# Multiscale Model Reduction to High-contrast Heterogeneous Flow Problems

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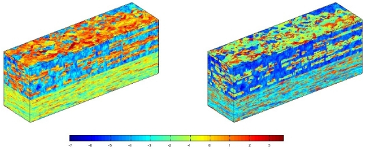
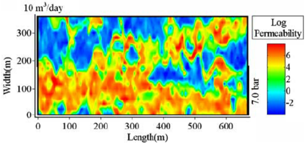
# Background

- Applications, e.g., subsurface flows, heat and mass transfer and filtration process, contain multiple scales and physical properties that vary over orders of magnitude and exhibit uncertainties
- Classical numerical approaches are infeasible or computationally inefficient *due to scale disparity!*



*https://www.sintef.no/projectweb/geoscale*




*Firoozabadi et al, computational geosciences, 2009*

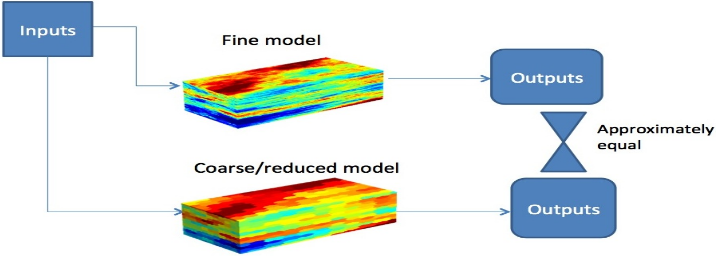
# Motivation

## Strategy

Solve the problem on the coarse-scale (affordable computational cost) with a certain accuracy.

## No free lunch!

Obtain the coarse-scale basis functions with fine-scale approximation properties, i.e., identify appropriate local problems.



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# Brief literature on multiscale methods

1. Homogenization theory *Sanchez-Plencia 80* periodic scale separable
2. Partition of Unity method (PUM) *Babuska, Caloz & Osborn, 94*
   • Generalized Finite Element Method (GFEM) *Strouboulis, Babuska & Copps 00* low contrast
3. Multiscale Finite Element methods (MsFEM) *Hou & Wu 97* scale separable, low contrast
4. Variational Multiscale methods (VMS) *Hughes 98* low contrast, expensive
   • Localized Orthogonal Decomposition (LOD) *Målqvist & Peterseim 13*
5. Heterogeneous Multiscale Methods (HMM) *E & Engquist 03* scale separable macroscale
6. Flux norm approach *Berlyand & Owhadi 10* low contrast, expensive
   • Localized version *Owhadi & Zhang 11*
7. Generalized Multiscale Finite Element methods (GMsFEM) *Efendiev, Galvis & Hou 13*
8. ...

# GMsFEM

*Efendiev, Galvis & Hou 13* **Efendiev, IL15.3, ICM 14**

**Offline computations:**

Step 1 Coarse grid generation.

Step 2 Construction of snapshot space that will be used to compute an offline space.

Step 3 Construction of a small dimensional offline space by performing dimension reduction in the space of local snapshots.

**Online computations:** *for parameter-dependent problems only!*

Step 1 For each input parameter, compute multiscale basis functions. (for parameter-dependent cases only)

Step 2 Solution of a coarse-grid problem for any force term and boundary condition.

# Local snapshot bases construction

- **Local spectral bases**

$$\begin{cases} -\nabla \cdot (\kappa \nabla \psi_\ell^{\text{snap}}) = \tilde{\kappa} \lambda_\ell^{-1} \psi_\ell^{\text{snap}} & \text{in } \omega_i \\ \dfrac{\partial}{\partial n} \psi_\ell^{\text{snap}} = 0 & \text{on } \partial\omega_i \end{cases}$$

Pros: Good approximation property • Cons: expensive, not available for every problem

- **Harmonic extension bases**

$$\begin{cases} -\nabla \cdot (\kappa \nabla \psi_\ell^{\text{snap}}) = 0 & \text{in } \omega_i \\ \psi_\ell^{\text{snap}} = \delta_\ell^k & \text{on } \partial\omega_i \end{cases}$$

