Multiscale Mortar Methods: Theory, Applications and Future Directions

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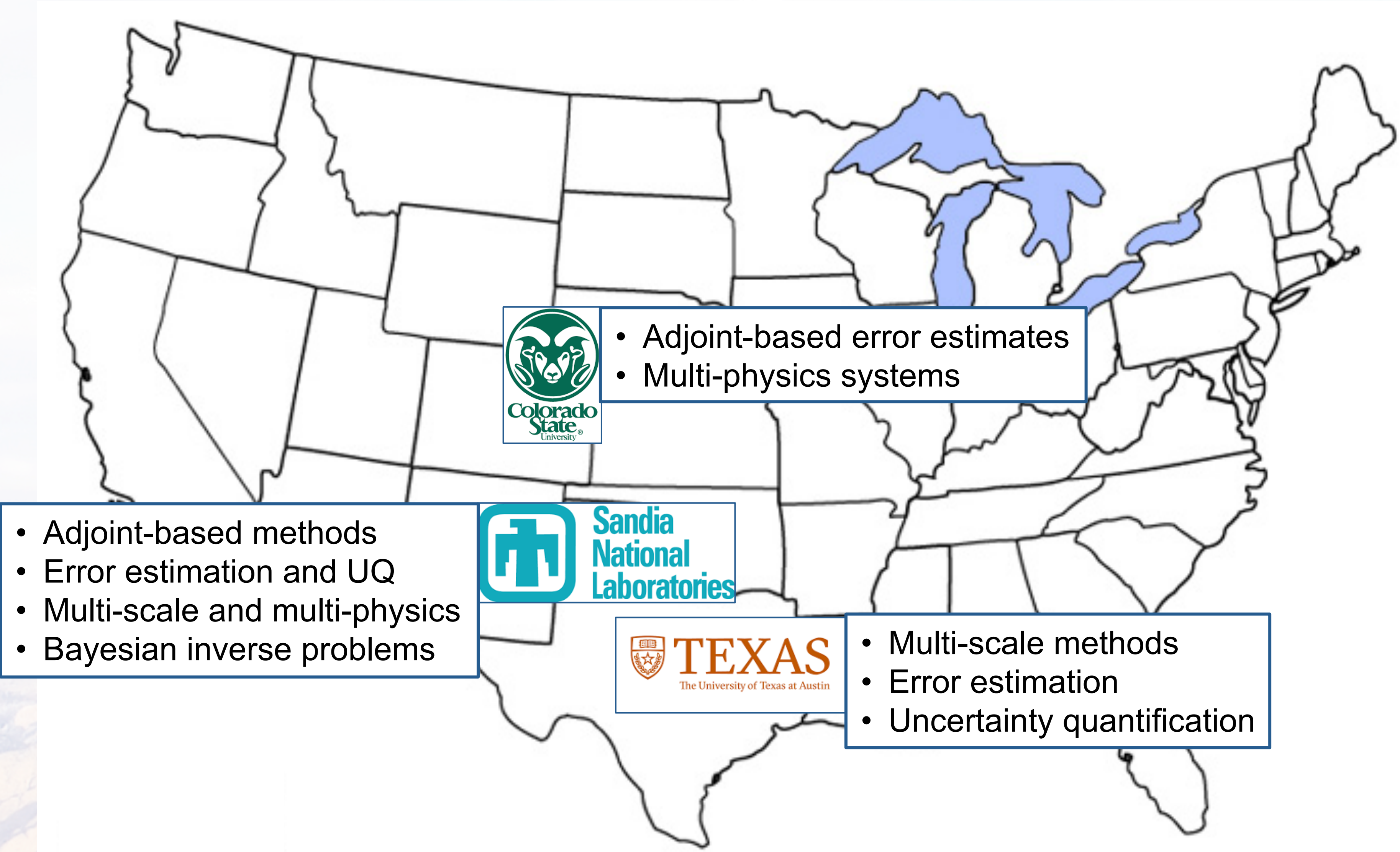
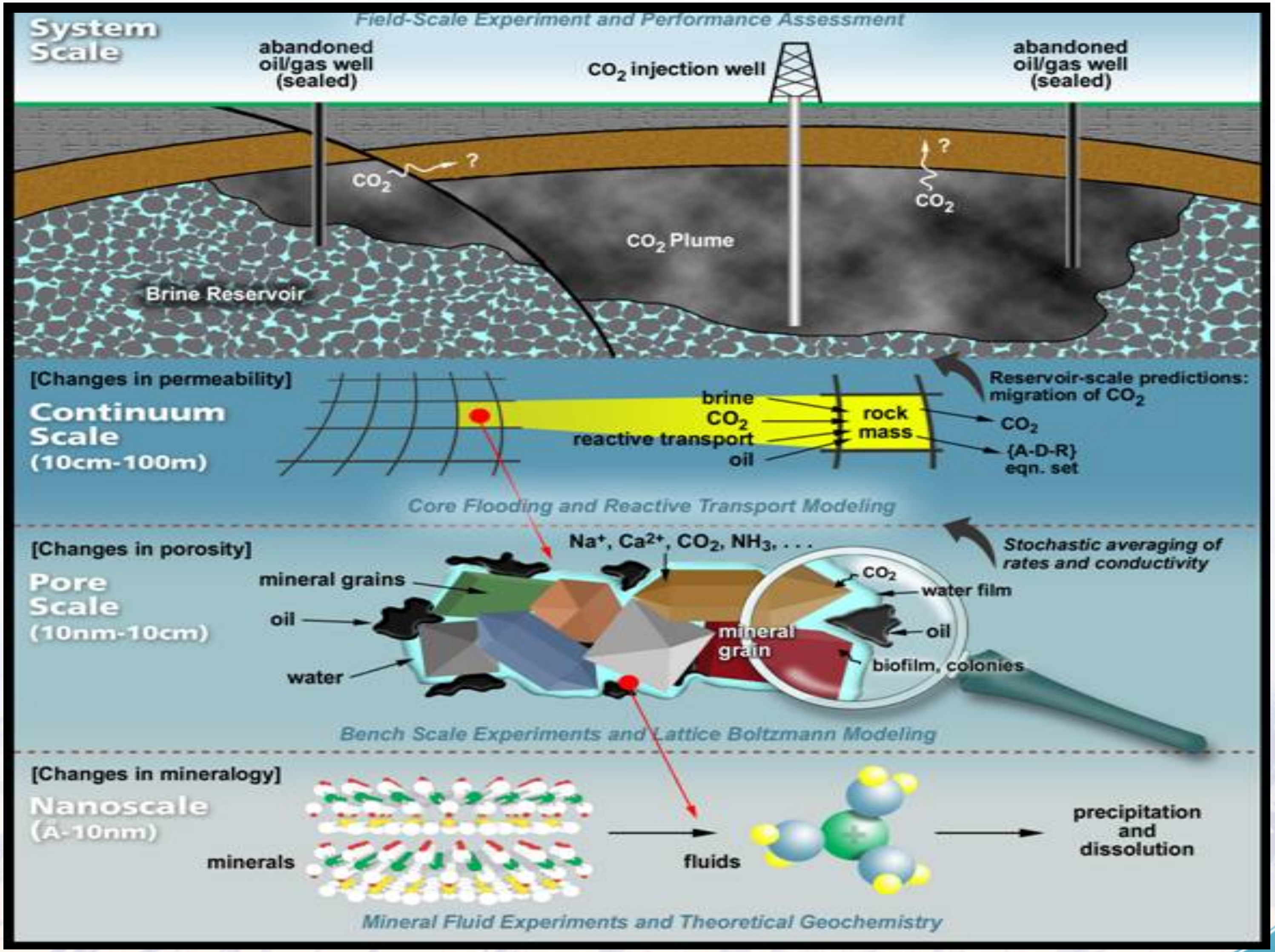


- Adjoint-based error estimates
- Multi-physics systems
- Adjoint-based methods
- Error estimation and UQ
- Multi-scale and multi-physics
- Bayesian inverse problems
- Multi-scale methods
- Error estimation
- Uncertainty quantification

Outline

- Introduction
  - Why do we care about multiscale methods?
  - What are mortar methods?
- Domain decomposition and multiscale mortar methods
- Applications
  - Incompressible single phase flow
  - IMPES and fully implicit formulations of two phase flow
  - Coupled flow and mechanics
- Goal-oriented a posteriori error estimate for multiscale/ multinumerics
- Current and Future Directions
- Conclusions

Scales in the Subsurface



Courtesy of D. Zhang (LANL)

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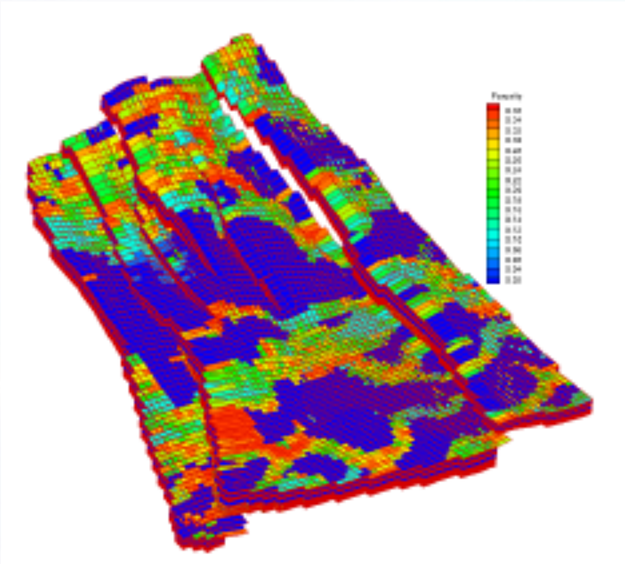
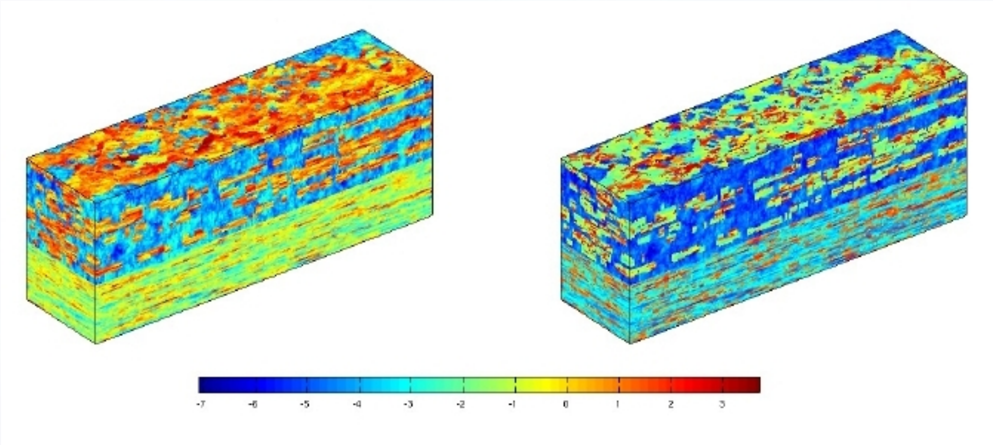
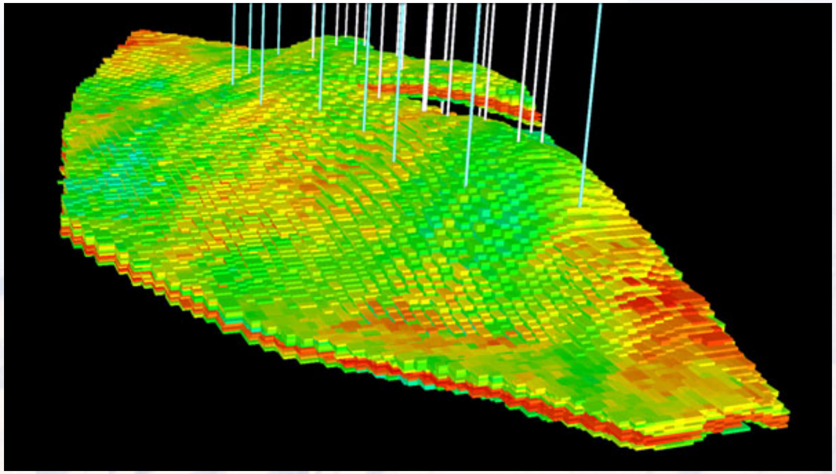
Typical Reservoir Models



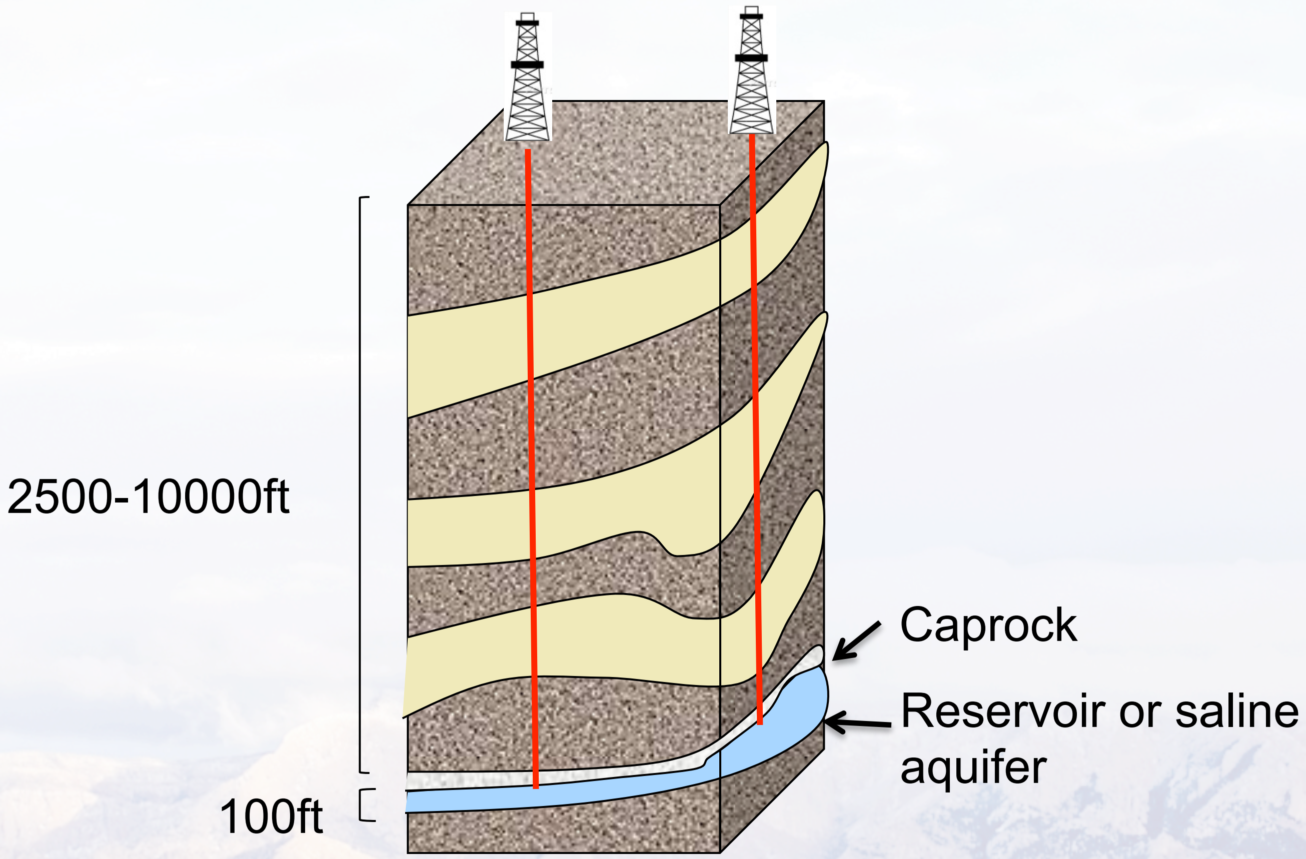




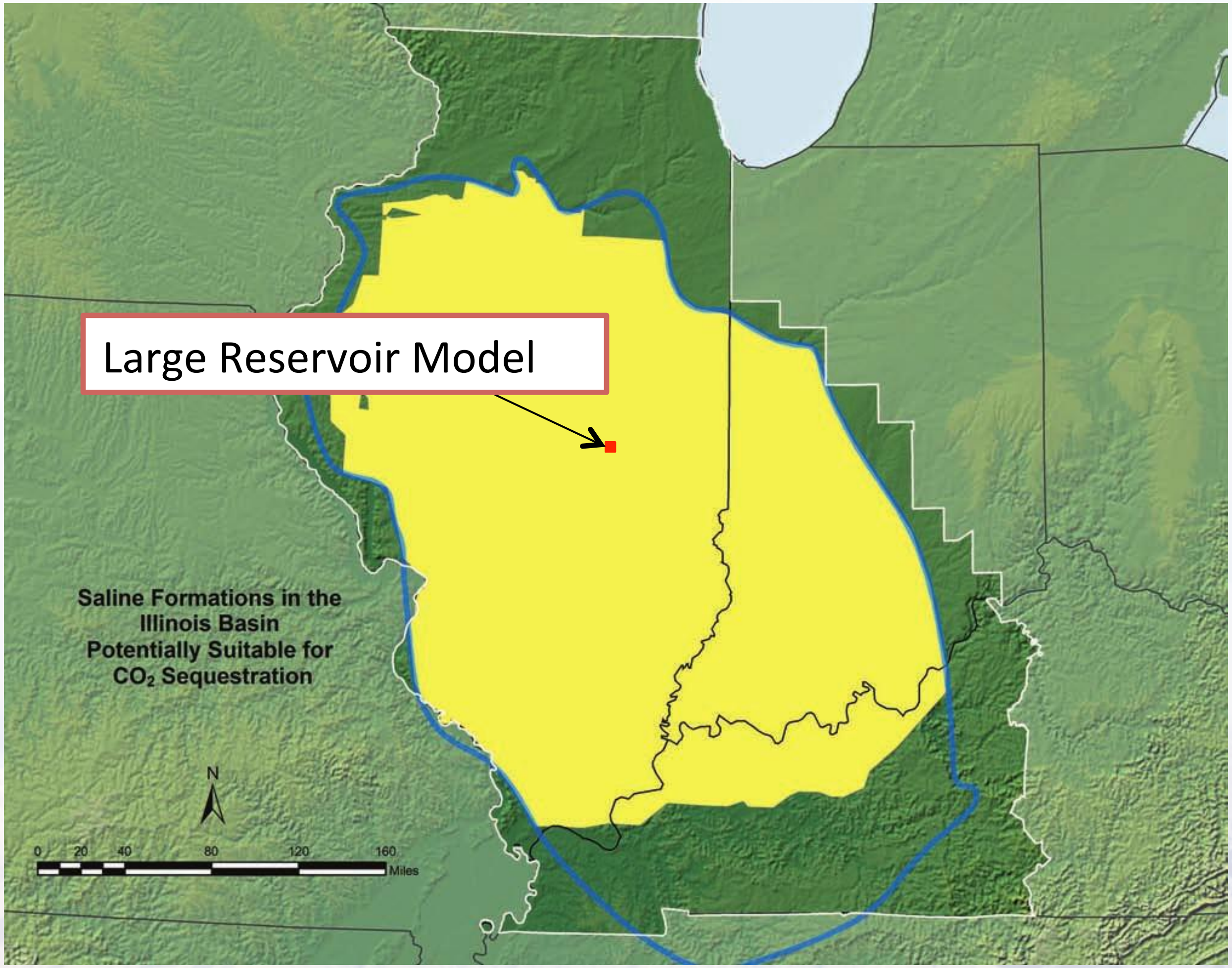
<u>Typical Dimensions</u>

- 1000ft x 1000ft x 100ft
- Approx. 1 million elements
- Degrees of freedom 1-40 million

Vertical Scales



Areal Scales



Courtesy of Midwest Geological Consortium

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Multiscale Approaches in Subsurface Modeling

Objective: Incorporate fine scale information into a coarse scale discretization.

