

Survey of new continuum numerical multiscale approaches and limitations

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Outline

- 1 Review: finite element method(s) for elliptic problems
 - Variational approach (conforming FE) and discretization
 - Numerical implementation and solving a linear system
 - Variational approach (mixed FE) and discretization
 - FE for multiscale problems: issues
- 2 Effective and upscaled coefficients
 - Use multigrid/multilevel approaches
 - Homogenization based methods
 - Upscaling by averaging or pressure-based
- 3 Survey of Multiscale FE methods for elliptic problems
 - MsFEM
 - Heterogeneous multiscale FEM
 - Variational and subgrid multiscale FEM
 - Mortar methods
- 4 Non-elliptic and/or nonlinear problems
 - Reconstruction and downscaling
 - Double-porosity approaches for parabolic problems
 - Methods of moments, pseudo-functions for transport problems
- 5 Recap and references

Model problem

Second order elliptic PDE on an open bounded $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$,
 $\mathbf{K} = \mathbf{K}^T$, $\mathbf{K} = \mathbf{K}(x)$ bounded, strictly elliptic: $\lambda_{\min}(x) \geq \lambda_0 > 0$

$$\begin{cases} -\nabla \cdot \mathbf{K} \nabla p = f, & x \in \Omega \\ p = 0, & x \in \partial\Omega \end{cases} \iff \begin{array}{l} A p = f \\ X, Y \text{ are Banach (Hilbert) spaces} \\ A : X \mapsto Y \text{ or } A : X \mapsto Y' \end{array}$$

- Sobolev spaces $H^m(\Omega)$, $m \geq 0$, ($\mathbf{K} \in C^1(\bar{\Omega})$, $\partial\Omega$ is C^2 smooth)

$$\underbrace{-\nabla \cdot \mathbf{K} \nabla}_A : H^{m+2}(\Omega) \cap H_0^1(\Omega) \mapsto H^m(\Omega), m \geq 0$$

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- a weaker notion ($\mathbf{K} = \mathbf{K}(x)$ can be discontinuous, $\partial\Omega$ is polygonal)

$$A : H_0^1(\Omega) \mapsto H^{-1}(\Omega)$$

- Sobolev spaces $W^{m,p}$, $1 \leq p < \infty$, when $\mathbf{K} = \mathbf{K}(x, \Theta)$ or is degenerate (also for transient problems)

Weak (variational) formulation and FE formulation

Use smooth $q : q|_{\partial\Omega} = 0$, integrate by parts $-\nabla \cdot \mathbf{K}\nabla p = f$,
use $p|_{\partial\Omega} = 0$ to get

$$\int_{\Omega} \mathbf{K}(x) \nabla p(x) \nabla q(x) dx = \int_{\Omega} f(x) q(x) dx,$$

Abstract setting

Define $V := H_0^1(\Omega)$, $a(p, q) := \int_{\Omega} \mathbf{K}\nabla p \nabla q dx$, $(f, q) := \int_{\Omega} f q dx$.

Find $p \in V : a(p, q) = (f, q), \forall q \in V$

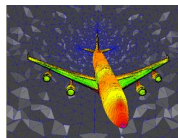
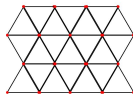
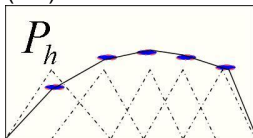
Theory: $\exists! p$: continuously depending on the data f, \mathbf{K}, Ω .

FE for the model elliptic problem

(D) PDE and b.c $-\nabla \cdot \mathbf{K} \nabla p = f, p|_{\partial\Omega} = 0$

(V): weak form: $a(p, q) = (f, q), \forall q \in V$

- Partition $\bar{\Omega}_h = \bigcup_{T \in \mathcal{T}_h} \bar{T} \approx \bar{\Omega} \subset \mathbb{R}^d$ into elements T : segments (1D) or triangles/quadrilaterals (2D), tetrahedra/prisms/bricks (3D)



- Define local polynomial basis (globally $C^0(\Omega)$ only) of degree $k = 1, 2, \dots$ for space $V_h^k(\Omega)$

