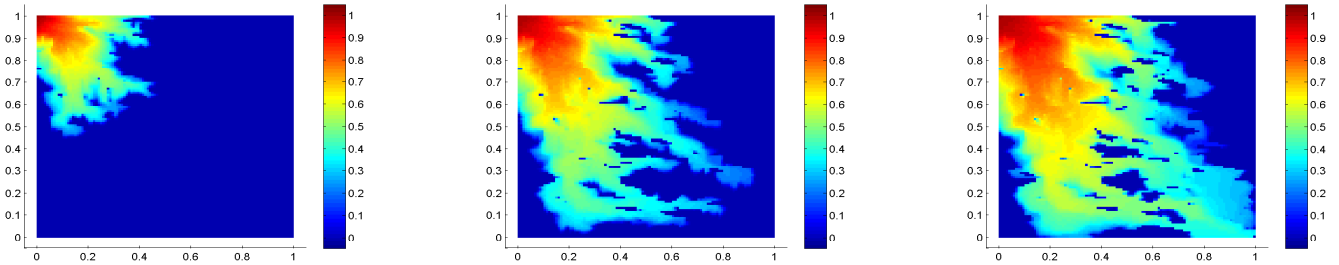


2 basis per edge



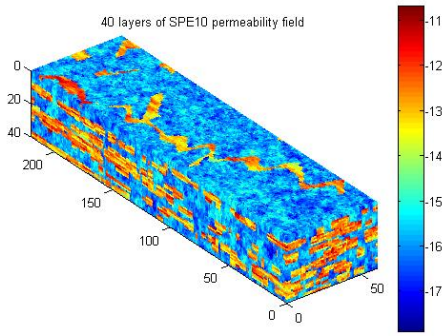
(a) Relative L^2 error = 11.7% (b) Relative L^2 error = 14.2% (c) Relative L^2 error = 11.3%