Pros: very general and available for every problem • Cons: expensive

# Randomized snapshots

*Carlo, Efendiev, Galvis & **GL**, Multiscale Modeling & simulation 16*

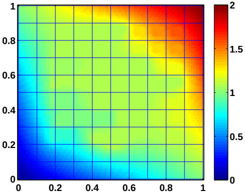
- Motivation: In many applications, the solution lives in a very low-dimensional manifold
- Technique: Randomized algorithm *Martinsen, Rockhlin & Tygert 06*
- Randomized snapshots

$$\begin{cases} -\nabla \cdot (\kappa \nabla \psi_\ell^{\text{rsnap}}) = 0 & \text{in } \omega_i \\ \psi_{\ell,\omega_i}^{\text{rsnap}} = r_\ell & \text{on } \partial\omega_i \end{cases}$$

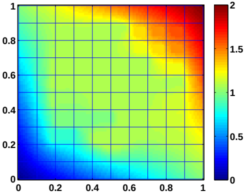
$r_\ell$ are i.i.d. standard Gaussian random vectors on the fine-grid nodes of the boundary

$$\int_D \kappa |\nabla(u - u_H)|^2 \preceq \left(\Lambda_* + (\Lambda_*)^2 \left(\left\|\mathcal{H}^{(-1)}\mathcal{S}\right\| + 1\right)^2\right) \int_D \kappa |\nabla u|^2 + H^2 \int_D f^2$$

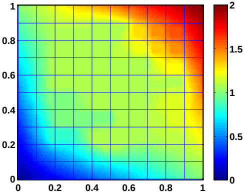
| dim($V_{\text{off}}$) | snapshot ratio (%) | all snapshots (%) | | using the randomized snapshots (%) | |
|---|---|---|---|---|---|
| | | $L^2_\kappa(D)$ | $H^1_\kappa(D)$ | $L^2_\kappa(D)$ | $H^1_\kappa(D)$ |
| 526 | 8.65(15.38) | 0.71 | 20.98 | 1.33(0.80) | 33.76(24.14) |
| 931 | 13.46 | 0.51 | 17.33 | 0.66 | 21.67 |
| 1336 | 18.27 | 0.45 | 15.83 | 0.53 | 18.26 |
| 1741 | 23.08 | 0.40 | 14.66 | 0.48 | 17.13 |
| 2146 | 23.88 | – | – | 0.43 | 15.39 |




Fine-scale




Coarse-scale, full




Coarse-scale, randomized

# Adaptive GMsFEM

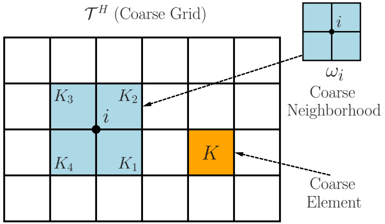
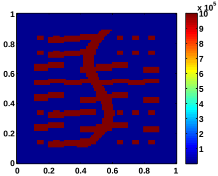



illustration of neighborhoods and elements subordinated to the coarse discretization.
$i$—the i-th coarse node.




$$-\mathrm{div}\big(\kappa(x)\,\nabla u\big) = f \quad \text{in} \quad D,$$

$\kappa(x)$–multiple scales and high contrast.
$H^{-1}$ – *based* residual for each coarse node $i$.

$$R_i(v) = \int_{\omega_i} fv - \int_{\omega_i} a\nabla u_{\text{ms}} \cdot \nabla v.$$

According to the Riez representation theorem, $\|R_i\|_{V_i^*} = \|z_i\|_{V_i}$, where $z_i$ is defined

$$\int_{\omega_i} a\nabla z_i \cdot \nabla v = R_i(v), \quad \text{for all} \quad v \in V_i.$$

$V_i = H_0^1(\omega_i)$ and $\|v\|_{V_i} = (\int_{\omega_i} \kappa(x)\nabla v \cdot \nabla v\, dx)^{\frac{1}{2}}$.