(FE) Finite element solution:

find $p_h \in V_h^k$: $a(p_h, q_h) = (f, q_h), \forall q_h \in V_h^k$

Error analysis

- $a(\cdot, \cdot)$ continuous: $a(p, q) \leq C \|p\|_V \|q\|_V$
- $a(\cdot, \cdot)$ elliptic: $a(u, u) \geq \alpha_0 \|u\|_V^2$
- Conforming FE: $V_h \subsetneq V$ (nonconforming \approx variational crimes)
- Galerkin orthogonality $a(p - p_h, v_h) = 0$
- Céa's lemma $\|p - p_h\|_V \leq \inf_{q_h \in V_h} \|p - q_h\|_V$
- Interpolation estimate(s) $\|u - I_h u\|_V \leq Ch \|u\|_{H^2(\Omega)}$

lead to ...

$$\|p - p_h\|_{H^1(\Omega)} \leq Ch \|p\|_{H^2(\Omega)}$$

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lead to ...

$$\|p - p_h\|_{H^1(\Omega)} \leq Ch \|p\|_{H^2(\Omega)}$$

- use of Aubin-Nitzche duality “trick” based on $\|p\|_{H^2(\Omega)} \leq \|f\|_{L^2(\Omega)}$:

$$\|p - p_h\|_{L^2(\Omega)} \leq Ch^2 \|p\|_{H^2(\Omega)}$$

Finding p_h : implementation

Use $\{\phi_1(\mathbf{x}), \dots, \phi_{N_h}(\mathbf{x})\}$ as the (piecewise polynomial) basis for V_h^k

Write $p_h = \sum_i p_i \phi_i(\mathbf{x})$ and $p_h \equiv \mathbf{P} = (p_i)_{i=1}^{N_h}$

(FE) Finite element solution $p_h \equiv \mathbf{P}$

$$a(p_h, q_h) = (f, q_h), \forall q_h \in V_h^k \leftrightarrow \sum_i p_i a(\phi_i, \phi_j) = (f, \phi_j), \forall j$$

Note: the system $\mathbf{AP} = \mathcal{F}$ has dimension N_h .

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Note: the system $\mathbf{AP} = \mathcal{F}$ has dimension N_h .

In practice the matrix entries $A_{ij} := a(\phi_i, \phi_j) = \int_{\Omega} \mathbf{K}(\mathbf{x}) \nabla \phi_i(\mathbf{x}) \nabla \phi_j(\mathbf{x}) dA = \sum_T \int_T \mathbf{K}(\mathbf{x}) \nabla \phi_i(\mathbf{x}) \nabla \phi_j(\mathbf{x}) dA$

are computed approximately using numerical integration (quadrature): $A_{ij} \approx \sum_T (\int_T \mathbf{K}(\mathbf{x}) \nabla \phi_i(\mathbf{x}) \nabla \phi_j(\mathbf{x}) dA)_h$

Numerical implementation and solving a linear system

- **Discretize**: define Ω_h , choose V_h^k
- **Assembly** process with **quadrature**: compute for each T the approximation

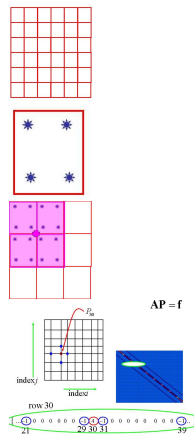
$$\int_T (\mathbf{K}(\mathbf{x}) \nabla \phi_i(\mathbf{x}) \nabla \phi_j(\mathbf{x}) dA)_h := \sum_m w_m \mathbf{K}(\mathbf{x}_m) \nabla \phi_i(\mathbf{x}_m) \nabla \phi_j(\mathbf{x}_m)$$

Add over all elements T adjacent to **node j** for each j (cost is $O(N_h)$)

- **Solve linear system** (\mathbf{A} is sparse spd)

$$\mathbf{A} \mathbf{p} = \mathcal{F}$$

...this requires $O(N_h^r)$ computational time $r=3$ for full GE ... to ... $r=1$ for Full Multigrid solvers,



Mixed formulation: $\mathbf{u} = -\mathbf{K}\nabla p, \nabla \cdot \mathbf{u} = f$