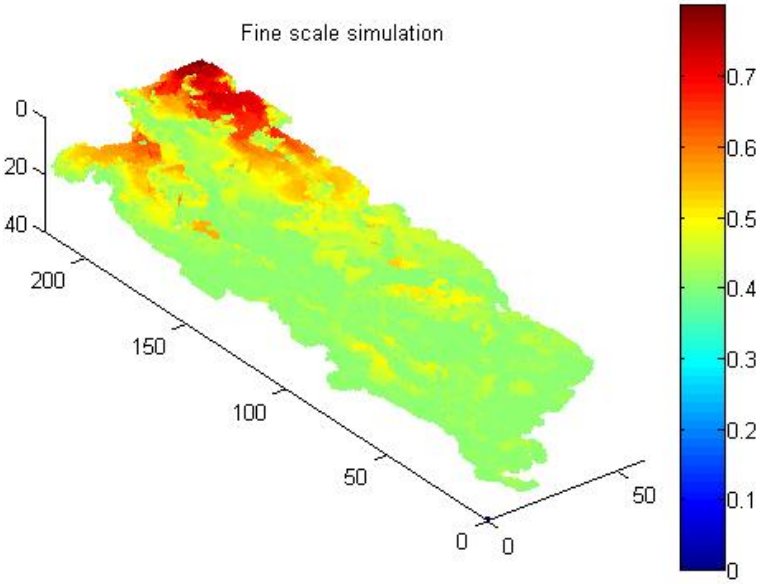
4 basis per edge

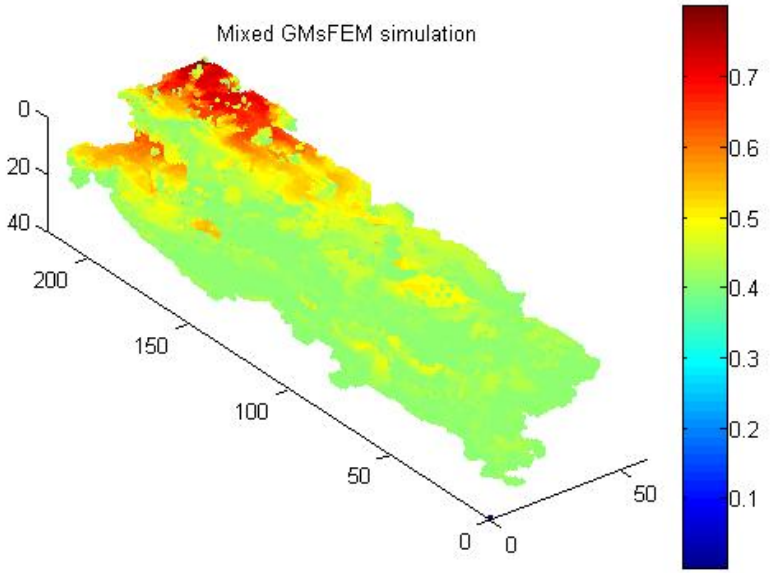


(a) Relative L^2 error = 4.2% (b) Relative L^2 error = 4.8% (c) Relative L^2 error = 5.7%

Numerical Results





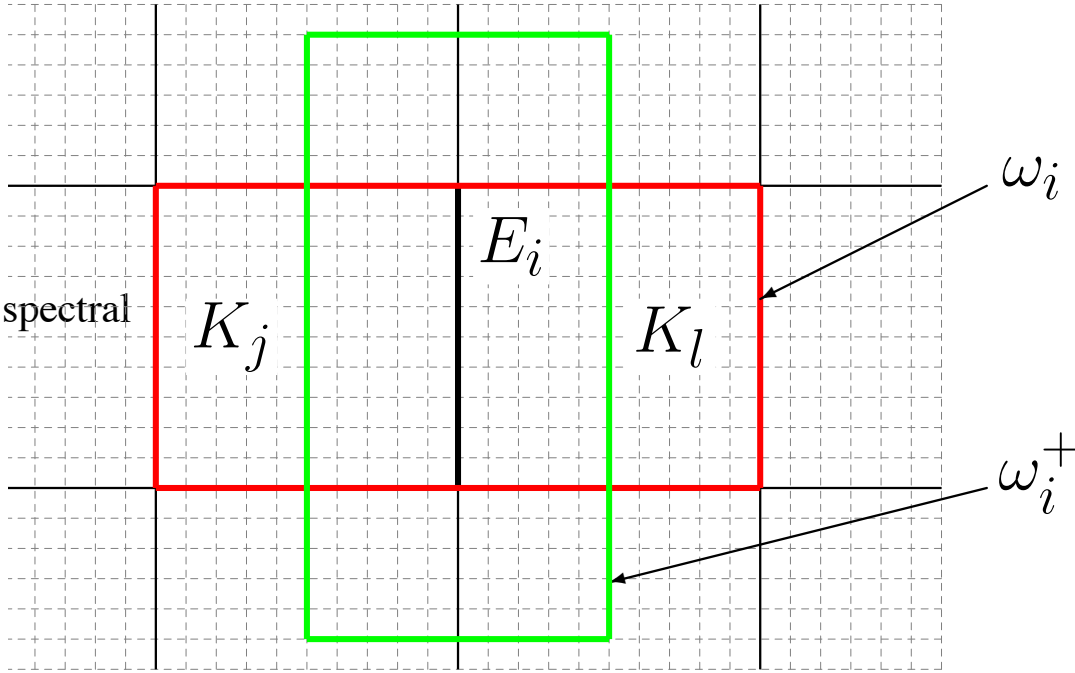


Error~7%

Mixed GMsFEM. Oversampling.

- Oversampling is important to reduce the degrees of freedom.