- Generalized Finite Elements
  - Babuska, Osborn 1983
- Heterogeneous Multiscale Methods
  - E, Engquist 2003
- Multiscale finite elements
  - Babuska, Caloz, Osborn 1994
  - Hou, Wu 1997
  - Hou, Wu, Cai 1999
  - Efendiev, Hou, Wu 2000
  - Aarnes 2004
  - Aarnes, Krogstad, Lie 2006
- Multiscale finite volumes
  - Jenny, Lee, Tchelepi 2003
  - Tchelepi, Jenny, Lee, Wolfsteiner 2007
  - Lunati, Jenny 2006, 2008
- Variational multiscale methods
  - Hughes 1995
  - Brezzi 1999
  - Arbogast 2004
  - Arbogast, Boyd 2006
- Multiscale mortar methods
  - Arbogast, Pencheva, Wheeler, Yotov 2007
  - Girault, Sun, Wheeler, Yotov 2007
  - Ganis, Yotov 2009
  - Wheeler, Wildey, Yotov 2010
  - Tavener, Wildey 2013
- Multiscale domain decomposition methods
  - Aarnes, Hou 2002
  - Graham, Scheichl 2007
  - Nordbotten, Bjorstad 2008

What Are Mortar Methods?

Mortar: a workable paste used to bind construction blocks together and fill the gaps between them.

-Wikipedia

ICAC16, 2016 Int'l Conference on Advances in Concrete Construction

Dear Colleagues:

We are very happy to announce the "**2016 International Conference on Advances in Concrete Construction (ICAC16)**" as a participating conference of **ACEM16/Structures16** to be held on August 28 - September 1, 2016, in Jeju Island, Korea. The congress venue is International Convention Center Jeju (ICC Jeju).

What Are Mortar Methods?

Mortar: a *workable* paste used to *bind* construction blocks together and fill the gaps between them.

-Wikipedia

Mortar methods: discretization methods for partial differential equations, which use interface variables to connect/couple discretizations on non-overlapping subdomains.

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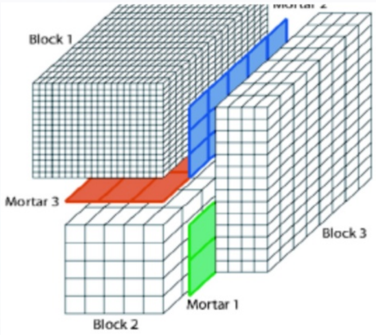
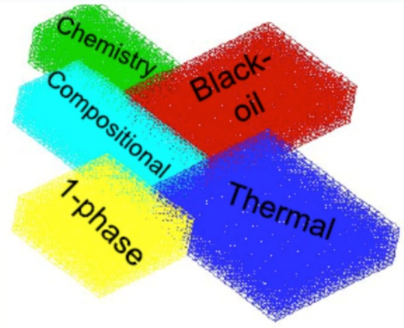
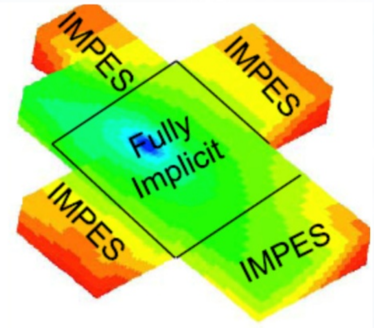
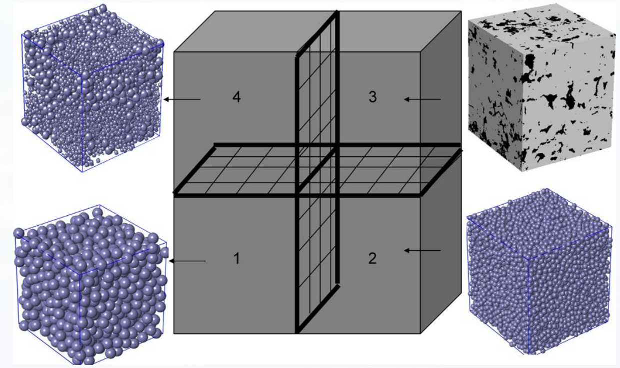
Multiscale Modeling with Mortar Methods









M. Balhoff (UT-Austin)

Features of Multiscale Mortar Approach

- Solid mathematical foundation *[Arbogast et al 2007]*
- Enables different discretizations, physics, and/or numerical methods *[Pencheva et al 2013, Girault et al 2008, Tavener, W. 2013]*
- Easily incorporates non-PDE based models *[Balhoff, Wheeler 2008]*
- No upscaling/homogenization of parameters *[Peszyńska et al 2002]*
- Provides a concurrent multi-scale formulation
- Hierarchical structure easily extended to finer or coarser levels
- Related to hybridizable discontinuous Galerkin
- Provides new opportunities for V&V/UQ/optimization
- Straightforward to define continuous/discrete adjoints *[Tavener, W. 2013]*

Domain Decomposition and Multiscale Mortar Methods

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Mixed Formulation

Model for flow in porous media:

$$\boldsymbol{u} = -K\nabla p, \qquad \text{(Darcy's Law)}$$
$$\nabla \cdot \boldsymbol{u} = f, \qquad \text{(Conservation of Mass)}$$

over Ω with $p = g$ on $\partial\Omega$.

Weak formulation: Find $\boldsymbol{u} \in H(\text{div}, \Omega)$ and $p \in L^2(\Omega)$ such that

$$\left(K^{-1}\boldsymbol{u}, \boldsymbol{v}\right) - (p, \nabla \cdot \boldsymbol{v}) = -\langle g, \boldsymbol{v} \cdot \boldsymbol{n} \rangle_{\partial\Omega}$$
$$(\nabla \cdot \boldsymbol{u}, w) = (f, w)$$

for all $\boldsymbol{v} \in H(\text{div}, \Omega)$ and $w \in L^2(\Omega)$.

Model Domain Decomposition Problem

Domain Decomposition: P nonoverlapping subdomains,

$$\Omega = \bigcup_{i=1}^{P} \Omega_i.$$

Interfaces: $\Gamma_{i,j} = \partial\Omega_i \cap \partial\Omega_j$ with $\Gamma = \bigcup_{1 \le i < j \le P} \Gamma_{i,j}$. Introduce $\lambda \in L^2(\Gamma)$.

Weak Formulation: On each subdomain,

$$\left(K^{-1}\boldsymbol{u}, \boldsymbol{v}\right)_{\Omega_i} - (p, \nabla \cdot \boldsymbol{v})_{\Omega_i} + \langle \lambda, \boldsymbol{v} \cdot \boldsymbol{n} \rangle_{\partial\Omega_i \cap \Gamma} = -\langle g, \boldsymbol{v} \cdot \boldsymbol{n} \rangle_{\partial\Omega_i \setminus \Gamma}$$

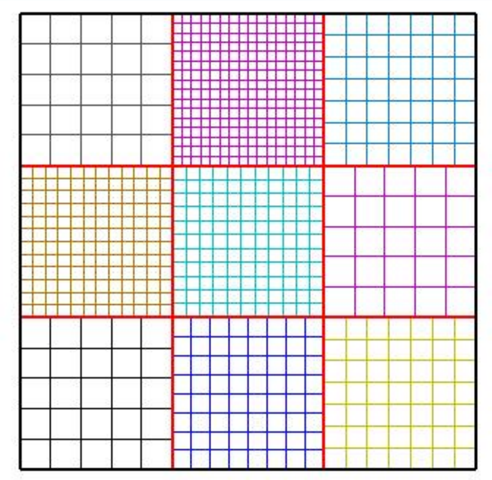
$$(\nabla \cdot \boldsymbol{u}, w)_{\Omega_i} = (f, w)_{\Omega_i}$$

Interface Conditions: Define $[\boldsymbol{u}]_{ij} = \boldsymbol{u}_i \cdot \boldsymbol{n}_i - \boldsymbol{u}_j \cdot \boldsymbol{n}_i$:

$$\sum_{1 \le i < j \le P} \langle [\boldsymbol{u}]_{ij}, \mu \rangle_{\Gamma_{i,j}}, \quad \mu \in L^2(\Gamma).$$

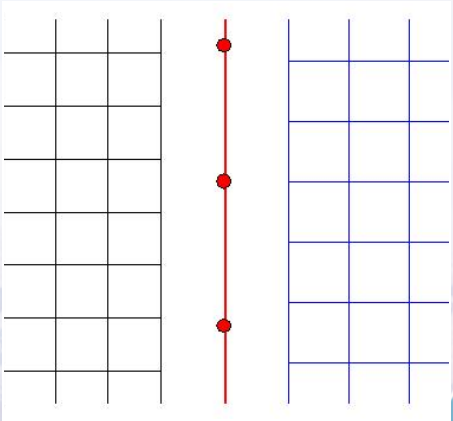
Multiscale Mortar Mixed Finite Element Method

Define a partition of each subdomain.



Let $\boldsymbol{V}_{h,i} \subset H(\mathrm{div}, \Omega_i)$ and $W_{h,i} \subset L^2(\Omega_i)$ be mixed finite element spaces.

Define a coarse partition of each $\Gamma_{i,j}$.



Let $M_H \subset L^2(\Gamma)$ be space of (dis)continuous polynomials.

MSMMFEM: Find $\boldsymbol{u}_{h,i} \in \boldsymbol{V}_{h,i}$, $p_{h,i} \in W_{h,i}$ and $\lambda_H \in M_H$ such that weak formulation is satisfied for all $\boldsymbol{v} \in \boldsymbol{V}_{h,i}$, $w \in W_{h,i}$ and $\mu \in M_H$.

Multiscale Mortar Mixed Finite Element Method

A priori error estimate for pressure:

$$\|p - p_h\| \le C \sum_{i=1}^{P} \big(\|p\|_{t,\Omega_i} h^t + \|p\|_{s+1/2,\Omega_i} H^{s+1/2} + \|\nabla \cdot \boldsymbol{u}\|_{t,\Omega_i} h^t H + \|\boldsymbol{u}\|_{r,\Omega_i} h^r H + \|\boldsymbol{u}\|_{r+1/2} h^r H^{3/2} \big)$$

A priori error estimate for velocity:

$$\|\boldsymbol{u} - \boldsymbol{u}_h\| \le C \sum_{i=1}^{P} \big(\|\boldsymbol{u}\|_{r,\Omega_i} h^r + \|p\|_{s+1/2,\Omega_i} H^{s-1/2} + \|\boldsymbol{u}\|_{r+1/2,\Omega_i} h^r H^{1/2} \big)$$

Optimal convergence can be maintained by choosing $H = \mathcal{O}(h^\beta)$.

For example, with lowest order RTN mixed FEM and quadratic mortars we take $H \approx h^{2/5}$.

The Interface Operator

Since the subdomain problems are independent, we can reduce the problem down to a **coarse-scale interface problem**.

In the case of two subdomains, the global discrete problem has the form:

$$\begin{bmatrix} A_1 & 0 & B_1 \\ 0 & A_2 & B_2 \\ B_1^T & B_2^T & 0 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ \lambda \end{bmatrix} = \begin{bmatrix} l_1 \\ l_2 \\ 0 \end{bmatrix}$$

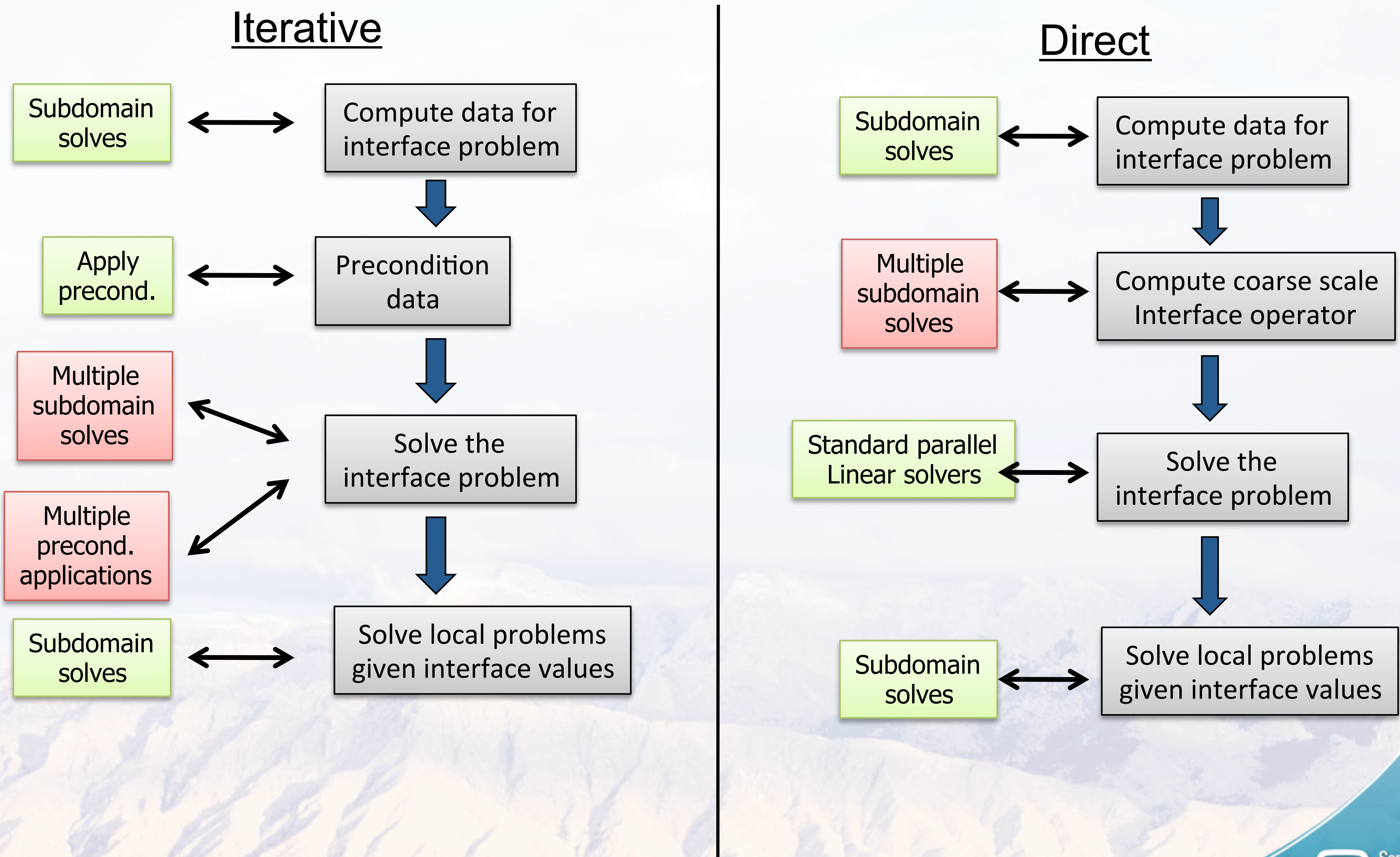
where A_i, z_i and l_i are the matrix, solution and source term corresponding to Ω_i.

Clearly a compatibility condition is required to guarantee a unique solution.

Reduction to an interface problem: $S\lambda = q$.

$$S = -B_1^T A_1^{-1} B_1 - B_2^T A_2^{-1} B_2, \quad q = -B_1^T A_1^{-1} l_1 - B_2^T A_2^{-1} l_2.$$

Iterative vs Direct



Applications

Slightly Compressible Flow with Transport

Conservation of mass and Darcy's law:

$$\frac{\partial}{\partial t}(\phi\rho) + \nabla \cdot \boldsymbol{u} = q,$$

$$\boldsymbol{u} = -\frac{\rho}{\mu} K(\nabla p - \rho \boldsymbol{g} \nabla D),$$

where ρ is density, μ is viscosity and ϕ is porosity.