$W := L^2(\Omega)$ and $\mathbf{V} := \mathbf{H}(\mathbf{div}; \Omega)$. Find $\Theta := (\mathbf{u}, p) \in \mathbf{V} \times W$

$$(K^{-1}\mathbf{u}, \mathbf{v}) = (p, \nabla \cdot \mathbf{v}) - \langle g, \mathbf{v} \cdot \mathbf{n} \rangle, \quad \forall \mathbf{v} \in \mathbf{V}$$

$$(\nabla \cdot \mathbf{u}, w) = (f, w), \quad \forall w \in W$$

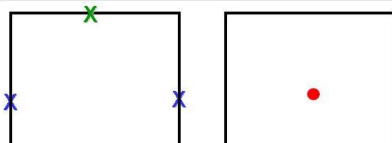
Discrete mixed formulation

$W_h \subset W, \mathbf{V}_h \subset \mathbf{V}$ are $\mathbf{RT}_{[0]}$ spaces. Find $\Theta_h := (\mathbf{u}_h, p_h) \in \mathbf{V}_h \times W_h$:

$$(K^{-1}\mathbf{u}_h, \mathbf{v}_h) = (p_h, \nabla \cdot \mathbf{v}_h) - \langle g_h, \mathbf{v}_h \cdot \mathbf{n} \rangle_{\partial\Omega}, \quad \forall \mathbf{v}_h \in \mathbf{V}_h,$$

$$(\nabla \cdot \mathbf{u}_h, w_h) = (f, w_h), \quad \forall w_h \in W_h.$$

Error estimates: $\|p - p_h\|_{L^2(\Omega)} = O(h), \quad \|\mathbf{u} - \mathbf{u}_h\|_K = O(h)$

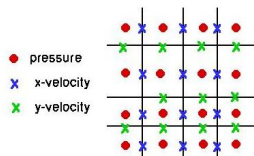


Discrete mixed $\mathbf{RT}_{[0]}$ spaces \equiv cell-centered FD

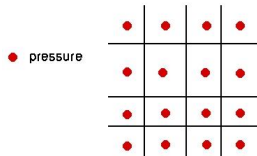
Basis functions for $\mathbf{RT}_{[0]}$ spaces [RavTho77]

$\mathbf{u}_h \in \mathbf{V}_h \subset \mathbf{V}$ are piecewise linear \times piecewise constants
 $p_h \in \mathbf{W}_h \subset \mathbf{W}$ are piecewise constants

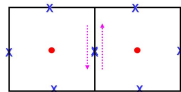
$\mathbf{u}_h \cdot \mathbf{n}$ are continuous



Equivalent to CCFD
 (up to quadrature)



$\mathbf{u}_h \cdot \mathbf{t}$ are NOT continuous



Reality of FE computations vs theory

For optimal convergence of numerical methods

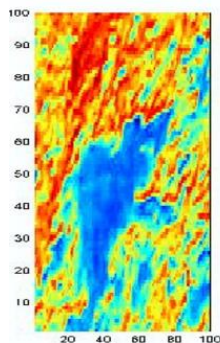
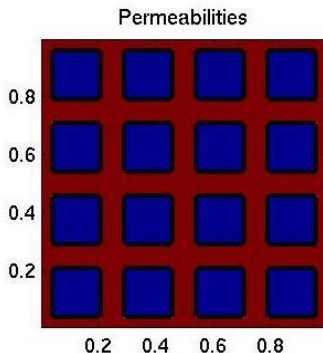
$$\| p - p_h \|_{L^2(\Omega)} \leq Ch^2 \| p \|_{H^2(\Omega)}$$

one needs (at least local) smoothness of the true solution p ... but in practice

- f, Ω possibly not smooth
- \mathbf{K} not smooth: multiscale character

What is $\mathbf{K} = \mathbf{K}(x)$ like ?

$\mathbf{K} = \mathbf{K}^T$ (permeability, conductivity, mobility,...) is in general anisotropic. Here we focus on two sources of difficulties:



two scales $K_{fast} / K_{slow} = 10^\beta, \beta \geq 1$
periodic character of \mathbf{K}

strong heterogeneity
no separation of scales ?