*Chung, Efendiev & **GL**, J. Comput. Phys., 2014.*

## SOLVE→ ESTIMATE→ MARK→ ENRICH

Choose $0 < \theta < 1$. For each $m = 1, 2, \cdots$,

Step 1: Find the solution in the current space. That is, find $u_{\text{ms}}^m \in V_{\text{off}}^m$ such that

$$a(u_{\text{ms}}^m, v) = (f, v) \quad \text{for all } \; v \in V_{\text{off}}^m.$$

Step 2: Compute the local residual. For each coarse region $\omega_i$, we compute

$$\eta_i^2 = \|R_i\|_{V_i^*}^2 \lambda_{l_i^m+1}^{\omega_i},$$

and we re-enumerate them in the decreasing order, that is, $\eta_1^2 \geq \eta_2^2 \geq \cdots \geq \eta_N^2$.

Step 3: Find the coarse region where enrichment is needed. We choose the smallest integer $k$ such that

$$\theta \sum_{i=1}^{N} \eta_i^2 \leq \sum_{i=1}^{k} \eta_i^2.$$

Step 4: Enrich the space.

Let $V$ be the fine scale space. We recall that the fine scale solution $u$ satisfies

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

and the multiscale solution $u_{\text{ms}}$ satisfies

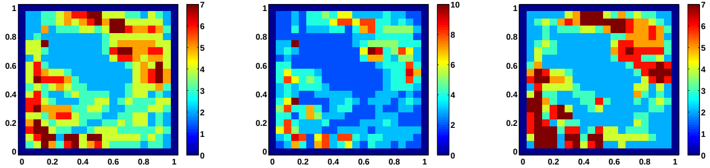
$$a(u_{\text{ms}}, v) = (f, v) \quad \text{for all} \quad v \in V_{\text{off}}$$

$$\|u - u_{\text{ms}}\|_V^2 \leq C_{\text{err}} \sum_{i=1}^{N} \|R_i\|_{V_i^*}^2 \lambda_{\ell_i+1}^{\omega_i}$$

$$\|u - u_{\text{ms}}^{m+1}\|_V^2 + \frac{\tau}{1+\tau\delta L_2} \sum_{i=1}^{N} S_{m+1}(\omega_i)^2 \leq \varepsilon\Big(\|u - u_{\text{ms}}^{m}\|_V^2 + \frac{\tau}{1+\tau\delta L_2} \sum_{i=1}^{N} S_m(\omega_i)^2\Big)$$

$$\varepsilon = \max(1 - \frac{\theta^2}{L_1(1+\tau\delta L_2)}, \frac{2C_{\text{err}}}{\tau L_1} + \rho)$$

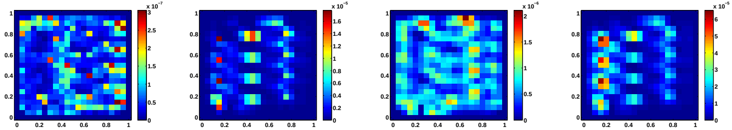
# Comparison with exact error indicator



(a) Proposed indicator with $\theta = 0.7$

(b) Proposed indicator with $\theta = 0.2$

(c) Exact indicator with $\theta = 0.7$



(d) Proposed indicator with the last offline space

(e) Proposed indicator with an intermediate of-

(f) Exact indicator with the last offline space

(g) Exact indicator with an intermediate offline

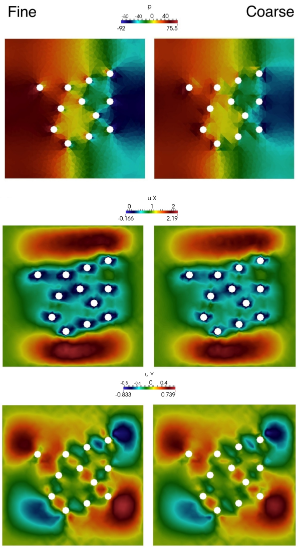
# Comparison and relative errors

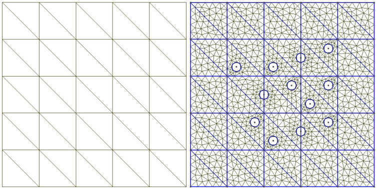
| $\dim(V_{\text{off}})$ | $\lVert u - u_{\text{off}} \rVert$ (%) | | $\lVert u_{\text{snap}} - u_{\text{off}} \rVert$ (%) | |
|---|---|---|---|---|
| | $L^2_\kappa(D)$ | $H^1_\kappa(D)$ | $L^2_\kappa(D)$ | $H^1_\kappa(D)$ |
| 802 | 0.87 | 20.15 | 0.87 | 19.94 |
| 868 | 0.83 | 16.51 | 0.83 | 16.26 |
| 979 | 0.33 | 12.62 | 0.33 | 12.30 |
| 1106 | 0.32 | 10.44 | 0.32 | 10.05 |
| 1410 | 0.10 | 7.43 | 0.10 | 6.87 |