1. We generate "harmonic snapshots" in ω_i^+
2. Use their traces on E_i and perform a local spectral decomposition
3. Extend the dominant traces to ω_i



For problems with scale separation, the snapshots in the neighborhood of E_i have a low dimensional structure.

$$\nabla_x \hat{u}_\varepsilon(x) \approx \nabla_x u_0(x) + \nabla_y N\left(x, y\right) \cdot \nabla_x u_0$$

Oversampling results

periodic

Coarse grid	10×10		20×20	
dof per E	Oversampling	w/o oversampling	Oversampling	w/o oversampling
1	0.0324	0.3422	0.0573	0.6733
2	0.0294	0.0222	0.0283	0.0057
3	0.0214	0.0214	0.0068	0.0054
4	0.0214	0.0214	0.0056	0.0054

Non-periodic

	Oversampling		w/o oversampling	
dof per E	Err wrt fine	Err wrt snapshot	Err wrt fine	Err wrt snapshot
1	0.1336	0.1333	0.7640	0.7718
2	0.0400	0.0345	0.0991	0.0979
3	0.0234	0.0106	0.0593	0.0561
4	0.0213	0.0046	0.0407	0.0353

Adaptive strategy

• The multiscale basis functions are added in each coarse region using an error indicator

Adaptive enrichment: Choose $0<\theta<1$.

1. Find $u_{ms}^{m} \in V_{off}^{m}$, $a(u_{ms}^{m}, v)=(f,v)$, $\forall v \in V_{off}^{m}$
2. For each coarse region ω_i compute

$$\eta_i^2 = \begin{cases} \| Q_i \|^2 \, (k_{\min,i} \lambda_{l_i+1}^{\omega_i})^{-1} \\ \| R_i \|^2 \, (\lambda_{l_i+1}^{\omega_i})^{-1} \end{cases}, \quad \eta_1^2 \geq \ldots \geq \eta_N^2$$

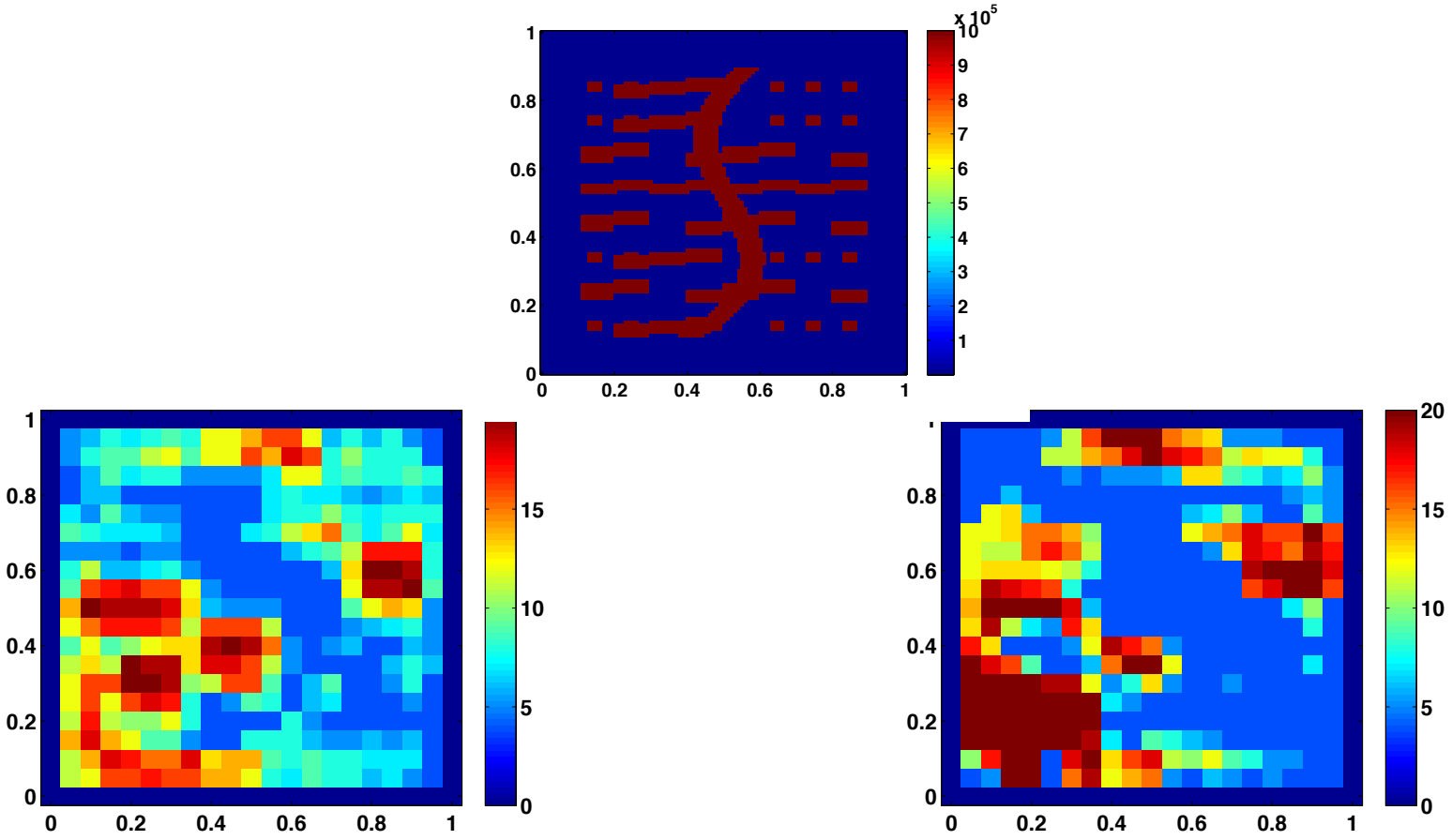
3. Choose the smallest integer k s.t., $\theta \sum_{i=1}^{N} \eta_i^2 \leq \sum_{i=1}^{k} \eta_i^2$
4. Enrich the space by adding next modes