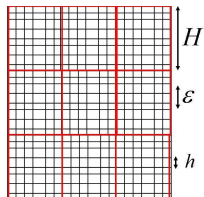
Numerical simulation: periodic multiscale case

Assume $\mathbf{K}(\mathbf{x}) = \mathbf{K}^\epsilon(\mathbf{x}) = \mathbf{K}(\mathbf{x}, \frac{\mathbf{x}}{\epsilon})$



Numerical simulation: periodic multiscale case

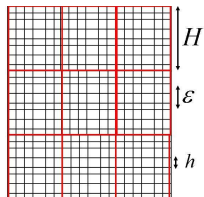
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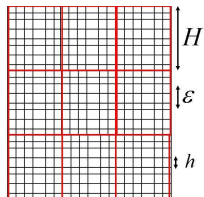
To resolve the **scales** in $\mathbf{K}(\mathbf{x})$, we need a grid with $h \ll \epsilon$.. this means solving $\mathbf{A}\mathbf{P} = \mathcal{F}$ with $O(N_h^r)$ complexity and may be prohibitively complex in $\mathbb{R}^2, \mathbb{R}^3$.^a

^aKeep in mind the big picture and solving nonlinear transient problems
 $\mathbf{K} = \mathbf{K}(\mathbf{x}, p, \nabla p)$

How not to solve with h



How not to solve with h



Some solutions and ideas when using $\epsilon < H$

- use a special linear solver technique (multigrid ?)
- find effective \mathbf{K}^*_H and solve for $p^*_H \approx p^0$
- solve for $p^*_H \approx p^0$ using multiscale FE
- if needed, recover (reconstruct) next order effects (correctors, downscaling)

Multigrid/multilevel methods

Well suited to handle large systems

$$\mathbf{A}\mathbf{P} = \mathcal{F}$$

- Standard multigrid not useful for problems with highly varying coefficients:
- Must use a special grid transfer operator (not bilinear)
- Idea: construct an effective \mathbf{K} using a special grid transfer operator [*Knapek, Moutlon, Dendy*]

Find effective \mathbf{K}^*_H by homogenization

- Homogenization formulas for \mathbf{K}^*

$$\mathbf{K}^*_{jk} = \frac{1}{|\Omega_0|} \int_{\Omega_0} K_{jk}(\mathbf{y})(\delta_{jk} + \partial_k \omega_j(\mathbf{y})) dA$$

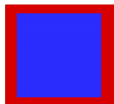
$$\begin{cases} -\nabla \cdot \mathbf{K} \nabla \omega_j(\mathbf{y}) & = \nabla \cdot (\mathbf{K} \mathbf{e}_j), \quad \mathbf{y} \in \Omega_0 \\ \omega_j & \Omega_0 - \text{periodic} \end{cases}$$

- Analytical formulas and bounds² available for special geometries only
- Finding \mathbf{K}^* numerically: for every T_H , solve a local problem with grid h for $\mathbf{K}^*_H(\mathbf{x})$
- exploit two-scale numerical FE approaches [Matache/Schwab]

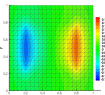
²Wiener, Matheron, Cardwell, Parsons, Torquato, Rubinstein, Hashin, Shtrikman, Dagan

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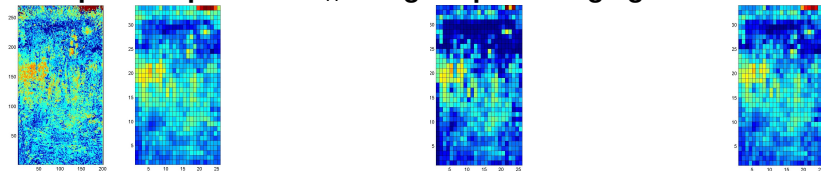
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Find an effective \mathbf{K}^*_H by upscaling

Examples of upscaled \mathbf{K}^*_H using simple averaging:

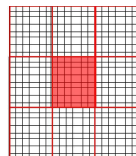


Original field \mathbf{K}_h with $h \approx 217 \times 201$, upscaled \mathbf{K}_H with $H \approx 34 \times 26$ by arithmetic, harmonic averaging, and renormalization [King]

(P)ressure based upscaling: solve

$$-\nabla \cdot \mathbf{K}^\epsilon(\mathbf{x}) \nabla w = 0, \quad \mathbf{y} \in T_H$$

$$w|_{\partial T_H} = ?$$



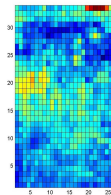
Then get $\mathbf{K}^*_H|_{T_H}$ by matching fluxes with $\langle \nabla w \rangle$.