Table: history for spectral basis with $\theta = 0.7$ and 5 iterations. The snapshot space has dimension 3690 giving 0.01% and 2.84% weighted $L^2$ and weighted energy errors. When using 5 basis per interior coarse node, the weighted $L^2$ and the weighted energy errors will be 0.09% and 7.40%, respectively, and the dimension of offline space is 1885.

# Applications

1. Homogenization of high-contrast Brinkman flow *Brown, Efendiev,* **GL***& Savatorova, Multiscale Modeling & Simulation, 2015.*
2. Nonlinear heterogeneous high-contrast elliptic flows *Efendiev, Galvis,* **GL***& Presho, Commun. Comput. Phys., 2014.*
3. High-contrast heterogeneous Brinkman flow *Galvis,* **GL***& Shi, J. Comput. Appl. Math. 2015.*
4. Hierarchical multiscale modeling for flows in fractured media *Efendiev, Lee,* **GL***, Yao, Zhang, GEM, 2015.*
5. Heterogeneous perforated media *Chung, Efendiev,* **GL***& Vasilyeva, Applicable Analysis, 2015.*
6. Sparse GMsFEM *Chung, Efendiev, Leung &* **GL***, INT J MULTISCALE COM, 2016.*



| $N_b^p$ | dim | velocity error $L^2$ | pressure error $L^2$ |
|---|---|---|---|
| number of velocity basis, $N_b^u = 12$ | | | |
| 1 | 2190 | 0.25 | 0.36 |
| 2 | 2340 | 0.18 | 0.24 |
| 4 | 2640 | 0.11 | 0.13 |
| 8 | 3240 | 0.08 | 0.09 |
| number of velocity basis, $N_b^u = 16$ | | | |
| 1 | 2870 | 0.22 | 0.45 |
| 2 | 3020 | 0.16 | 0.32 |
| 4 | 3320 | 0.09 | 0.19 |
| 8 | 3920 | 0.05 | 0.11 |
| 12 | 4520 | 0.05 | 0.11 |

# Fundamental issue

**Question:** How to construct the local problems, and why the corresponding local solutions are capable of characterizing the local solution space?

• local solvers: highest order operator coupled with all possible boundary data *Efendiev, Galvis,* **GL***& Presho 14* randomized snapshots *Carlo, Efendiev, Galvis &* **GL***16* local spectral bases, etc.

$$\begin{cases} -\nabla \cdot (\kappa \nabla \psi_\ell^{\text{snap}}) = 0 & \text{in } \omega_i \\ \psi_\ell^{\text{snap}} = \delta_\ell^k & \text{on } \partial\omega_i \end{cases}$$

Consequently, the local snapshot space is generated.

• approximation property: measured by **Komolgrov n-width** *Pinkus 1985, Pietsch 1987, Bebedorf & Hackbusch 03* — 'worst case optimal approximation space' *Wozniakowiski, 85*

Given a tolerance $\delta > 0$, we aim at finding a linear subspace $X_N \subset V := H_0^1(D)$ of dimension $N$, dependent of $\delta$, satisfying

$$d_N(\mathcal{S}(W); V) := \sup_{u \in \mathcal{U}} \inf_{v \in X_N} \|u - v\|_{H^1_\kappa(D)} \leq C\delta,$$

where $C$ denotes a constant independent of $N$, $\mathcal{S} := \mathcal{L}^{-1}$ and $W = L^2(D)$.