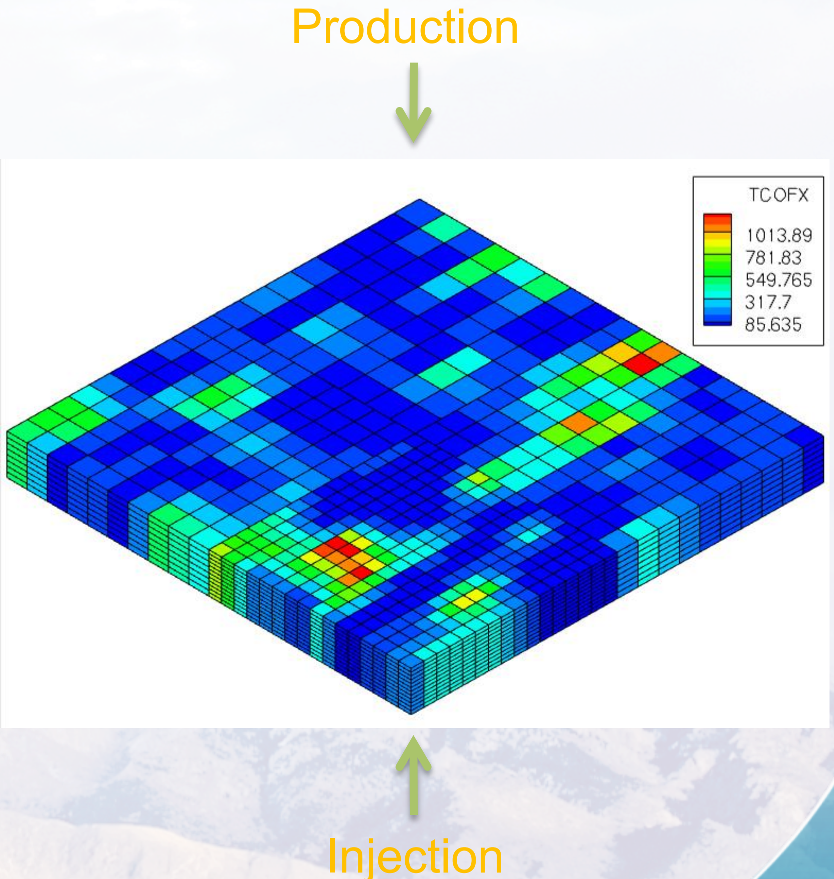
Equation of state: $\rho = \rho_{\text{ref}} e^{-c(p - p_{\text{ref}})}$.

Model for reactive transport,

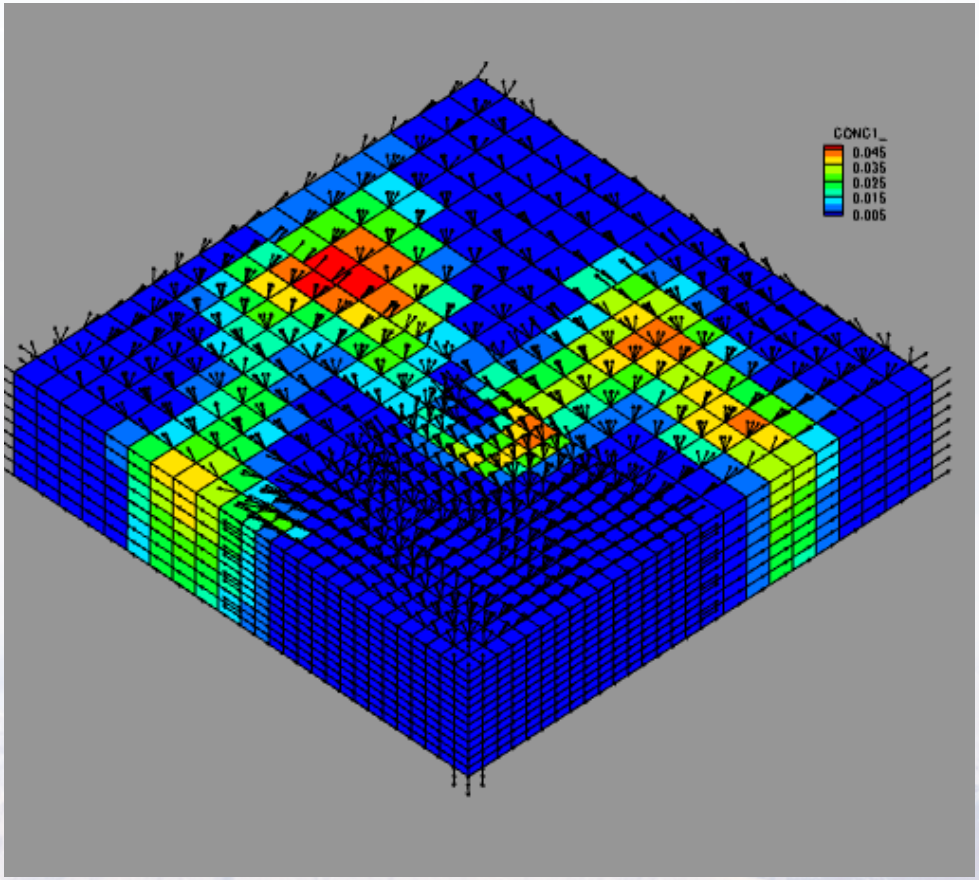
$$\frac{\partial c}{\partial t} + \nabla \cdot (c\boldsymbol{u} - D\nabla c) = q_c.$$

Numerical Results: Heterogeneous Permeability

- 24 ft x 400ft x 400ft
- Grid sizes
  - 2ft x 12.5ft x 12.5ft (12x16x16)
  - 3ft x 16.6ft x 16.6ft (8x12x12)
  - 3ft x 16.6ft x 16.6ft (8x12x12)
  - 4ft x 25ft x 25ft (6x8x8)
- Injection pressure: increase linearly
  - 505 [psi] (initially)
  - 1000 [psi] (50 days)
- Production pressure: decrease linearly
  - 480 [psi] (initially)
  - 350 [psi] (30 days)
- One species, initial concentrations:
  - 100 [M/cu-ft] in first grid cell
  - 0 everywhere else
- Continuous linear mortars
- High order Godunov for advection
- Van Leer slope limiting with parameter 0.85
- Molecular diffusivity: 1.0 [sq ft / day]
- Physical (Diffusion)-Dispersion:
  - Longitudinal: 1.0 [ft]
  - Transverse: 0.2 [ft]



Numerical Results: Heterogeneous Permeability



Two Phase Immiscible Slightly Compressible Flow

Mass conservation and Darcy's law:

$$\frac{\partial}{\partial t}(\phi S_\alpha \rho_\alpha) + \nabla \cdot \boldsymbol{u}_\alpha = q_\alpha, \quad \boldsymbol{u}_\alpha = -\frac{k_\alpha K}{\mu_\alpha}\rho_\alpha(\nabla p_\alpha - \rho_\alpha \boldsymbol{g})$$

Equation of state:

$$\rho_\alpha = \rho_\alpha^{\mathrm{ref}} e^{c_\alpha (p_\alpha - p_\alpha^{\mathrm{ref}})}$$

Physical constraints:

$$S_o + S_w = 1, \quad p_c(S_w) = p_o - p_w.$$

ϕ	porosity
S_α	saturation
ρ_α	density
q_α	source term
k_α	relative permeability
μ_α	viscosity

Equations can be solved using either IMPES or fully implicit.

Implicit Pressure – Explicit Saturation (IMPES) Formulation

Following *[Hoteit, Fizoozabado, 2008]*, define mobilities,

$$\eta_\alpha(S_w) = \frac{k_\alpha}{\mu_\alpha}, \quad \eta_t = \eta_w + \eta_o.$$

Define a primary and capillary velocity,

$$\boldsymbol{u}_a = -\eta_t \boldsymbol{K}(\nabla p_w - \rho_w \boldsymbol{g}), \quad \boldsymbol{u}_c = -\eta_o \boldsymbol{K}(\nabla p_c - (\rho_o - \rho_w)\boldsymbol{g})$$

Solve an **implicit** (elliptic) equation for primary velocity:

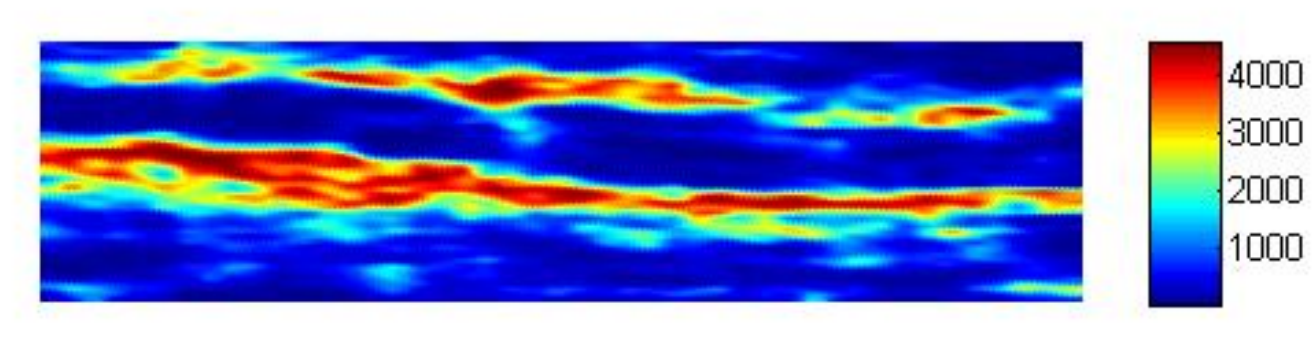
$$\nabla \cdot \boldsymbol{u}_a = q_t + q_c - \nabla \cdot \boldsymbol{u}_c$$

Solve an **explicit** equation for saturation:

$$\frac{\partial}{\partial t}(\phi S_w) + \left(\frac{\eta_w}{\eta_t}\boldsymbol{u}_a\right) = q_w.$$

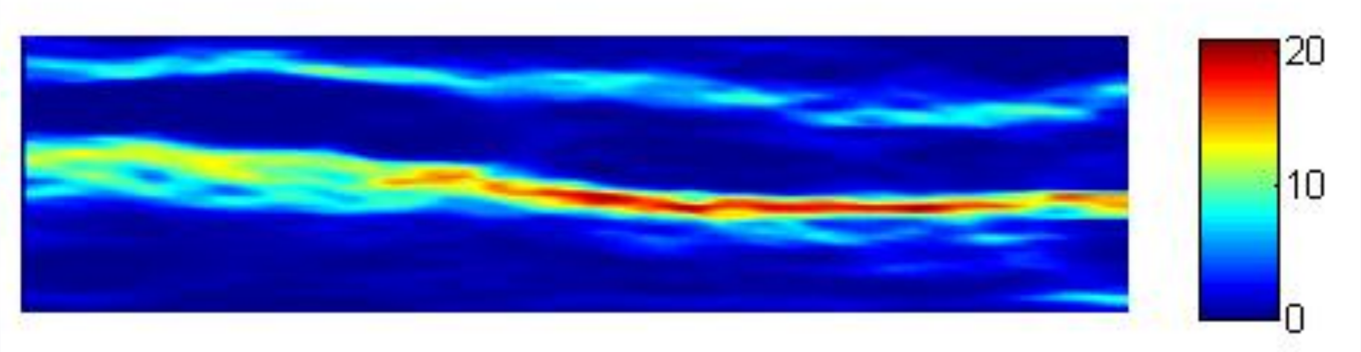
Example: Water Flood

- Compare multiscale mortar solution with fine scale solution.
- Fine scale: 180x180 → 32,400 fine scale degrees of freedom
- Coarse scale: 4x4 quadratic mortars → 456 degrees of freedom on coarse scale
- Channelized permeability.
- Inject at one end, produce at the other.
- Neglect gravity.
- 100 saturation time steps per pressure time step

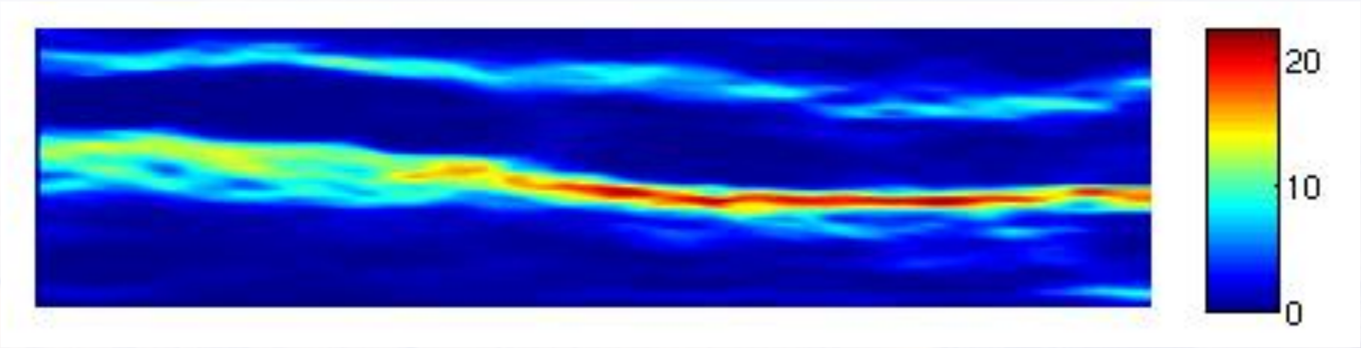


Fine scale permeability

Fine Scale and Multiscale Velocities

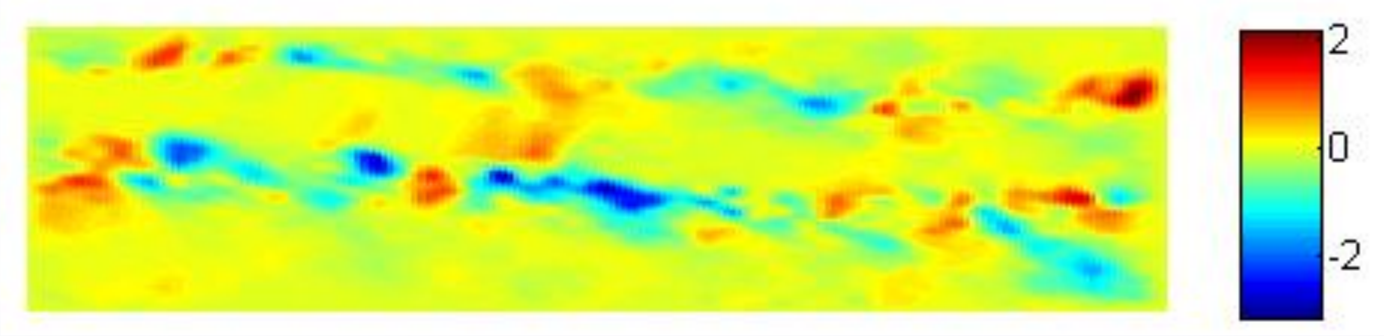


x-velocity from fine scale solution:

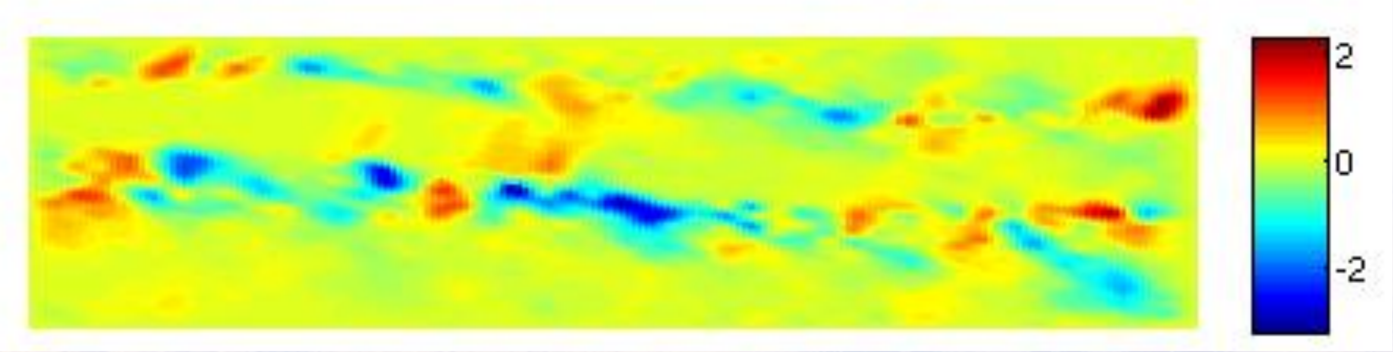


x-velocity from multiscale solution:

Fine Scale and Multiscale Velocities

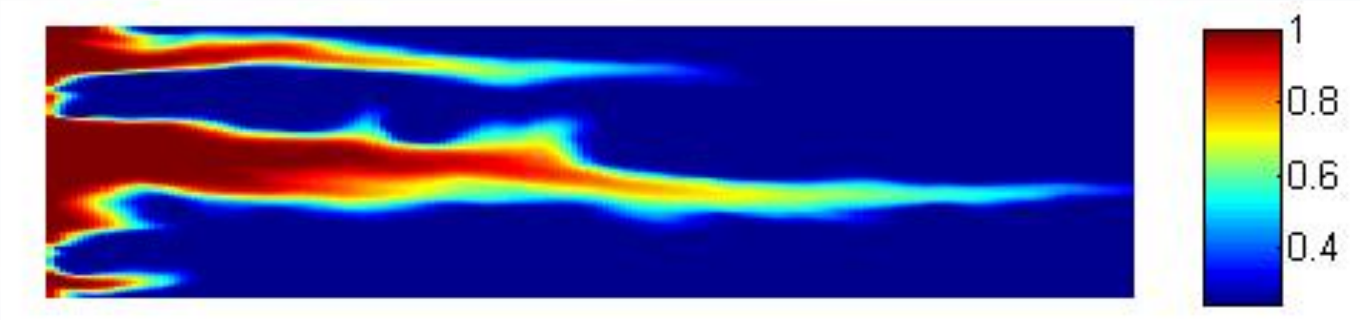


y-velocity from fine scale solution:

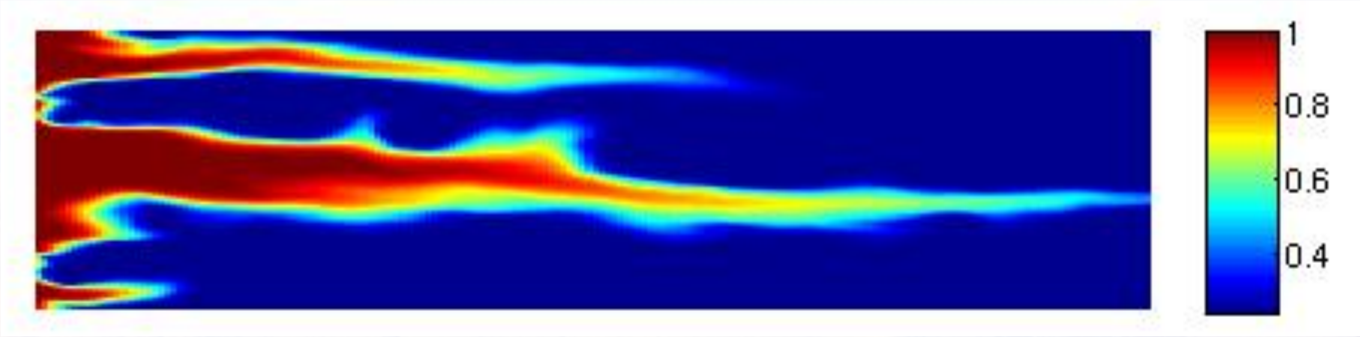


y-velocity from multiscale solution:

Fine Scale and Multiscale Saturations



Water saturation from fine scale solution:



Water saturation from multiscale solution:

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Fully Implicit Formulation

Mass conservation and Darcy's law:

$$\frac{\partial}{\partial t}(\phi S_\alpha \rho_\alpha) + \nabla \cdot \boldsymbol{u}_\alpha = q_\alpha, \quad \boldsymbol{u}_\alpha = -\frac{k_\alpha K}{\mu_\alpha}\rho_\alpha(\nabla p_\alpha - \rho_\alpha \boldsymbol{g})$$

On subdomains, solve for a pressure, p_w, and a concentration, $N_o = \rho_o S_o$.