Boundary conditions: Dirichlet (prevents crossflow) or periodic.

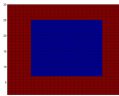
Comparison of upscaling methods

Given \mathbf{K}_h , $h \approx 34 \times 26 \dots$

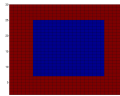
Heterogeneous case
 $\mathbf{K}_h \in [1.9, 242.2]$



Fracture cell
 $\mathbf{K}_h(\mathbf{x}) \in \{1, 1e - 2\}$



Fracture cell
 $\mathbf{K}_h(\mathbf{x}) \in \{1, 1e - 4\}$



... compute *effective* \mathbf{K}_H , $H \approx 1 \times 1$

method	heterogeneous	fracture 1e-2	fracture 1e-4
(A)rithmetic	89.5002	0.6436	0.6400
(H)armonic	79.3953	0.0273	0.000273
(R)enormalization (6x)	78.6652	0.4799	0.4703
(P)ressure based	86.5225, 81.5955	0.455825	0.446895

MsFEM

Idea: solve on scale H

incorporate ϵ -scale of $\mathbf{K}^\epsilon(\mathbf{x})$ into basis functions [Babuska, Osborn'83], [Hou, Wu'97-],[Efendiev, Hou, Wu, '00]

Given original test functions

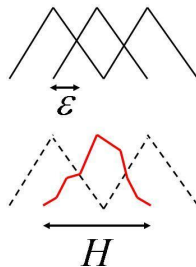
$\{\phi_1(\mathbf{x}), \dots, \phi_{N_H}(\mathbf{x})\} \dots$

solve local problem on T_H

$$-\nabla K^\epsilon(\mathbf{x}) \nabla \psi_i = 0, \quad \mathbf{y} \in T_H$$

$$\psi_i|_{\partial T_H} = \phi_i$$

Use ψ_i to construct basis for V_H .



MsFEM and oversampling

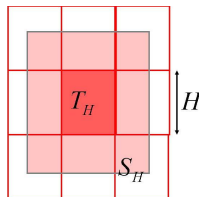
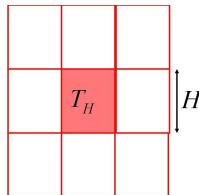
MsFEM: solve on T_H

$$-\nabla K^\epsilon(\mathbf{x}) \nabla \psi_i^T = 0, \quad \mathbf{y} \in T_H$$
$$\psi_i|_{\partial T_H} = \phi_i$$

Use ψ_i to construct basis for V_H .

Oversampling MsFEM: solve on S_H

$$-\nabla K^\epsilon(\mathbf{x}) \nabla \psi_i^S = 0,$$
$$\psi_i|_{\partial S} = \phi_i$$



Analysis of MsFEM (periodic \mathbf{K})

Error estimates [*Hou, Wu'97*],[*Efendiev, Hou, Wu, '00*]:

$$\| \boldsymbol{p} - \boldsymbol{p}_H \|_{L^2(\Omega)} \leq C(H^2 + \frac{\epsilon}{H})$$

$$\| \boldsymbol{p} - \boldsymbol{p}_H \|_{H^1(\Omega)} \leq C(H + \epsilon + \sqrt{\frac{\epsilon}{H}})$$

Difficulties:

- **Resonance effect** partially removed by oversampling.
- Efficiency ... still solving on every \mathbf{T}_H ...
- Applied in practice to non-periodic problems
- Extensions to nonlinear and transient cases [*Efendiev, Pankov*]

Also [*Chen'05, Chen, Hou'02*], for mixed FE methods.