• $d_N(\mathcal{S}(W); V) = \sqrt{\lambda_{N+1}}$

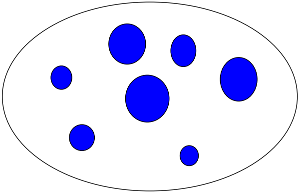
# model

**GL**, *2017: submitted*

Let $\mathcal{L} : H_0^1(D) \to L^2(D)$ be defined by

$$\mathcal{L}u := -\nabla \cdot (\kappa \nabla u) = f \qquad \text{in } D$$
$$u = 0 \qquad \text{on } \partial D.$$

- $\kappa$ low-contrast, then $\lambda_n = \mathcal{O}(n^{-\frac{2}{d}})$—algebraic decay rate *Li & Yau, Acta Math 1986*
- contrast increases, then the estimate above will become inaccurate!



# Motivation

## Proposition (GL, 2017)

*Let $D_i := B(O_i, \epsilon_i)$ and $v \in V$. If $v = \sin k_i\theta$ on the interface $\Gamma_i$, where $k_i \in \mathbb{N}_+$ and $i = 1, \cdots, m$, then*

$$R(v) := \frac{\int_D v^2 \mathrm{d}x}{\int_D \kappa |\nabla v|^2 \mathrm{d}x} \leq \frac{1}{\pi \sum_{i=1}^{m} k_i \eta_{min}}$$

$$V := V_m \oplus V^h \oplus V^b \oplus V_0^b$$

$$V_m = \mathrm{span}\{w_1, w_2, \cdots, w_m\}$$

$$V^h = \{v \in V : -\Delta v = 0 \text{ in } D_i \text{ and } \int_{\Gamma_i} \frac{\partial}{\partial n_i^+} v = 0, \text{ for } i = 1, 2, \cdots, m\}$$

$$V^b = \{v \in V : v = 0 \text{ in } \bar{D}_0\}$$

$$V_0^b = \{v \in V : v = 0 \text{ in } \bar{D}_i \text{ for } i = 1, 2, \cdots, m\}$$

# Lower bound in $V_m$

$$\begin{cases} -\Delta w_i = 0 & \text{in } D_0 \\ w_i = \delta_{ik} & \text{on } \Gamma_k, k = 1, 2, \cdots, m \\ w_i = 0 & \text{on } \partial D \end{cases}$$

**Theorem (GL, *2017*)**

*For $i = 1, 2, \cdots, m$, there holds*

$$R(w_i) \geq \begin{cases} [\pi(1 + 2\frac{\epsilon_i}{\delta_i})]^{-1}|D_i| & \textit{if } d = 2 \\ [\frac{4}{3}\pi(\delta_i + 3\epsilon_i + 3\frac{\epsilon_i^2}{\delta_i})]^{-1}|D_i| & \textit{if } d = 3 \end{cases}$$

# Upper bounds in $V^b$ and $V^h$

Poincaré inequality in each inclusion and the asymptotic extension yield

$$R(v) \leq \max_i \{\eta_i^{-1} C_{\text{poin}}(D_i)\} \qquad \text{for } v \in V^b$$

$$R(v) \leq \frac{1}{\pi \sum_{i=1}^{m} k_i \eta_{\min}} \qquad \text{for } v \in V^h$$

However, little is known for $R(v)$ with $v \in V_0^b$! *Cioranescu & Murat 82; Tartar, 09*

- $\epsilon_i \ll \delta_i$ and $\epsilon_i \to 0$, then $C_{\text{poin}}(D_0) \approx C_{\text{poin}}(D)$ *algebraic decay rate!*
- Periodic case and $\epsilon_i \to 0$, then $C_{\text{poin}}(D_0) \lesssim \epsilon_i^2$ *spectral gap!*

# Spectral gap under certain assumption

**Proposition (GL, 2017)**

*Assume that*

$$C_{poin}(D_0) \ll \min\{R(w_i)\}.$$

*Then it holds*

$$d_i(\mathcal{S}(W); V) \begin{cases} \geq \sqrt{\dfrac{|D_{i+1}|}{\pi}} & i \leq m-1 \\ \lesssim \eta_{min}^{-\frac{1}{2}}(C_{poin}(D) + \max\{C_{poin}(D_j)\}) & i = m. \end{cases}$$

# Future work

- Extend the classical homogenization theory to scale non-separable problems; seek for a more general assumption and a sharp convergence rate
- Derive the eigenvalue decay rate of the elliptic operators with $L^\infty$ coefficient

## Questions

Thank you for your attention!