Interface variables: $\lambda_1 = p_w$, and $\lambda_2 = N_o$.

Interface conditions: $[\boldsymbol{u}_\alpha] = 0$

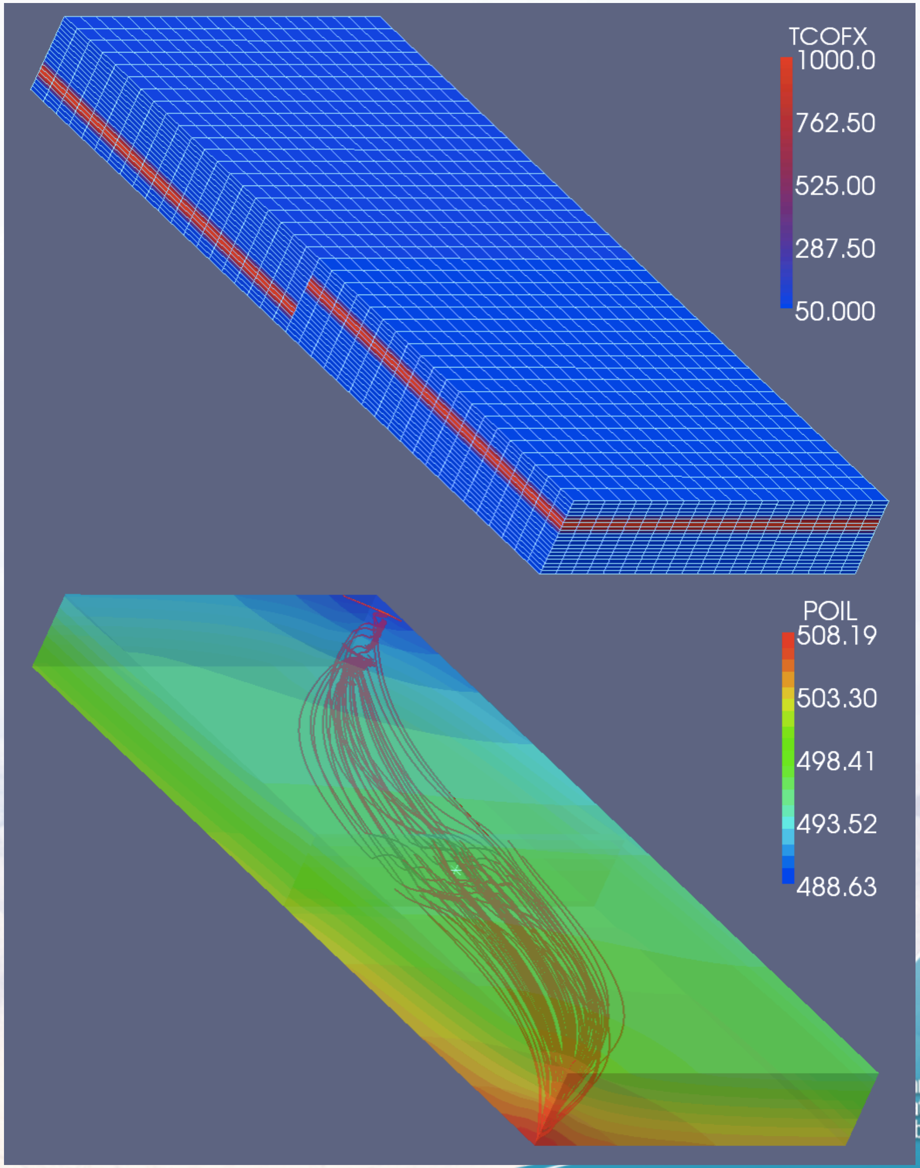
Interface Jacobian has block structure:

$$\frac{\partial}{\partial \boldsymbol{\lambda}} F(\boldsymbol{\lambda}) = \begin{pmatrix} \frac{\partial \boldsymbol{u}_w}{\partial \lambda_1} & \frac{\partial \boldsymbol{u}_w}{\partial \lambda_2} \\ \frac{\partial \boldsymbol{u}_o}{\partial \lambda_1} & \frac{\partial \boldsymbol{u}_o}{\partial \lambda_2} \end{pmatrix}$$

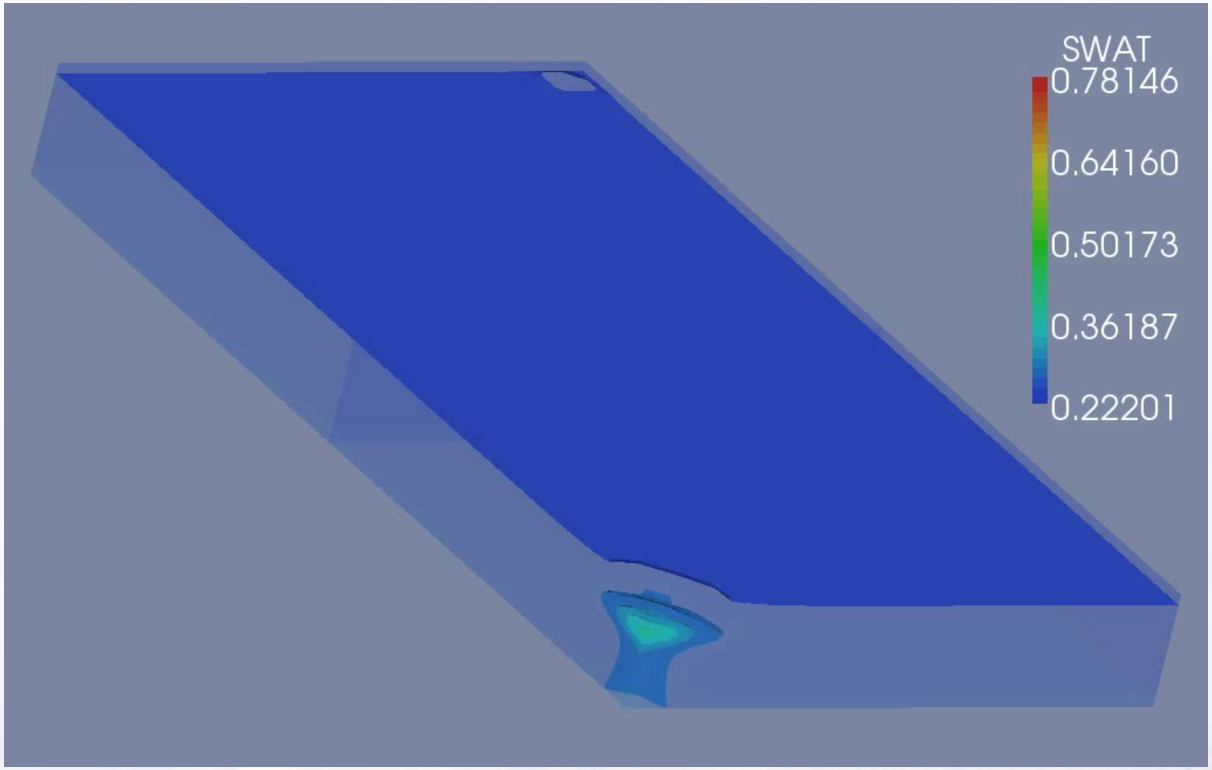
We use a finite difference method to approximate Jacobian.

Numerical Results: Two Phase Flow

- 20 [ft] x 100 [ft] x 200 [ft]
- Second grid (finer)
    - 1 [ft] x 5 [ft] x 5 [ft] (20x20x20)
    - 1 [ft] x 5 [ft] x 5 [ft] (20x20x20)
- Layered permeability
- Initial pressure: 500 [psi]
- Initial water saturation: 0.22
- Injection pressure: 505 [psi]
- Production pressure: 495 [psi]
- Includes gravity and capillary pressure
- Discontinuous constant mortars



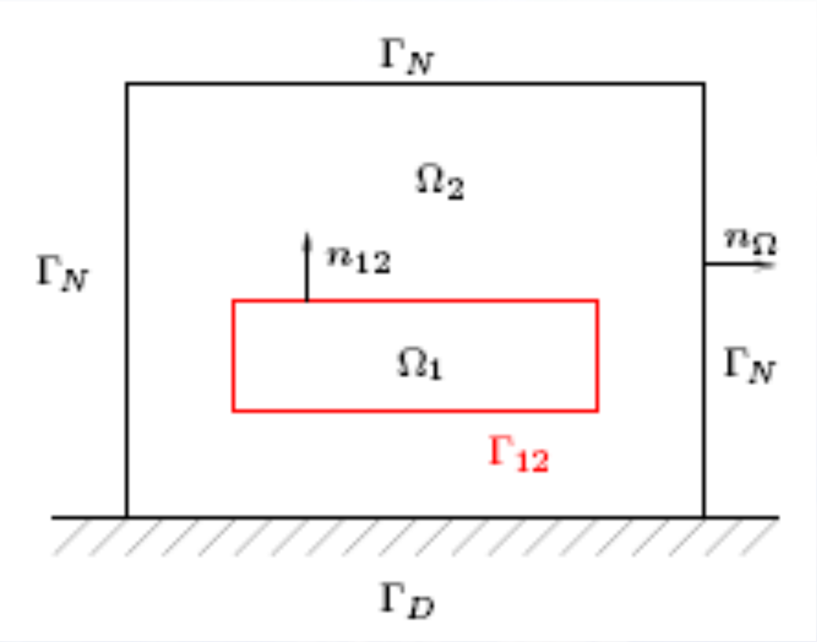
Numerical Results: Two Phase Flow

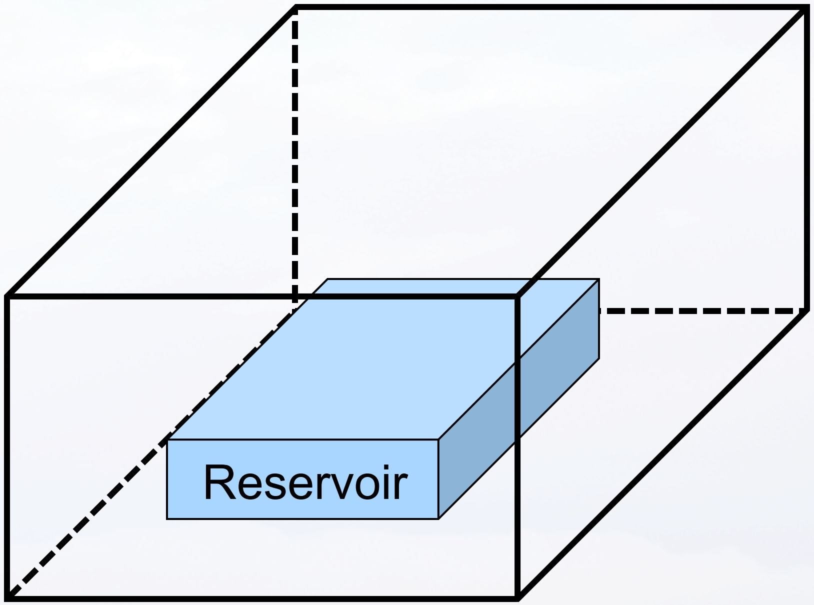


Finer Grid	Avg. Interface Iterations	Time Per Newton Step (min)	Multiscale Precond. Assembly Time (min)	Total Time (min)
No Precond.	157.7	7.86	-	1730.3
Multiscale Precond.	7.2	0.41	15.7	105.7

Mortar Coupling for Elasticity and Poroelasticity

Domain Decomposition





Ω_1	Reservoir (pay-zone)
Ω_2	Nonpay-zone
Ω	$\Omega_1 \cup \Omega_2$
Γ_{12}	Interface between Ω_1 and Ω_2

Pay-zone Model: Poroelasticity

- Equation for Cauchy stress tensor: $\tilde{\boldsymbol{\sigma}} = \boldsymbol{\sigma} - \alpha p \boldsymbol{I}$

$\boldsymbol{u}$	displacement
p	fluid pressure
$\boldsymbol{\sigma}(\boldsymbol{u}) = \lambda(\operatorname{div}\boldsymbol{u})\boldsymbol{I} + 2\mu\,\epsilon(\boldsymbol{u})$	effective stress tensor
$\epsilon(\boldsymbol{u}) = \frac{1}{2}\left(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T\right)$	strain tensor
$\boldsymbol{I}$	identity tensor
$\lambda > 0,\ \mu > 0$	Lame coefficients
$\alpha > 0,$	Biot-Willis constant

- Balance of linear momentum: $\nabla \cdot \hat{\boldsymbol{\sigma}} = \boldsymbol{f}_1$

- Darcy's Law: $\boldsymbol{v}_f = -\dfrac{\boldsymbol{K}}{\mu_f}\left(\nabla p - \rho_f \boldsymbol{g}\right)$

$\boldsymbol{v}_f$	fluid flux
$\boldsymbol{K}$	permeability tensor (SPD)
$\mu_f > 0,\ \rho_f > 0$	fluid viscocity and density
$\boldsymbol{g}$	gravitational force

- Mass conservation: $\nabla \cdot \boldsymbol{v}_f = q$

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Nonpay-zone Model and Interface Conditions

- Linear elastic model in nonpay-zone: $\nabla \cdot \boldsymbol{\sigma} = \boldsymbol{f}_2$

$$\begin{array}{r|l} \boldsymbol{f}_2 & \text{body force in } \Omega_2 \\ \boldsymbol{u} = \boldsymbol{0} & \text{Displacement on } \Gamma_D \\ \boldsymbol{\sigma}(\boldsymbol{u})\,\boldsymbol{n}_\Omega = \boldsymbol{t}_N & \text{Traction on } \Gamma_N \end{array}$$

- Define the jump and average along interface

$$[v] = \left(v|_{\Omega_1} - v|_{\Omega_2}\right)|_{\Gamma_{12}}$$

$$\{v\} = \frac{1}{2}\left(v|_{\Omega_1} + v|_{\Omega_2}\right)|_{\Gamma_{12}}$$

- Prescribe the following transmission conditions:

$$\begin{array}{r|l} [\boldsymbol{u}] = \boldsymbol{0} & \text{continuity of the medium} \\ [\boldsymbol{\sigma}(\boldsymbol{u})]\,\boldsymbol{n}_{12} = \alpha p\,\boldsymbol{n}_{12} & \text{continuity of normal stresses} \\ -\frac{\boldsymbol{K}}{\mu_f}\left(\nabla p - \rho_f \boldsymbol{g}\right) \cdot \boldsymbol{n}_{12} = 0 & \text{no flow on the interface} \end{array}$$

Variational Formulation

Find $\boldsymbol{u} \in H_0^1(\Omega)^d$ and $p \in H^1(\Omega_1)$ such that

$$\int_\Omega \boldsymbol{\sigma}(\boldsymbol{u}) : \epsilon(\boldsymbol{v})\ d\boldsymbol{x} - \alpha \int_{\Omega_1} p \ \mathrm{div}\ \boldsymbol{v}\ d\boldsymbol{x} = \int_\Omega \boldsymbol{f} \cdot \boldsymbol{v}\ d\boldsymbol{x} + \int_{\Gamma_N} \boldsymbol{t}_N(s) \cdot \boldsymbol{v}(s)\ ds$$

$$\int_{\Omega_1} \frac{\boldsymbol{K}}{\mu_f} \nabla p \cdot \nabla \theta\ d\boldsymbol{x} = \int_{\Omega_1} q\ \theta\ d\boldsymbol{x} + \int_{\Omega_1} \frac{\boldsymbol{K}}{\mu_f} \rho_f \boldsymbol{g} \cdot \nabla \theta\ d\boldsymbol{x}$$

for all $\boldsymbol{v} \in H_0^1(\Omega)^d$ and $\theta \in H^1(\Omega_1)$.