Heterogeneous multiscale FEM

Idea: [E, Engquist'02], [Ming, Yue'03, E, Ming, Zhnag'04]

Solve with H , incorporate ϵ -scale of $\mathbf{K}^\epsilon(\mathbf{x})$ at quadrature points.

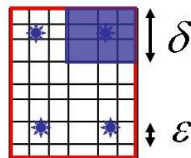
$$\int_T (\mathbf{K}(\mathbf{x}) \nabla \phi_i(\mathbf{x}) \nabla \phi_j(\mathbf{x}) dA)_h := \sum_m w_m \mathbf{K}(\mathbf{x}_m) \nabla \phi_i(\mathbf{x}_m) \nabla \phi_j(\mathbf{x}_m)$$

$$\approx \sum_m w_m \mathbf{K}_{ij}^\epsilon(\mathbf{x}_m) \nabla \hat{\phi}_i(\mathbf{x}_m) \nabla \hat{\phi}_j(\mathbf{x}_m)$$

Need to capture variation in $\mathbf{K}^\epsilon(\mathbf{x})$: solve for $\hat{\phi}$

$$-\nabla \cdot \mathbf{K}^\epsilon(\mathbf{x}) \nabla \hat{\phi} = 0, \quad \mathbf{x} \in T_\delta$$

$$\hat{\phi} - \phi \text{ periodic on } T_\delta$$



Heterogeneous multiscale FEM: analysis

- Analysis: (periodic $\mathbf{K}^\epsilon(\mathbf{x})$)

$$\|p - p_H\|_{L^2\Omega} \leq C \left(H^2 + \begin{cases} O(\epsilon), & \delta = \epsilon \\ O(\delta + \frac{\epsilon}{\delta}), & \delta > \epsilon \end{cases} \right)$$

- Special error estimates for random \mathbf{K} .

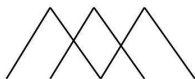
- Computational cost: smaller than using h , competitive with MsFEM.
- Extensions to nonlinear cases



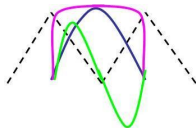
Variational and subgrid multiscale FEM

Idea of Bubbles:

provide enrichment of FE spaces [Hughes] used to stabilize convection-diffusion problems, CFD, or elasticity FE formulations, to resolve nonpolynomial behavior such as: boundary layers, numerical Green's functions



usual FE basis functions



basis functions plus bubbles

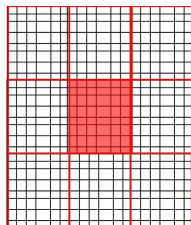
$$\text{Write } p_h = \bar{p} + p'$$

Subgrid methods for mixed FE methods [Arbogast, Keenan, Minkoff', Arbogast'00]

Idea: write $p_h = p_H + \delta p$, same for velocity variables.

Subgrid upscaling

- Write $p_h = p_H + \delta p$, $\mathbf{v}_h = \mathbf{v}_H + \delta \mathbf{v}$
- Decouple coarse problems by the closure assumptions: no flow for $\delta \mathbf{v}$ on the coarse boundaries ∂T_H .
- Use higher order FE for velocity v_H (BDDF) and lower order (RT) for δv .
- Use numerical Green's functions to precompute for influence of coarse on fine scale.

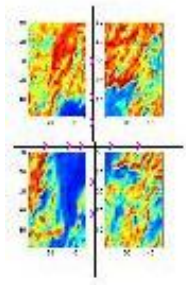


Error estimates and experiments for $\frac{H}{h}$ fixed

$$\| p - p_H \|_{L^2(\Omega)} = O(H), \quad \| \mathbf{v} - \mathbf{v}_H \|_{L^2(\Omega)} = O(H^2)$$

Recent extensions by [Aarnes et al] of Mixed MsFEM and Subgrid methods

Mortar based methods



- Complete decoupling of problems on T_H : they are connected by mortars on interfaces
- optimal convergence: a-priori analysis [ACWY'00] and a-posteriori analysis [P05], [APWY'07] available
- mortar upscaling [PWY02]
- Computational savings achieved when efficient interface solvers are available
- No reconstruction necessary: solution at grid h available
- Automatic implementation of transient nonlinear problems