We show (Chung, Efendiev, Li, JCP 2014)

$$\|u-u_{ms}^{m+1}\|_V^2 + c \sum_{i=1}^{N} S_{m+1}(\omega_i)^2 \leq \delta \left(\|u-u_{ms}^{m}\|_V^2 + c \sum_{i=1}^{N} S_{m}(\omega_i)^2 \right)$$

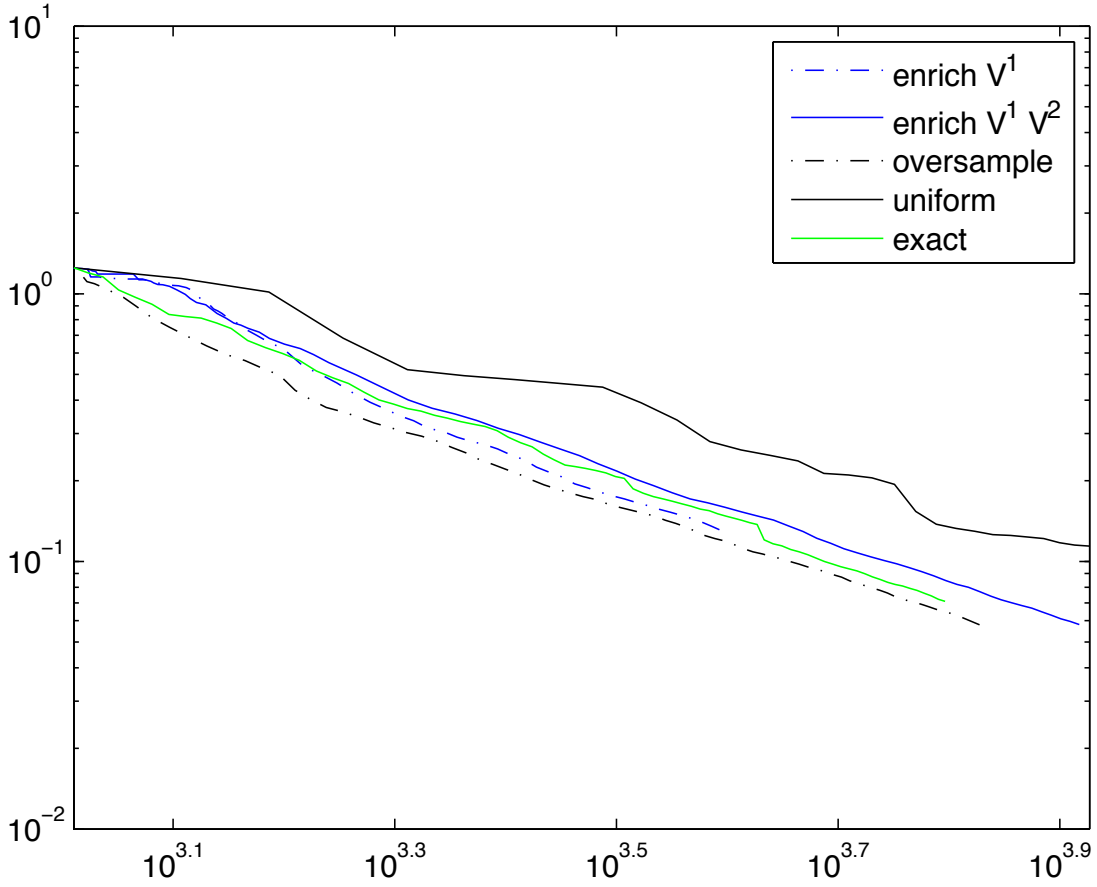
for some δ that depends on θ

Adaptive results



Dimension distributions of the offline space for theta=0.7