A unique solution exists under regularity assumptions.

DG with Lagrange Multipliers

Introduce the Lagrange multiplier $\boldsymbol{\lambda}$ on Γ_{12}.
Elasticity and poroelasticity equations become:

$$\sum_{i=1}^{2} \int_{\Omega_i} \boldsymbol{\sigma}(\boldsymbol{u}_i) : \boldsymbol{\epsilon}(\boldsymbol{v}_i)\ d\boldsymbol{x} - \int_{\Omega_1} \alpha p\ \nabla \cdot \boldsymbol{v}_1\ d\boldsymbol{x} +$$

Usual interior terms

$$\sum_{i=1}^{2} - \int_{\Gamma_{12}} \boldsymbol{\sigma}(\boldsymbol{u}_i)\boldsymbol{n}_i \cdot \boldsymbol{v}_i\ ds\ + \int_{\Gamma_{12}} \alpha p\ \boldsymbol{n}_1 \cdot \boldsymbol{v}_1\ ds\ +$$

Interface terms from integration by parts

$$\sum_{i=1}^{2} \int_{\Gamma_{12}} (\lambda + 2\mu)\frac{\sigma_i}{h_i}(\boldsymbol{u}_i - \boldsymbol{\lambda}) \cdot \boldsymbol{v}_i\ ds + \sum_{i=1}^{2} \int_{\Gamma_{12}} \boldsymbol{\sigma}(\boldsymbol{v}_i)\boldsymbol{n}_i \cdot (\boldsymbol{u}_i - \boldsymbol{\lambda})\ ds\ +$$

DG terms on interface

$$= \sum_{i=1}^{2} \int_{\Omega_i} \boldsymbol{f}_i \cdot \boldsymbol{v}_i\ d\boldsymbol{x} + \int_{\Gamma_N} \boldsymbol{t}_N \cdot \boldsymbol{v}_i\ ds$$

Usual source terms

DG with Lagrange Multipliers

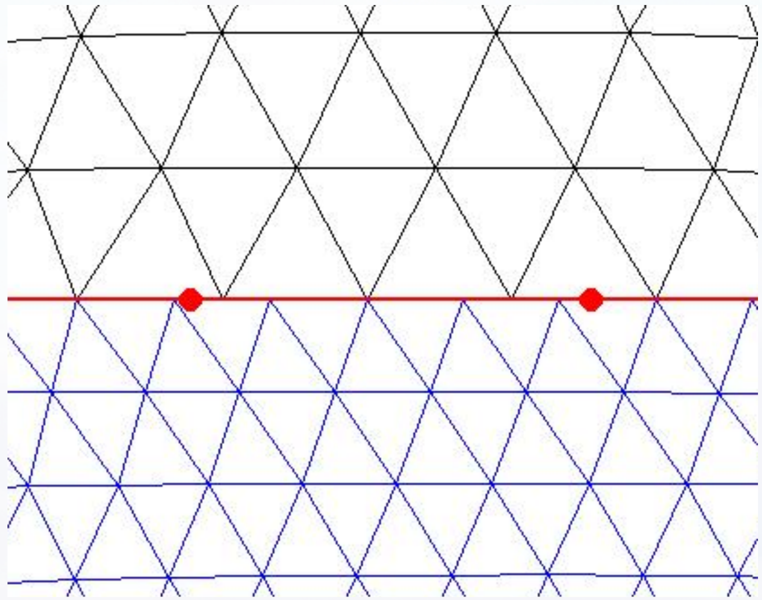
Interface equation:

$$\sum_{i=1}^{2} -\int_{\Gamma_{12}} (\lambda + 2\mu)\frac{\sigma_i}{h_i}(\boldsymbol{u}_i - \boldsymbol{\lambda}) \cdot \boldsymbol{\mu} \; ds + \int_{\Gamma_{12}} [\boldsymbol{\sigma}(\boldsymbol{u})] - \alpha p)\boldsymbol{n}_{12} \cdot \boldsymbol{\mu} \; ds$$

Pressure equation:

$$\int_{\Omega_1} \frac{\boldsymbol{K}}{\mu_f} \nabla p \cdot \nabla \theta \; d\boldsymbol{x} = \int_{\Omega_1} q \; \theta \; d\boldsymbol{x} + \int_{\Omega_1} \frac{\boldsymbol{K}}{\mu_f} \rho_f \boldsymbol{g} \cdot \nabla \theta \; d\boldsymbol{x}$$

Discretizations



$\mathcal{T}_{h,i}, i = 1, 2$	two independent regular triangulations of size h_i
Γ_H	triangulation of Γ_{12} of size H
$\boldsymbol{u}^n_{h_i} \in \boldsymbol{X}_{h,i}$	continuous in Ω_1 and Ω_2, piecewise $\mathbb{P}^d_k$, $k \geq 1$
$p^n_h \in M_{h,1}$	continuous in Ω_1, piecewise $\mathbb{P}_m$, $m \geq 1$
$\boldsymbol{\lambda}^n_H \in \boldsymbol{\Lambda}_H$	continuous in Γ_{12}, piecewise $\mathbb{P}^d_l$, $l \geq 1$

Error Estimates

Theorem

Assume the triangulations are regular in the sense of Ciarlet and satisfy a quasi-uniformity assumption along the interface†. Then there exists a constant $C > 0$ independent of h_1, h_2 and H such that

$$E_{\boldsymbol{u}}^2 + E_p^2 + E_{\Gamma_{12}}^2 + E_{\Gamma_D}^2 \leq C\left(h_1^{2(r_u-1)} + h_2^{2(r_u-1)} + \left(\frac{H}{h_1} + \frac{H}{h_2}\right) H^{2r_\lambda - 1}\right)$$

where $r_{\boldsymbol{u}} = \min(k+1, s_{\boldsymbol{u}})$, $r_p = \min(m+1, s_p)$, $r_{\boldsymbol{\lambda}} = \min(l+1, s_{\boldsymbol{u}} - 1/2)$.

† For details, see Girault et al, M^{3}AS, 2011.

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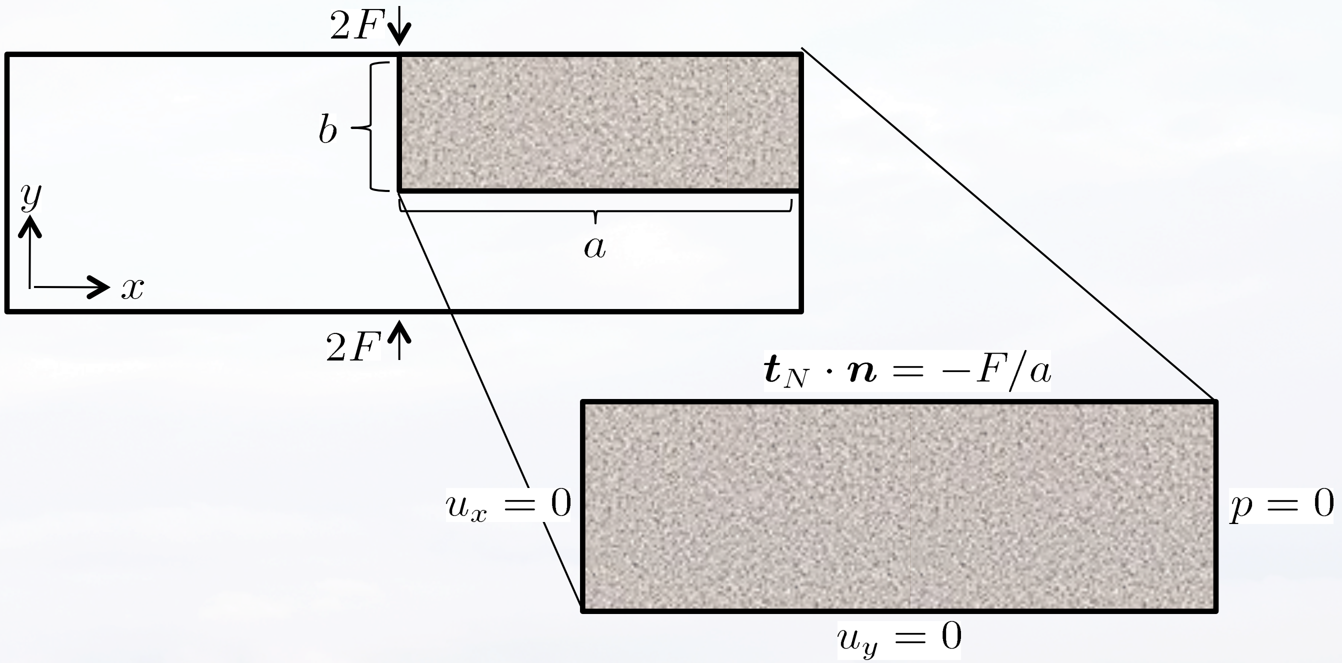
Mandel's Problem



- Infinite domain subjected to a loading of 2F from above and below
- Symmetry allows domain to be reduced to 2D upper right quadrant
- Analytical solution for pressure and displacements[1]
- Solution demonstrates the Mandel-Creyer effect.

[1] *Mandel 1953, Abouslieman et al 1996*

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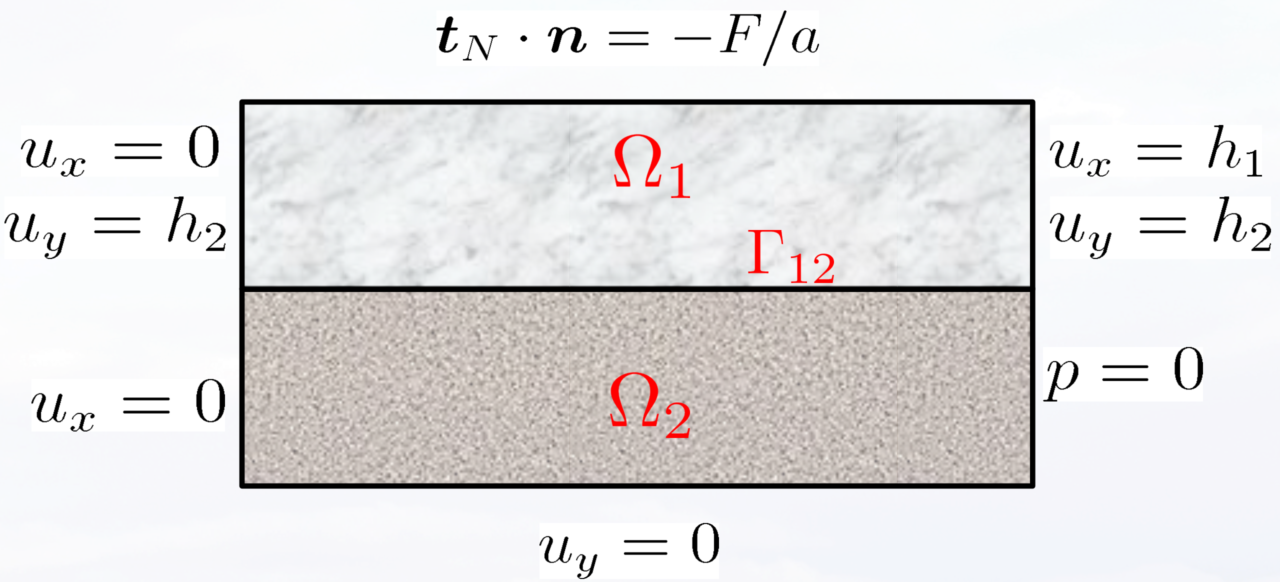
Extension of Mandel's Problem



α	1
E	1×10^4
ν	0.2
K	100
F	2000
c_0	0.1
Δt	1×10^{-8}

- Extend Mandel's problem to include an elastic domain

$$u_x^{\text{nonpay}} = u_x^{\text{pay}} \qquad u_y^{\text{nonpay}} = u_y^{\text{pay}} - \frac{\alpha}{\lambda + 2\mu}(y-b)p$$

- Piecewise linear finite elements and continuous linear mortars with H = h

Extension of Mandel's Problem

Total Degrees of Freedom	Error in Energy Norm	Predicted Rate	Observed Rate
1,197	1.07E-2		
4,387	4.91E-3	1	1.09
16,767	2.34E-3	1	1.05
65,527	1.14E-3	1	1.03
259,047	5.65E-4	1	1.01

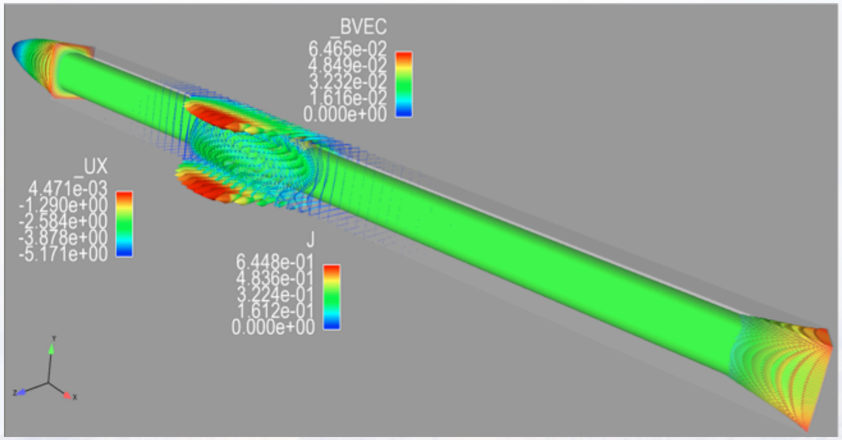
Goal Oriented Error Estimates

Goal Oriented Error Estimation

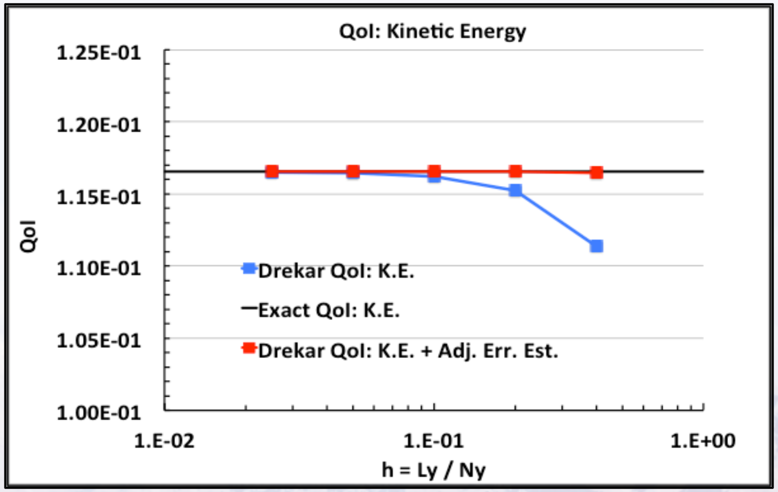
Our goal is often to compute a small number of *quantities of interest* from a simulation.

Understanding the error and sensitivity of a QoI is critical.

Adjoint-based methods can provide both!



Adjoint Solution for resistive MHD (Drekar::CFD)



Can we estimate the error in a QoI from a ms-mortar simulation?

Model Problem

For simplicity, we consider the model elliptic problem,

$$-\nabla \cdot (\boldsymbol{K}\nabla p) = f, \quad x \in \Omega$$
$$p = g_D, \quad x \in \partial\Omega$$

where $\boldsymbol{K}$ is a sym., bdd. and uniformly positive definite, and f and g_D are sufficiently smooth.

Domain Decomposition: $\Omega = \bigcup_{i=1}^{P} \Omega_i, \quad \Gamma_{i,j} = \partial\Omega_i \cap \partial\Omega_j.$

Let $\boldsymbol{V}_i$ and M denote appropriate Hilbert spaces.

Let $\mathcal{A}_i : \boldsymbol{V}_i \times \boldsymbol{V}_i \to \mathbb{R}$, $\mathcal{B}_i : M \times \boldsymbol{V}_i \to \mathbb{R}$, $\mathcal{C}_i : \boldsymbol{V}_i \times M \to \mathbb{R}$, and $\mathcal{D}_i : M \times M \to \mathbb{R}$ be appropriate continuous bilinear forms.

Variational formulation: seek $\boldsymbol{z}_i \in \boldsymbol{V}_i$ and $\lambda \in M$ such that

$$\mathcal{A}_i(\boldsymbol{z}_i, \boldsymbol{w}_i) = l_i(\boldsymbol{w}_i) - \mathcal{B}_i(\lambda, \boldsymbol{w}_i), \quad \forall \boldsymbol{w}_i \in \boldsymbol{V}_i, \quad i = 1, \ldots, P,$$
$$\sum_{i=1}^{P} (\mathcal{C}_i(\boldsymbol{z}_i, \mu) + \mathcal{D}_i(\lambda, \mu)) = 0, \quad \forall \mu \in M.$$

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Adjoint Problem

The continuous adjoint problem is given by

$$\begin{aligned} -\nabla \cdot (\boldsymbol{K} \nabla \phi) &= \psi, \quad x \in \Omega \\ \phi &= 0, \quad x \in \partial\Omega \end{aligned}$$

where ψ is chosen based on the quantity of interest.

Let $\mathcal{A}_i^* : \boldsymbol{V}_i \times \boldsymbol{V}_i \to \mathbb{R}$, $\mathcal{B}_i^* : \boldsymbol{V}_i \times M \to \mathbb{R}$, $\mathcal{C}_i^* : M \times \boldsymbol{V}_i \to \mathbb{R}$, and $\mathcal{D}_i^* : M \times M \to \mathbb{R}$ be appropriate continuous adjoint bilinear forms.