Example: adaptive mortar modeling [P05]

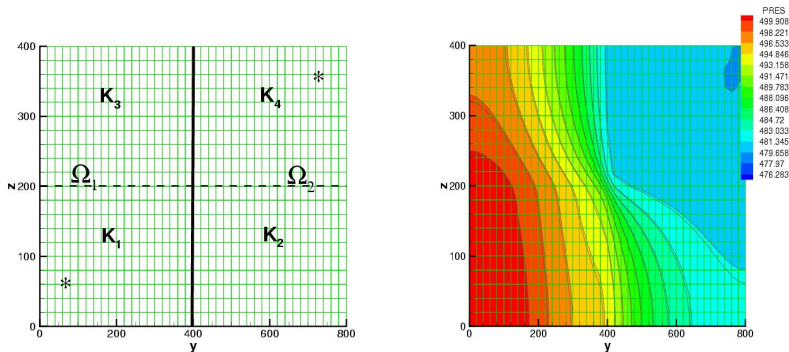
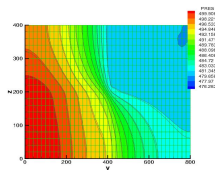
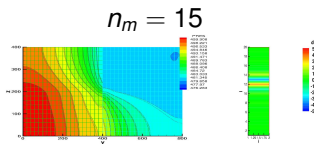
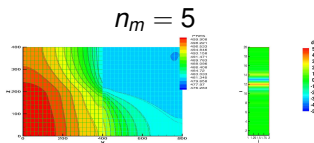
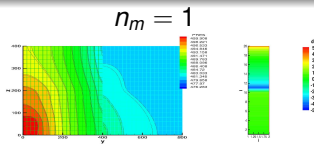


Figure: Left: $\Omega = \Omega_1 \cup \Omega_2 \cup \Gamma$. Right: solution $\Theta_h \equiv p_h$, no mortars

Results: mortars for single phase flow in porous media



Solution $\Theta_h \equiv p_h$
 (no mortars)



Solution $\tilde{\Theta}_h = \tilde{p}_h$ (with mortars). Right: $\eta_{\Gamma,*}$

Flow coupled to transport $\mathcal{F}(\Theta) = 0$ with $\Theta = (\mathbf{u}, p, c)$

Flow

$$\mathbf{u} = -\mathbf{K}\nabla p, \quad \nabla \cdot \mathbf{u} = 0$$

Diffusive-dispersive transport

$$\phi \frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u}c - \mathbf{D}(\mathbf{u})\nabla c) = 0$$

Definitions

$$\begin{aligned} \mathbf{D}(\mathbf{u}) &:= \text{diffusion} + \text{dispersion} \\ &:= d_{mol}\mathbf{I} + |\mathbf{u}|(d_{long}\mathbf{E}(\mathbf{u}) + d_{transv}(\mathbf{I} - \mathbf{E}(\mathbf{u}))). \\ \mathbf{E}(\mathbf{u}) &= \frac{1}{|\mathbf{u}|^2} u_i u_j \\ \mathbf{D}(\mathbf{u}) &\approx d_{mol}\mathbf{I} + d_{long}|\mathbf{u}|\mathbf{E}(\mathbf{u}) \end{aligned}$$

Reconstruction and downscaling

Flow coupled to transport

$$\mathbf{u} = -\mathbf{K}\nabla p, \quad \nabla \cdot \mathbf{u} = 0$$
$$\phi \frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u}c - \mathbf{D}(\mathbf{u})\nabla c) = 0$$

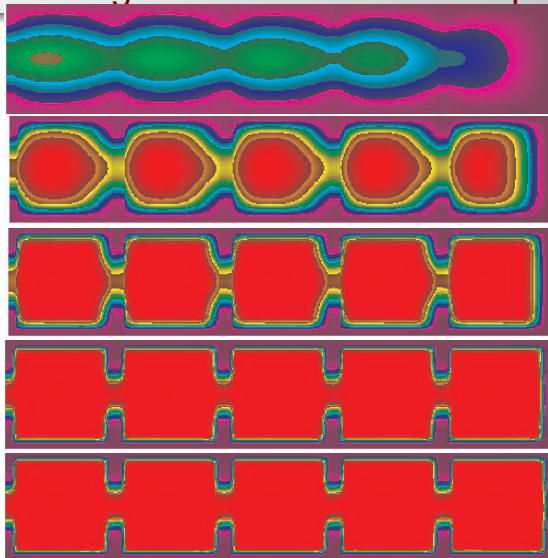
Need accurate fine scale \mathbf{u}_h !