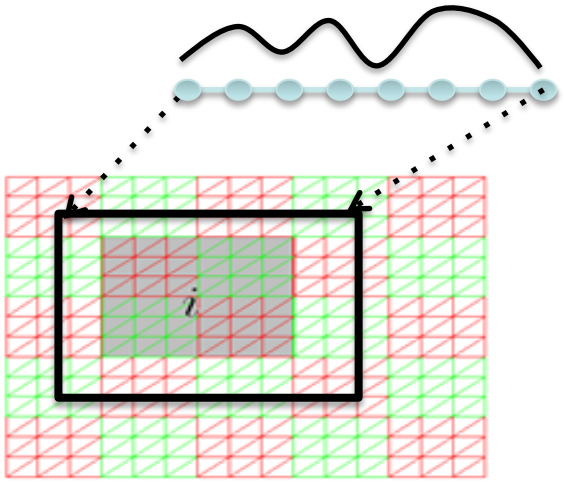
Adaptive for SIPDG discretization



Inexpensive snapshot computations

- Random boundary conditions on oversampled regions. To compute n basis, we choose n+4 snapshots

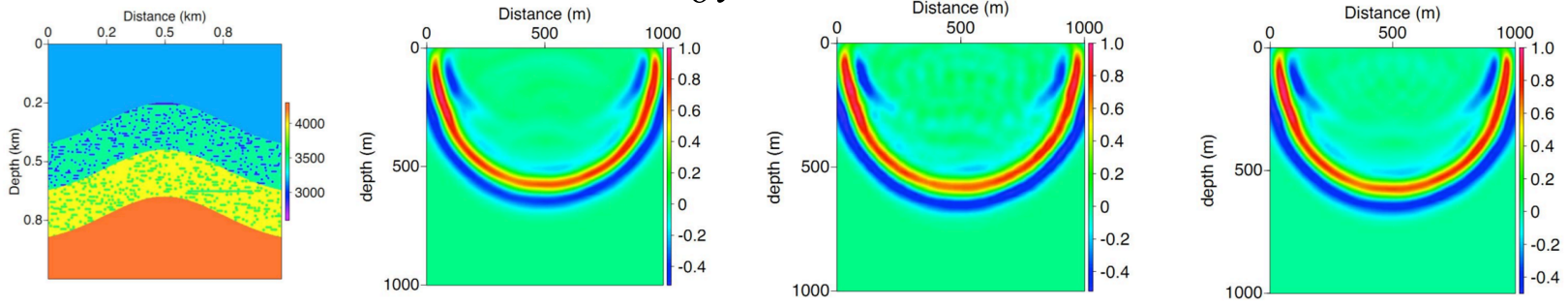
Dim	Ratio (%)	All (%)	Random (%)
536	6.81	0.71	1.33
931	9.62	0.5	0.66