Adjoint variational formulation: seek $\boldsymbol{\phi}_i \in \boldsymbol{V}_i$ and $\eta \in M$ such that

$$\begin{aligned} \mathcal{A}_i^*(\boldsymbol{z}_i, \boldsymbol{w}_i) = j_i(\boldsymbol{w}_i) - \mathcal{C}_i^*(\lambda, \boldsymbol{w}_i), \quad \forall \boldsymbol{w}_i \in \boldsymbol{V}_i, \quad i = 1, \ldots, P, \\ \sum_{i=1}^{P} \left(\mathcal{B}_i^*(\boldsymbol{\phi}_i, \mu) + \mathcal{D}_i^*(\eta, \mu)\right) = 0, \quad \forall \mu \in M. \end{aligned}$$

Adjoint-based Error Estimate

Let $\boldsymbol{z}_{h,i} \in \boldsymbol{V}_{h,i} \subset \boldsymbol{V}_i$ and $\lambda_H \in M_H \subset M$ be discrete approximations and let $\boldsymbol{\Pi}_{h,i} : \boldsymbol{V}_i \to \boldsymbol{V}_{h,i}$ and $Q_H : M \to M_H$ be projection operators.

Define $\boldsymbol{e}_{\boldsymbol{z},i} = \boldsymbol{z}_i - \boldsymbol{z}_{h,i}$ and $e_\lambda = \lambda - \lambda_H$.

The error in a linear functional of the solution satisfies,

$$\sum_{i=1}^{N} j_i(\boldsymbol{e}_{z,i}) = \sum_{i=1}^{N} \left(\mathcal{E}_{\mathrm{sub},i} + \mathcal{E}_{\mathrm{mort},i}\right),$$

where

$$\mathcal{E}_{\mathrm{sub},i} = l_i(\boldsymbol{\phi}_i - \boldsymbol{\Pi}_{h,i}\boldsymbol{\phi}_i) - \mathcal{A}_i(\boldsymbol{z}_{h,i}, \boldsymbol{\phi}_i - \boldsymbol{\Pi}_{h,i}\boldsymbol{\phi}_i) - \mathcal{B}_i(\lambda_H, \boldsymbol{\phi}_i - \boldsymbol{\Pi}_{h,i}\boldsymbol{\phi}_i),$$

represents the subdomain discretization error, and

$$\mathcal{E}_{\mathrm{mort},i} = -\mathcal{C}_i(\boldsymbol{z}_{h,i}, \eta - Q_H\eta) - \mathcal{D}_i(\lambda_H, \eta - Q_H\eta),$$

represents the contribution to the mortar discretization error.

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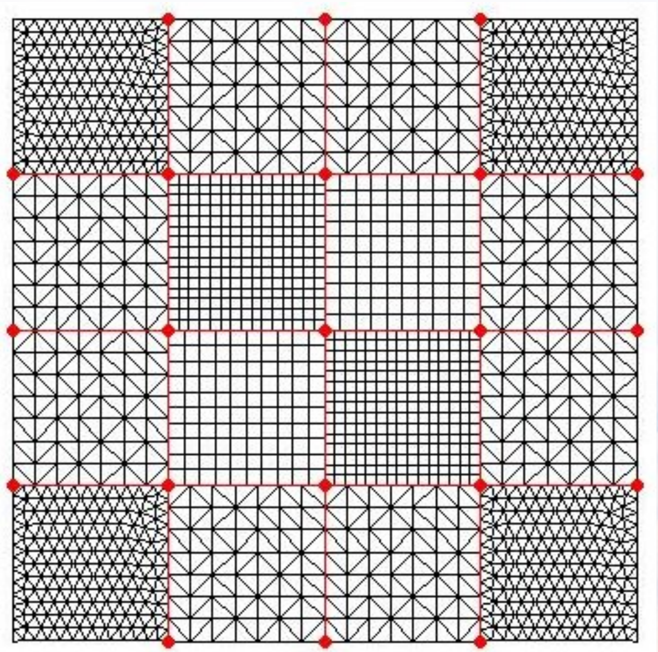
Example: Multiscale and Multinumerics

Let $\Omega = (0,1) \times (0,1)$ with

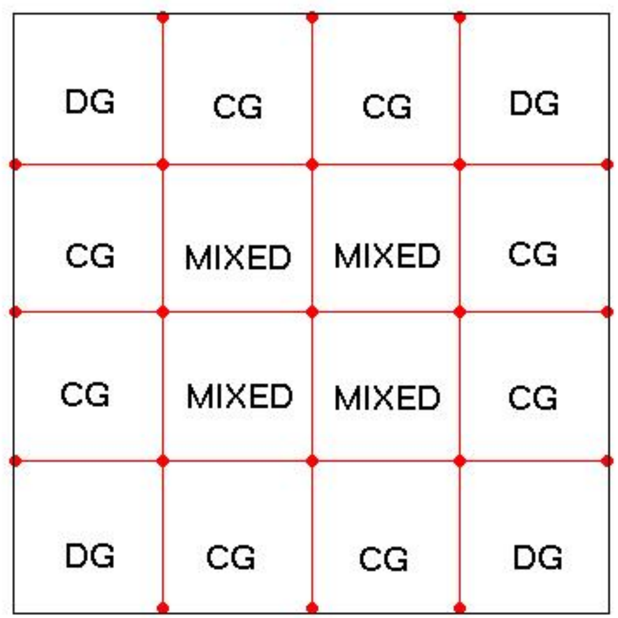
$$\boldsymbol{K}(x,y) = (1 + 0.8\sin(4\pi x)\cos(3\pi y))\mathbb{I}.$$

We choose f and g_D such that

$$p(x,y) = 10x(1-x)y(1-y)\exp(\sin(3\pi x)\sin(3\pi y)).$$



Domain decomposition



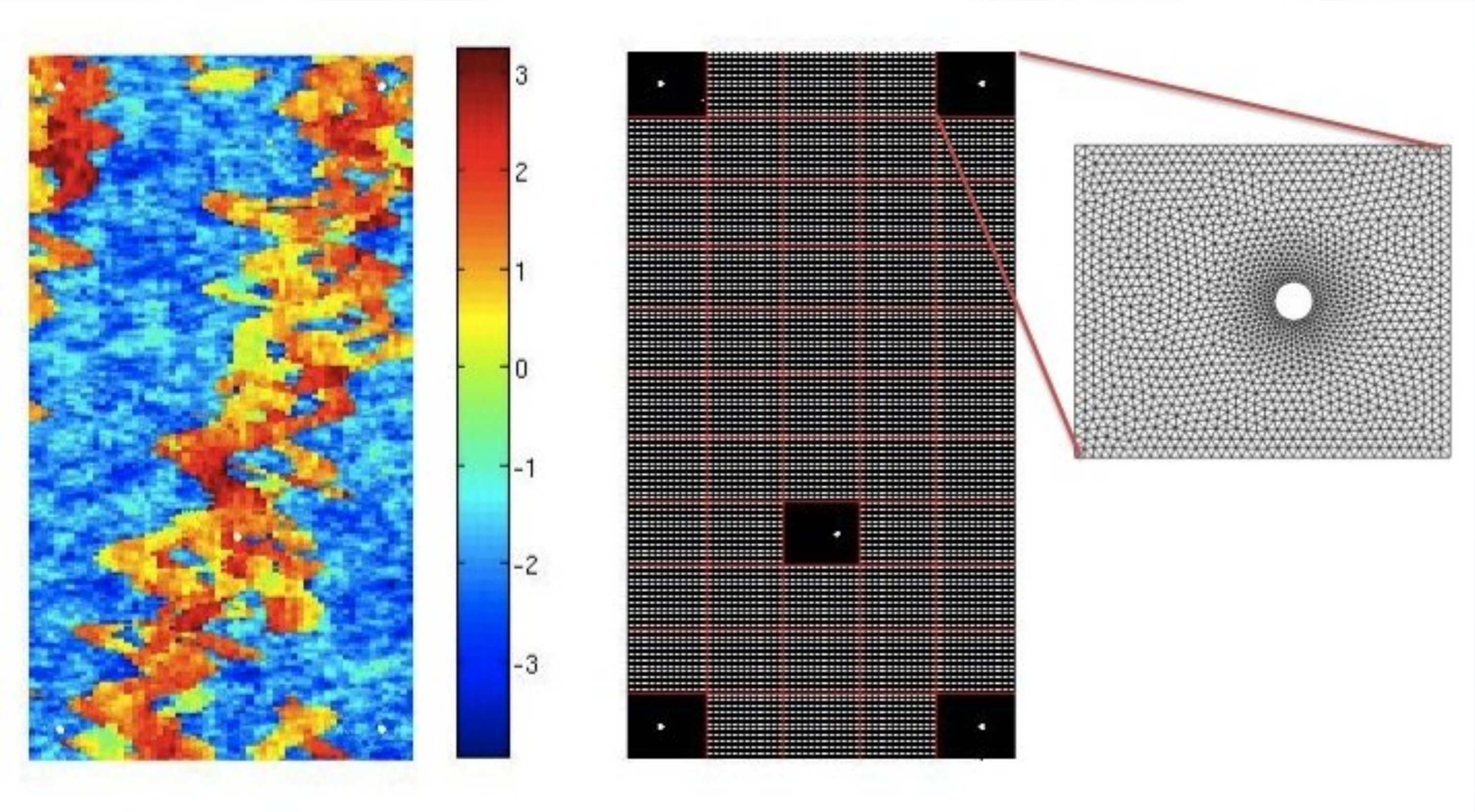
Subdomain numerical methods

Example: Multiscale and Multinumerics

QofI	$\mathcal{E}_{\text{sub}}$	$\mathcal{E}_{\text{mort}}$	True Error	Effectivity
1	-1.4960E-3	-4.1564E-4	-1.9166E-3	0.997
2	8.3416E-4	1.4993E-6	8.5018E-4	0.983
3	7.4364E-4	4.1535E-4	1.2002E-3	0.966

Table 1: Error estimates and effectivity ratios using three different quantities of interest using multinumerics.

Example: Mortar Adaptivity



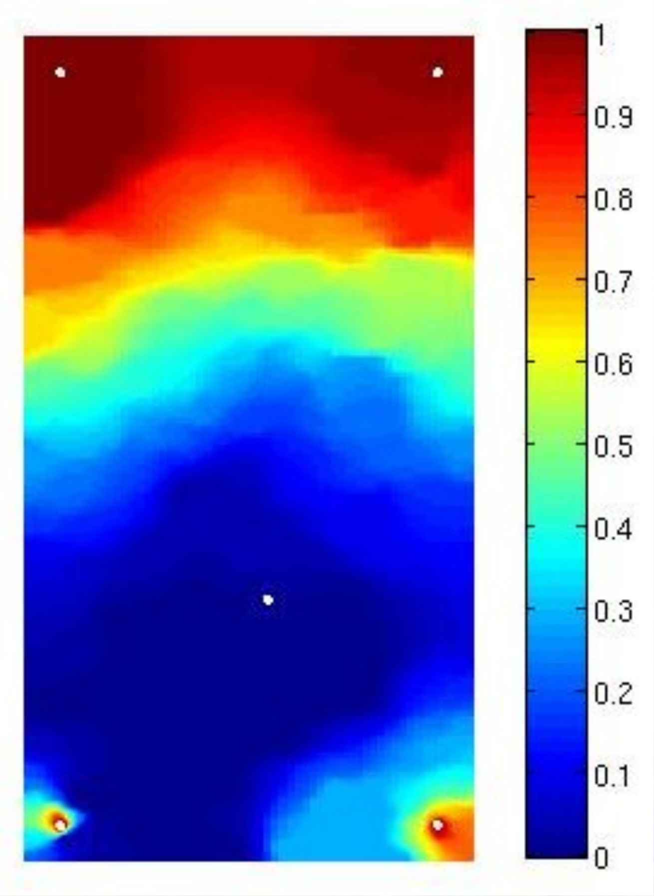
Consider layer 75 of SPE10 permeability field.

Decompose $\Omega = (0, 1200) \times (0, 2200)$ into 55 subdomains (5×11)

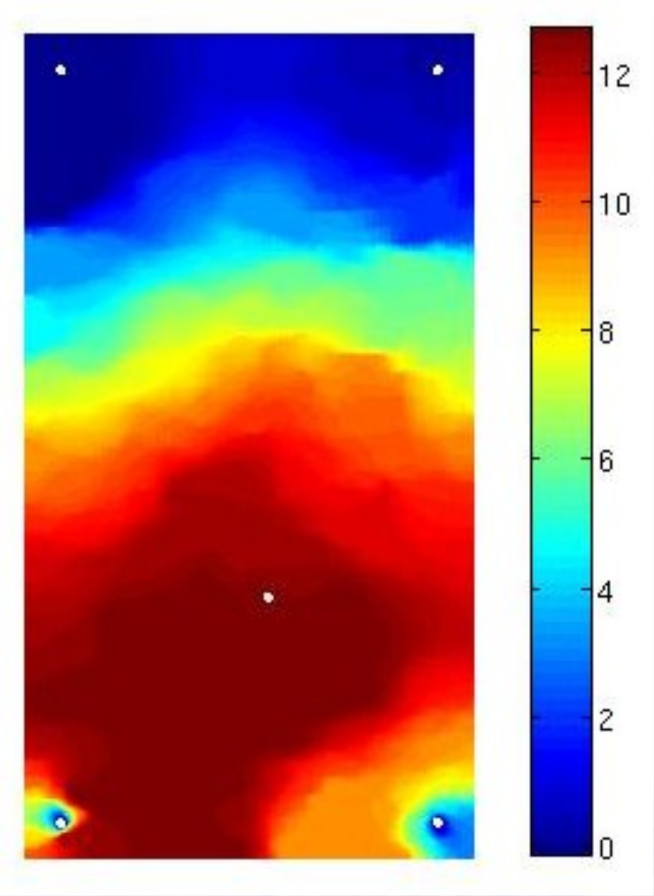
Subdomains with wells are refined up to well-bore and use DG (SIPG)

Remaining subdomains discretized using mixed method

Example: Mortar Adaptivity

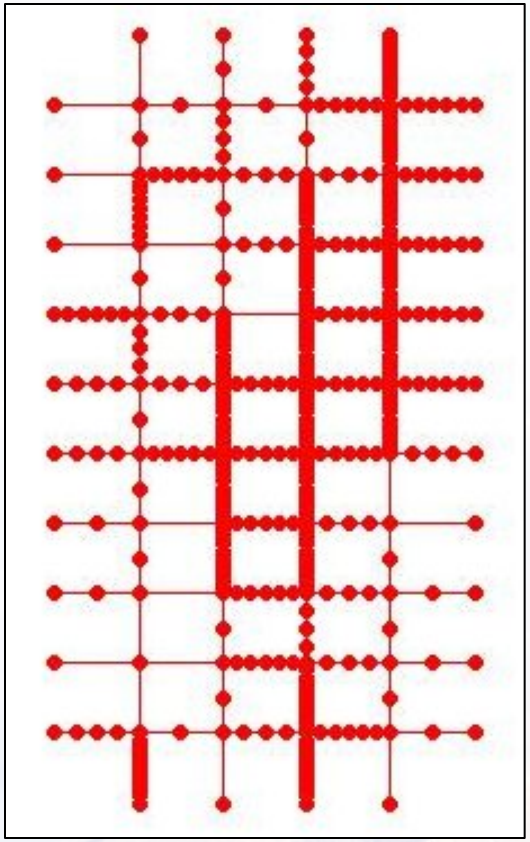


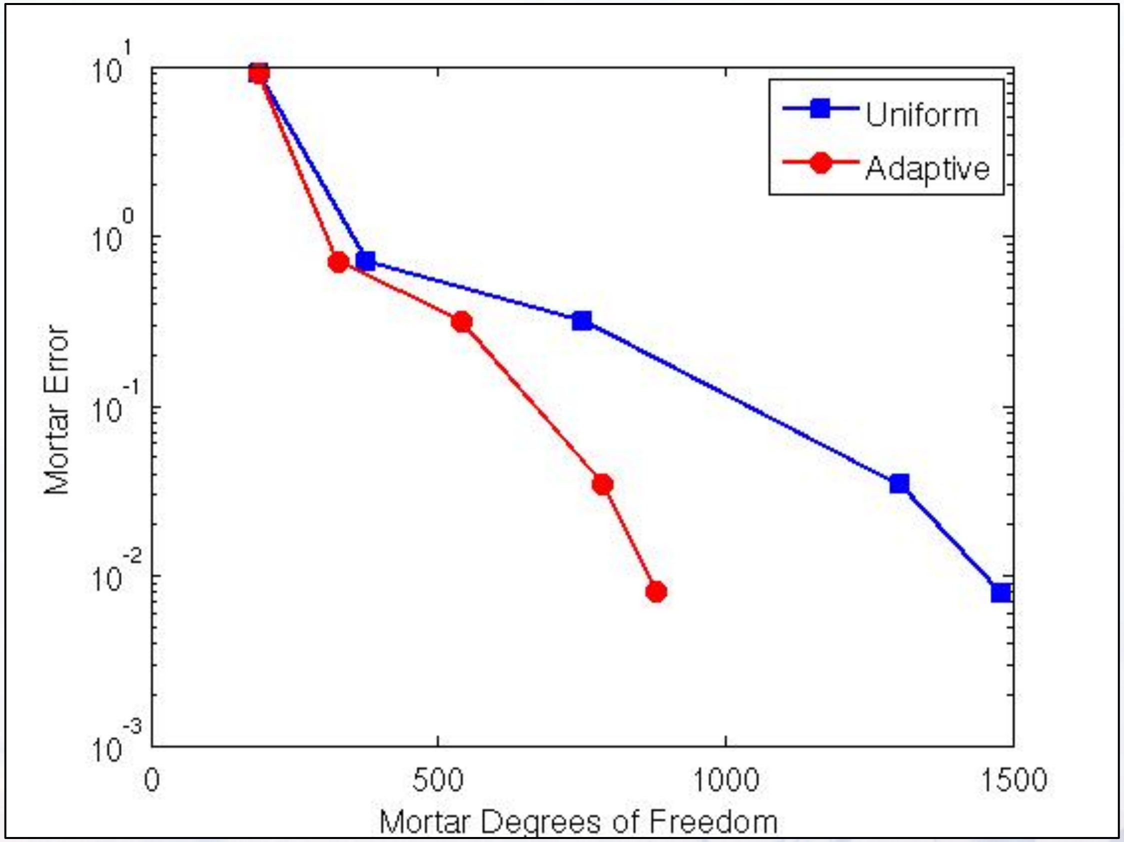
Forward solution



Adjoint solution. QofI is the average pressure at the production well.