... have to reconstruct \mathbf{u}_h from \mathbf{u}_H

Ideas

- [Oden, Vemaganti]: use the coarse solution p_H as boundary conditions for the local problem solved for p_h
- global-local upscaling [Durlafsky, Chen, Gerritsen]
- use global information [Efendiev'06,'07]

Small/large contrast diffusive-dispersive transport



Multi-phase flow problems, phases $\alpha = w, n$

$$\frac{\partial}{\partial t} \phi S_{\alpha} \rho_{\alpha} - \nabla \cdot \mathbf{K} \lambda_{\alpha} \nabla P_{\alpha} = q_{\alpha}, \quad (1)$$

$$P_n - P_w = P_c(S_w) \quad (2)$$

$$S_n + S_w \equiv 1 \quad (3)$$

Well-posedness results and character of solutions

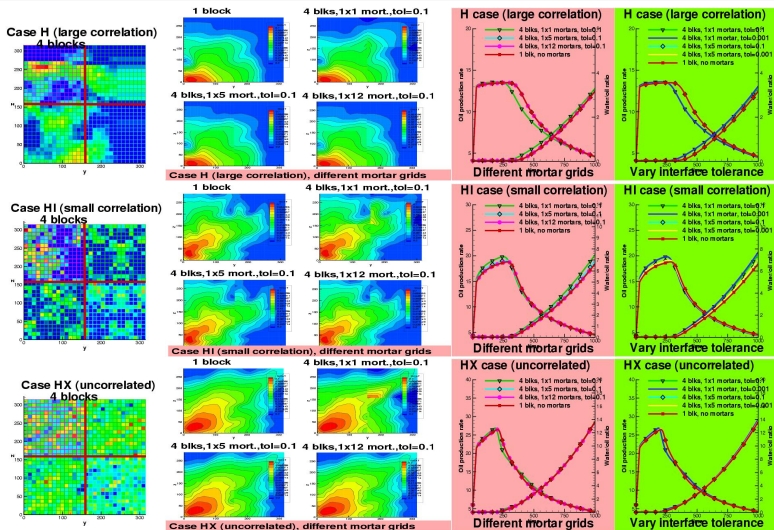
degenerate parabolic/elliptic + parabolic/hyperbolic

[altdibene, Arbogast, Chen]

Handling transient nonlinearities

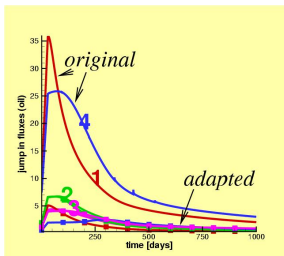
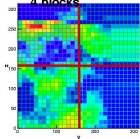
- use upscaled \mathbf{K} ; how to handle λ_{α}, P_c ? [Durlafsky et al, Trykozko and Zijl]
- if heterogeneity is \approx periodic, use homogenization [Arbogast97, Bourgeat, BourKozMik95]

Example: mortar upscaling for multi-phase flow

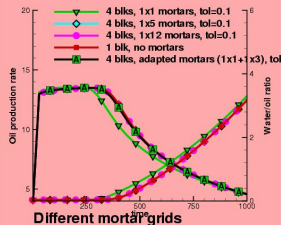


Example: mortar adaptivity [P05]

Case H (large correlation)
4 blocks



H case (large correlation) ADAPTED



Recap

- Elliptic problems with multiscale coefficients lead to large linear systems
- Multiscale FE aim to reduce computational complexity
- Not all are applicable and/or perform equally well when applied to transient coupled nonlinear problems