- Similar (to using all snapshots) convergence rate can be shown
- More accurate non-random snapshot spaces can be designed at a higher cost
- For adaptivity, each new iterate requires computing a few extra snapshots

Some applications

- Acoustic Wave equations $\frac{\partial^2}{\partial t^2} u - \mathrm{div}(a \nabla u) = f$



- Brinkman flow $\nabla p - \mu \Delta v + k^{-1} v = f, \quad \mathrm{div}(v) = 0$
- Elasticity equations and elastic wave equations using Symmetric Interior Penalty Discontinuous Galerkin
- Applications to multilevel MC and multilevel MCMC
- Nonlinear problems (nonlinear diffusion, monotone operators). Estimating nonlinear response.
- Representing fractures on a coarse grid
- Applications to preconditioners.
- …

Nonlinear problems. Multiscale Empirical Interpolation

- The residual on the fine grid: $R(u,\nu,\mu)=0$.
- Newton method requires the calculations of Jacobians $J(u,\nu,\mu)$ and $R(u,\nu,\mu)$.
- How can we calculate the nonlinear functions without incurring the cost of the fine grid calculation in the online stage?

- Empirical Interpolation Technique (Chaturantabut and Sorensen, 2010):

  (1) Compute modes for the approximation $R(u)$

  (2) Define spatial points that can be used to approximate

  $$R(u) \approx \sum_i d_i(u)\Psi_i,$$ where $d_i(u)$'s are defined based on a few locations.

Nonlinear problems. Multiscale Empirical Interpolation using GMsFEM

- Divide the computation of nonlinear function into coarse regions

$$\mathrm{R(u)=R}\left(\sum_i z_i\phi_i\right)=\sum_i \Theta_{\omega_i}\mathrm{R}_{\omega_i}(\Phi^{\omega_i}z^{\omega_i})$$

- Multiscale POD for finding the empirical modes

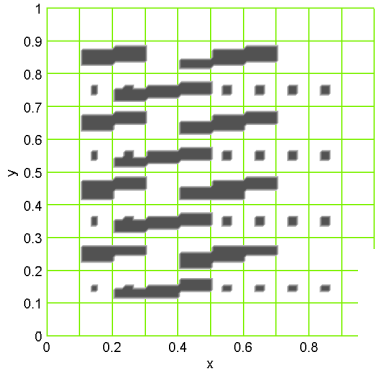
$$(\mathrm{R}_{\omega_i}^T A\mathrm{R}_{\omega_i})\Psi^{\omega_i}=\Lambda(\mathrm{R}_{\omega_i}^T M\mathrm{R}_{\omega_i})\Psi^{\omega_i}$$

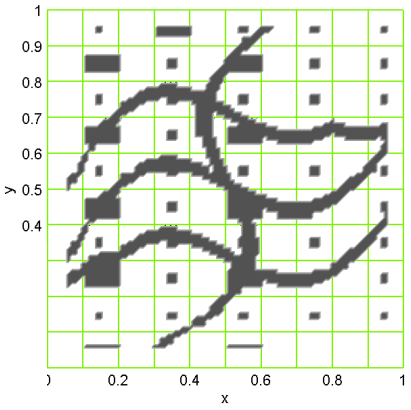
for A and M that depend on multiscale conductiviy field.