Example: Mortar Adaptivity



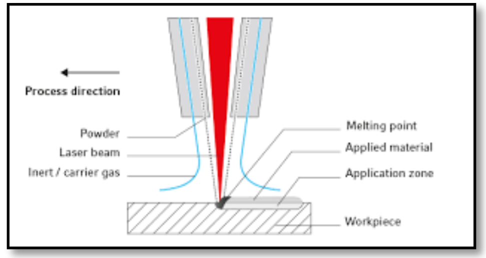


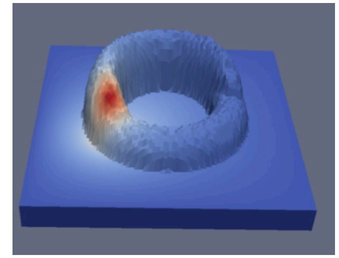
We fix the subdomain meshes and refine mortars until mortar error is comparable to subdomain error.

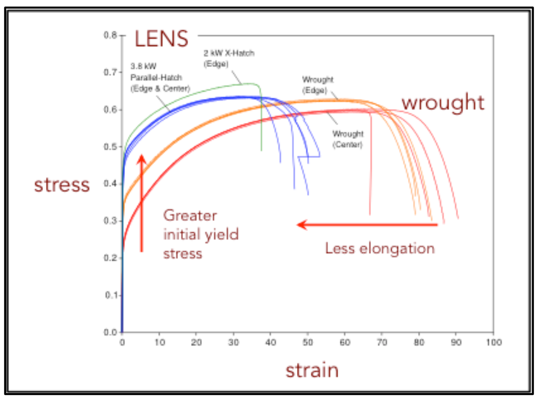
Current and Future Directions

Predict/Control Performance of Additive Manufacturing of Materials and Components with Quantified Uncertainty

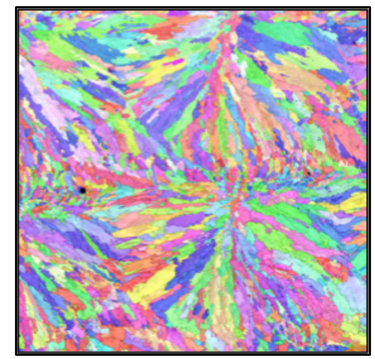
AM Process Modeling



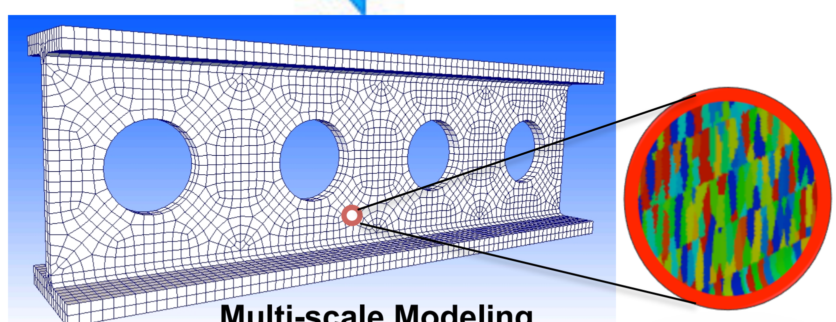




Component performance assessment
- J. Carroll (SNL)



Material characterization with quantified uncertainty
- J. Michael and D. Adams (SNL)

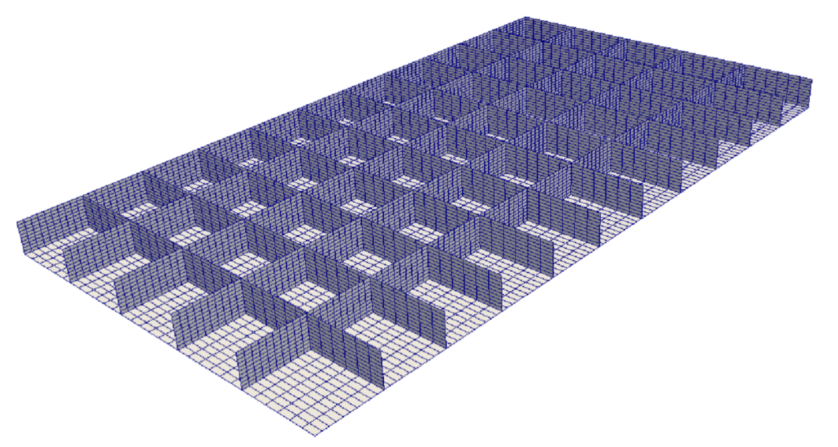


Multi-scale Modeling

Multiscale Modeling for Materials

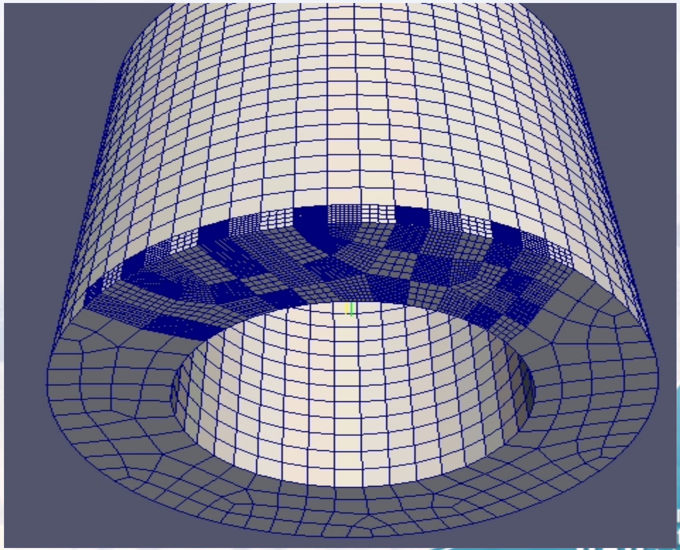
Previous work:

- Small number of subdomains: $\mathcal{O}(10)$
- Many DOFs per subdomain/mortar: $\mathcal{O}(10^3)$
- Iterative DD methods applicable



Current work:

- Large number of subdomains: $\mathcal{O}(10^6)$
- Few DOFs per mortar: $\mathcal{O}(10)$
- Iterative DD methods **NOT** applicable



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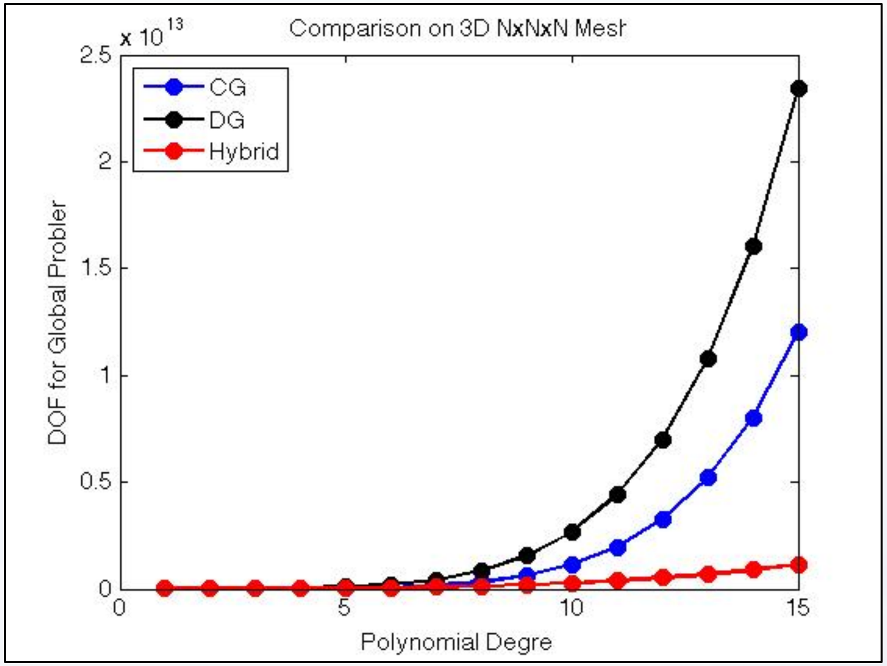
Relationship to Hybridizable DG Methods

At this extreme, we are very close to another method

Hybridizable DG methods are conceptually very similar

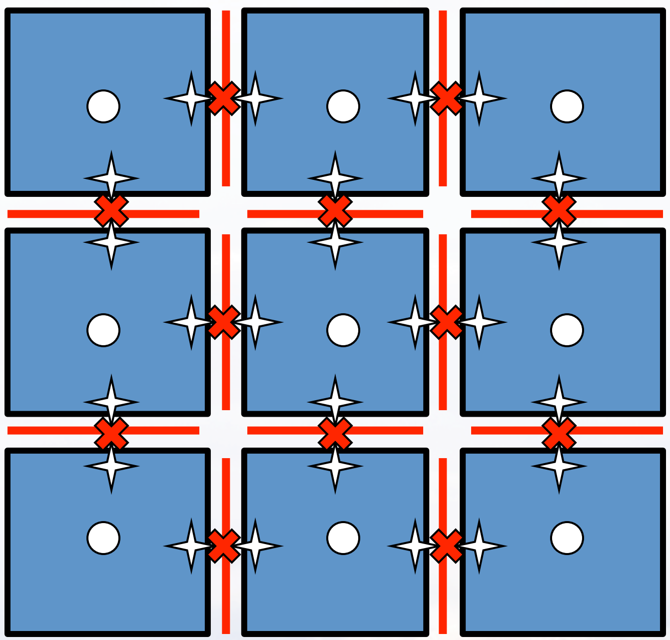
HDG methods have grown in popularity in recent years



Current work to show HDG is special case of multiscale mortar methods (with Tan Bui - UT Austin)

Multilevel Solvers for Hybridized Formulations

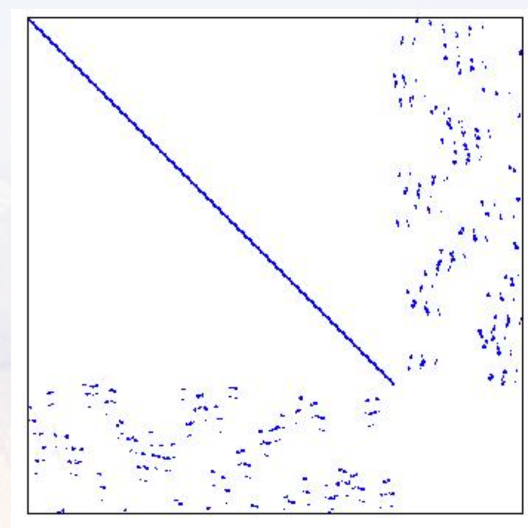
Hybridization of Mixed Methods



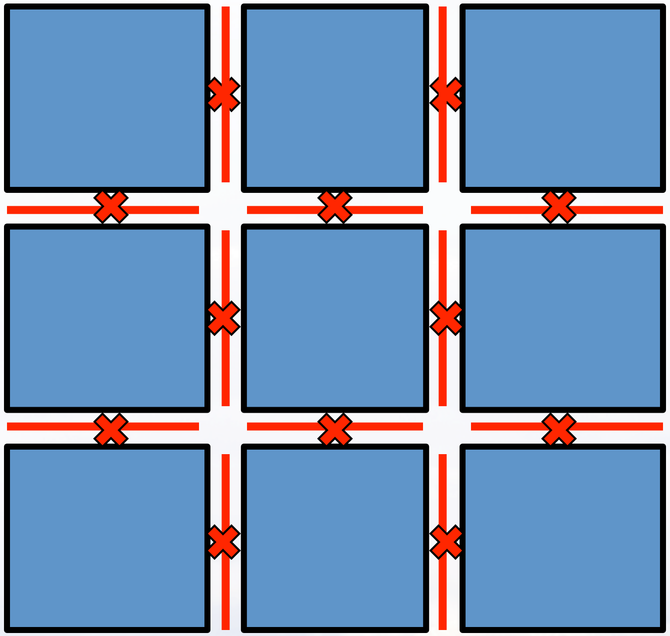
○ Pressure degree of freedom
✧ Velocity degree of freedom
✖ Lagrange multiplier dof

Introduce Lagrange multipliers on the element boundaries:

$$\begin{pmatrix} M & B & C \\ B^T & 0 & 0 \\ C^T & 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ p \\ \lambda \end{pmatrix} = \begin{pmatrix} \mathbf{g} \\ -f \\ 0 \end{pmatrix}$$



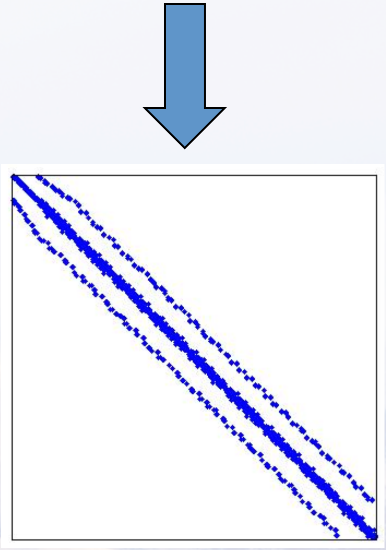
Hybridization of Mixed Methods



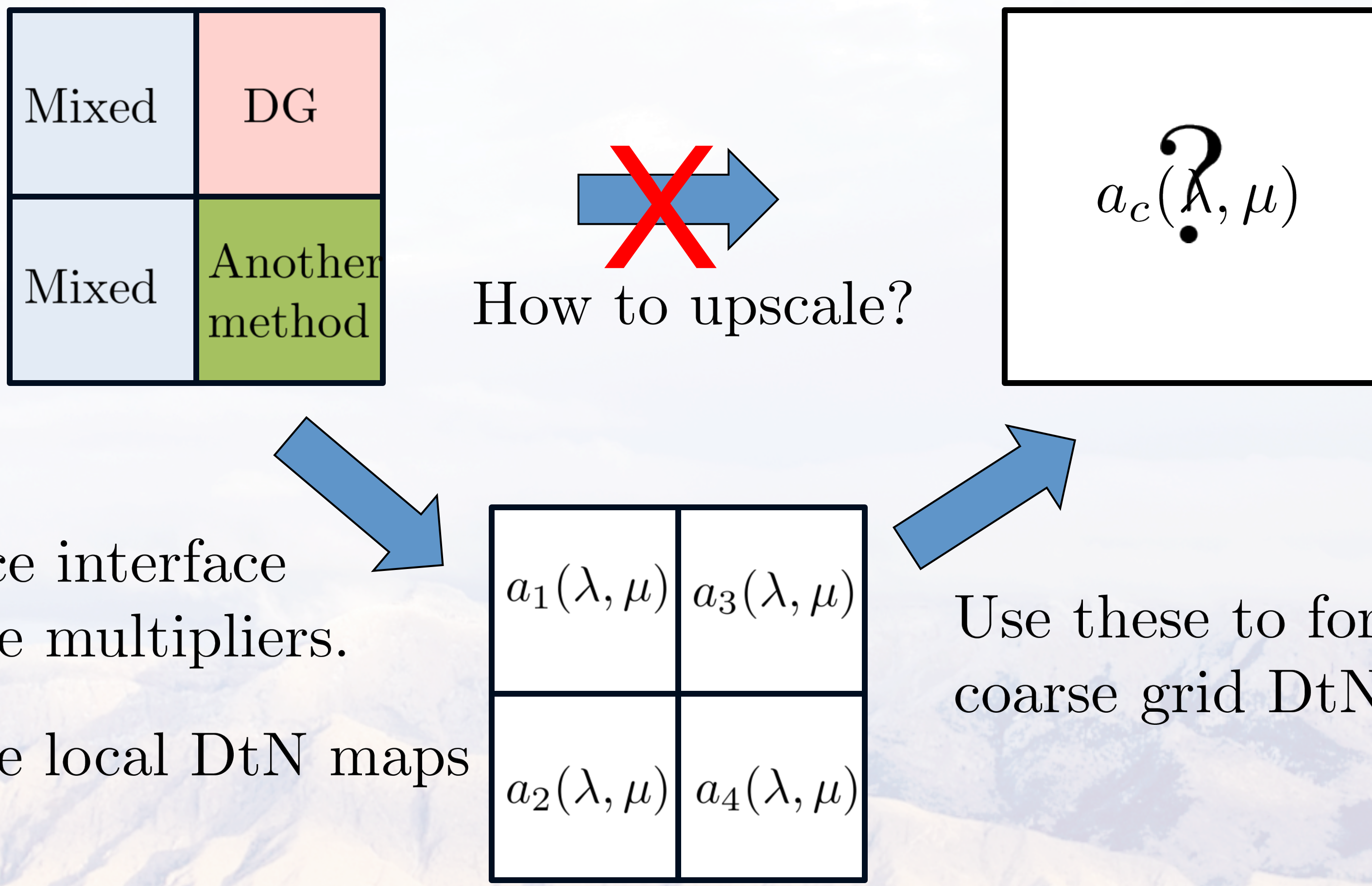
Lagrange multiplier dof

Reduce to Schur complement for Lagrange multipliers:

$$A\lambda = g$$



Defining Coarse Grid Operators



Introduce interface Lagrange multipliers.

Compute local DtN maps

Use these to form coarse grid DtN map?

A Multigrid Algorithm

Define a sequence of partitions

$$\mathcal{T}_1, \mathcal{T}_2, \ldots, \mathcal{T}_N = \mathcal{T}_h,$$

where each element $E_{k,i} \in \mathcal{T}_k$ consists of a union of fine grid elements.

To prove convergence, we need to assume each $E_{k,i}$ is sufficiently regular to allow $\mathrm{H}^{3/2+\alpha}$ regularity.

Assume there exists constants $0 < c \leq C$ such that

$$c h_k \leq h_{k-1} \leq C h_k, \quad 1 \leq k \leq N.$$

Define interface grids

$$\mathcal{E}_1, \mathcal{E}_2, \ldots, \mathcal{E}_N = \mathcal{E}_h,$$

with the corresponding nonnested Lagrange multiplier spaces,

$$M_1, M_2, \ldots, M_N = M_h.$$

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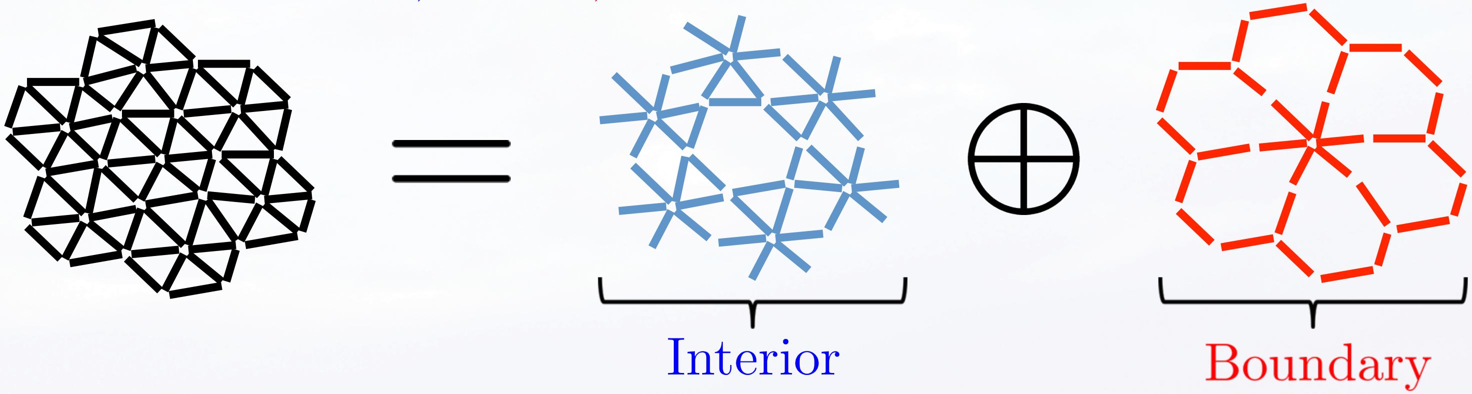
A Multigrid Algorithm

Decompose each $M_k = M_{k,I} \oplus M_{k,B}$.



Note that $M_{k-1} \subset M_{k,B}$ for $2 \leq k \leq N$.

Define a sequence of symmetric positive definite bilinear forms and energy norms,

$$a_k(\cdot,\cdot) : M_k \times M_k \to \mathbb{R}, \quad |||\mu|||_k^2 = a_k(\mu,\mu), \quad 1 \leq k \leq N,$$

We associate with $a_k(\cdot,\cdot)$ an operator $A_k : M_k \to M_k$ satisfying for any $\lambda \in M_k$,

$$\langle A_k \lambda, \mu \rangle_k = a_k(\lambda,\mu), \quad \forall\, \mu \in M_k.$$

A Multigrid Algorithm

Given $M_k = M_{k,I} \oplus M_{k,B}$, the operator A_k can be written as,

$$A_k = \begin{pmatrix} A_{k,II} & A_{k,IB} \\ A_{k,BI} & A_{k,BB} \end{pmatrix}$$

The intergrid transfer operators $I_k : M_{k-1} \to M_k$ are defined by

$$I_k := \begin{pmatrix} -A_{k,II}^{-1} A_{k,IB} J_k \\ J_k \end{pmatrix}$$

where $J_k : M_{k-1} \to M_{k,B}$ is the natural injection.

Each $a_k(\cdot, \cdot)$ is constructed such that the variational equality and norm equivalence

$$a_{k-1}(\lambda, \mu) = a_k(I_k \lambda, I_k \mu), \quad |||\lambda|||_{k-1} = |||I_k \lambda|||_k,$$

hold for all $\lambda, \mu \in M_{k-1}$.

A Multigrid Algorithm

On M_1 we define $B_1 = A_1^{-1}$.

On level k, $2 \leq k \leq N$, assume B_{k-1} is defined.

Define $B_k g$ as follows:

$$
\begin{array}{r|l}
\textit{Initialization} & x^{\{0\}} = 0, \\
& \\
\textit{Presmoothing} & x^{\{1\}} = x^{\{0\}} + G_{k,m}\left(g - A_k x^{\{0\}}\right), \\
\textit{Local Correction} & x^{\{2\}} = x^{\{1\}} + T_k\left(g - A_k x^{\{1\}}\right), \\
\textit{Coarse Grid Correction} & x^{\{3\}} = x^{\{2\}} + I_k B_{k-1} Q_{k-1}\left(g - A_k x^{\{2\}}\right), \\
\textit{Local Correction} & x^{\{4\}} = x^{\{3\}} + T_k\left(g - A_k x^{\{3\}}\right), \\
\textit{Postsmoothing} & x^{\{5\}} = x^{\{4\}} + G_{k,m}\left(g - A_k x^{\{4\}}\right). \\
& \\
\textit{Final result} & B_k g = x^{\{5\}}
\end{array}
$$

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A Multigrid Algorithm

Theorem

If all of the above assumptions are satisfied and if the number of smoothing steps on each level satisfy

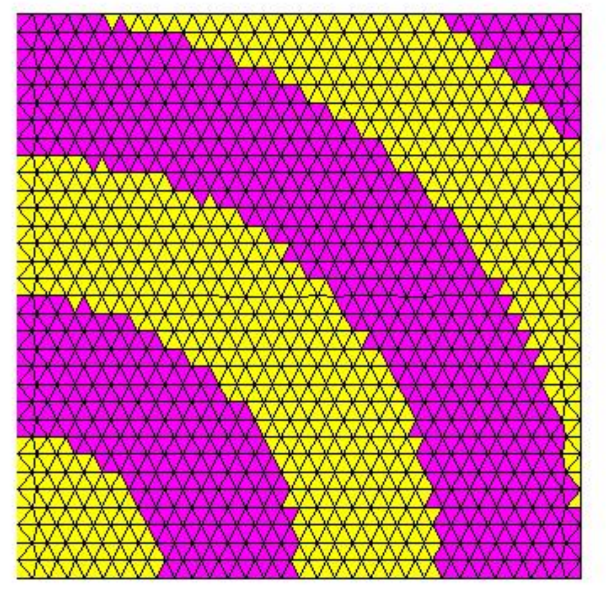
$$\beta_0 m_k \leq m_{k-1} \leq \beta_1 m_k,$$

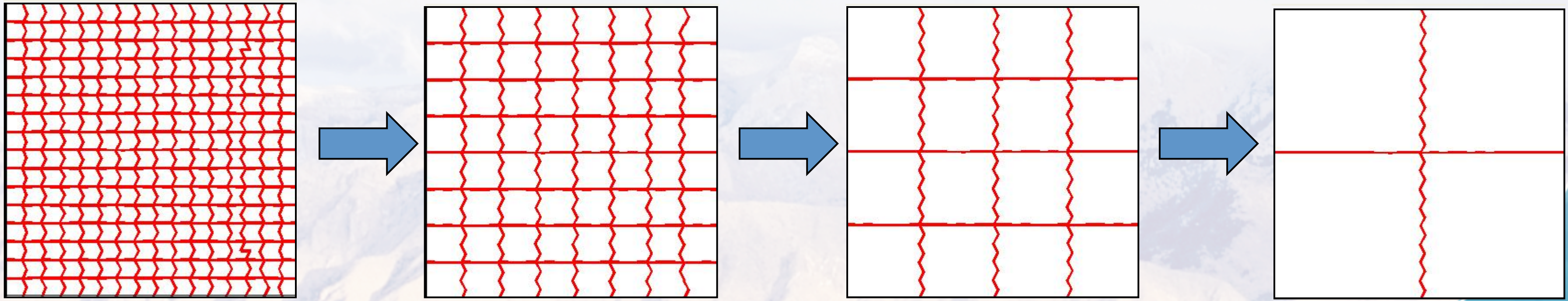
for some $1 < \beta_0 \leq \beta_1$, then there exists $0 < \delta < 1$ independent of h such that,

$$a_N((I - B_N A_N)\mu, \mu) \leq \delta a_N(\mu, \mu), \quad \forall\, \mu \in M_N.$$

Laplace Equation – Multinumerics

Model	Laplace equation
Domain	$(0,1) \times (0,1)$
Method	DG-NIPG$_1$ (Yellow)
Method	Mixed-RT$_1$ (Pink)
Mesh	Triangles
True solution	$p = xye^{x^2 y^3}$
Tolerance	1×10^{-6}





Laplace Equation – Multinumerics

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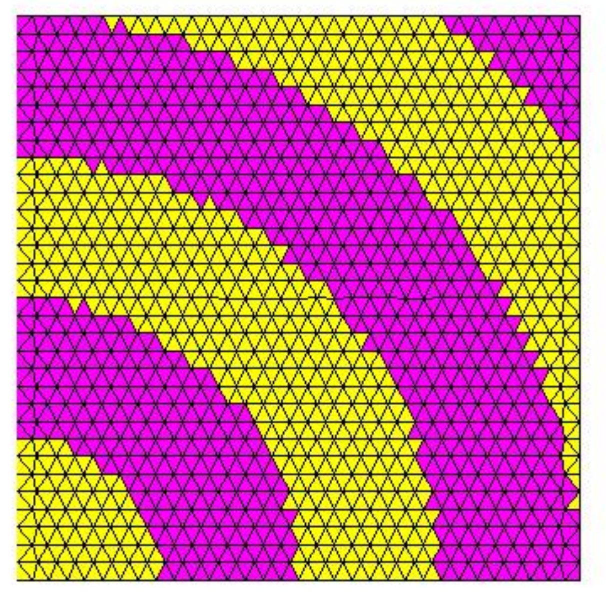
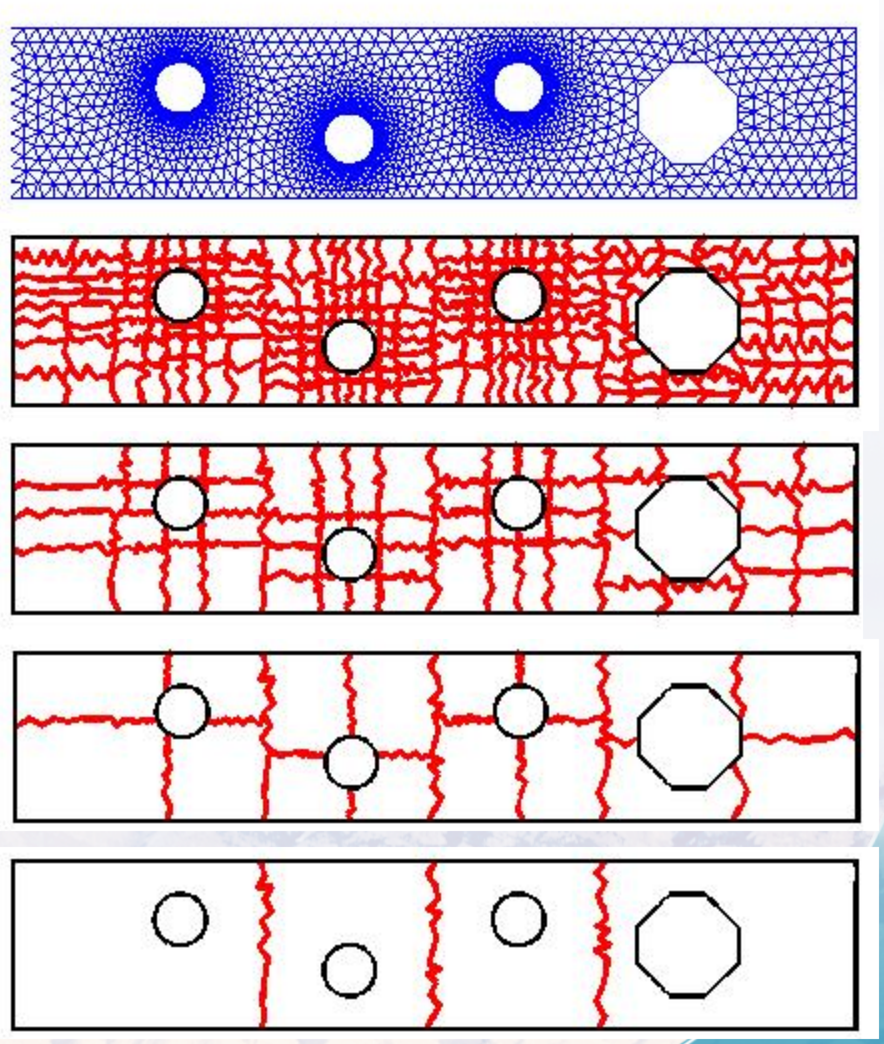


Levels	DOF	V-cycles	MG Factor
3	224	8	0.19
4	960	8	0.19
5	3968	8	0.20
6	16128	8	0.20

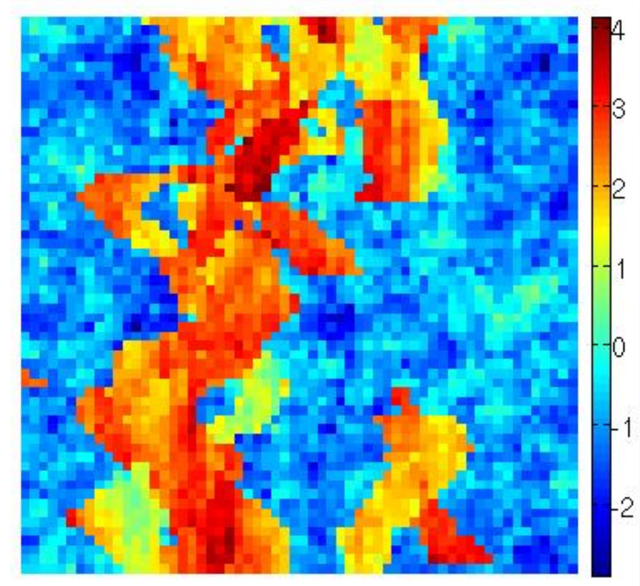
Poisson Equation – Unstructured Mesh

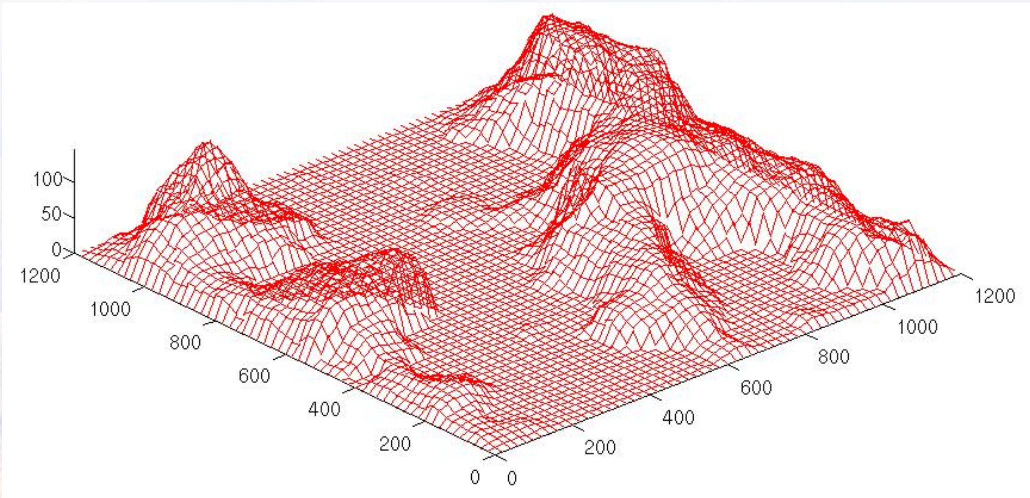
Model	Poisson equation
Permeability	$5.5e^{\sin(2\pi x)}$
Method	Mixed RT_1
Tolerance	1×10^{-6}
Degrees of freedom	11492
Levels	5
V-cycles	29
Convergence rate	0.51
PCG Iters	11



Single Phase Flow with Heterogeneities

Model	Single phase - incompr.
Domain	$(0, 1200) \times (0, 1200)$
Method	Mixed RT_1
Mesh	Quadrilaterals
Permeability	Layer 75 from SPE10
Tolerance	1×10^{-6}
Degrees of freedom	52240
Levels	8
V-cycles	27
Convergence rate	0.57
PGMRES Iters.	8





Conclusions

Conclusions

- Multiscale mortar methods provide a flexible modeling framework with a solid mathematical foundation
- Avoids the need to upscale model parameters
- Applicable to multiphysics and multinumerics
- Related to non-overlapping domain decomposition and HDG
- Variational framework well-suited for
  - Goal-oriented error estimates
  - Optimization
  - Embedded UQ
- New opportunities for modeling and simulation

Thank you for your attention!
Questions?