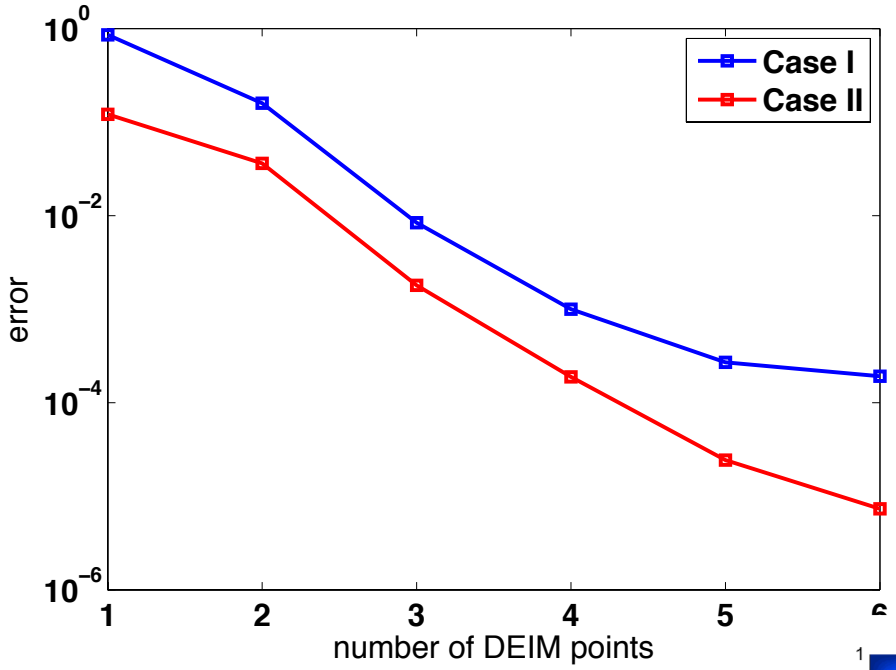
- Evaluate the contribution of nonlinear function in each coarse region inexpensively

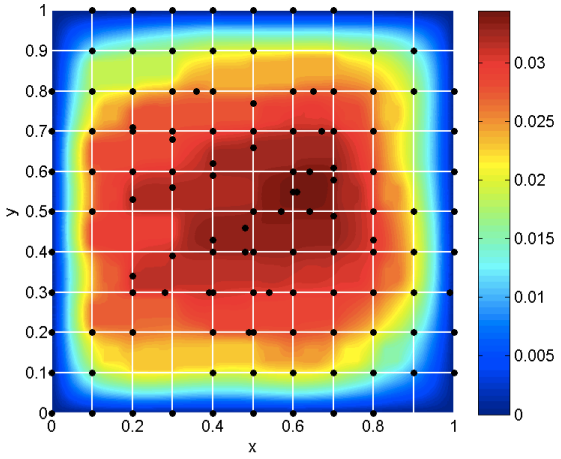
$$\mathrm{R}_{\omega_i}(\Phi^{\omega_i}z^{\omega_i})\approx\Psi^{\omega_i}d(z^{\omega_i})$$

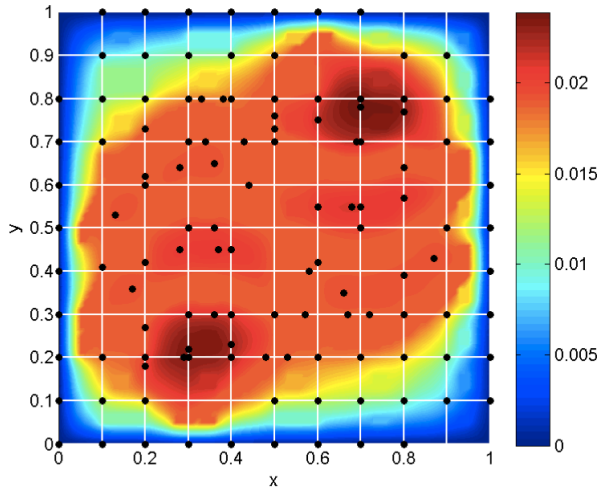
Numerical Result











Conclusions and current work

- Local multiscale methods.
- Generalized MsFEM. Oversampling. Examples
- Mixed, Discontinuous Galerkin,…
- Nonlinear problems
- Aposteriori error estimates
- Applications to two-phase, wave equations, Brinkman,..

Collaborators

- V. Calo (KAUST)
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Thank You !
Questions?