Multilevel Modeling: Multigrid's Lost Twin

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Single-Phase Flow

Steady-state flow of a fluid that entirely fills the pore-space of a porous medium (e.g., porous rock), may be described by,

$$
\begin{aligned}
\nabla \cdot \mathbf{u} &= Q(\mathbf{r}) \qquad \textit{(mass conservation)} \\
\mathbf{u} &= -\frac{\mathcal{K}(\mathbf{r})}{\mu} \nabla p \qquad \textit{(Darcy's law)}
\end{aligned}
$$

for $\mathbf{r} \in \Omega$ and subject to appropriate boundary conditions.
Here the variables are defined as follows:

$\mathbf{u}$	fluid velocity
p	pressure
$\mathcal{K}(\mathbf{r})$	absolute permeability
μ	fluid viscosity

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Motivation for Multilevel Methods

Multilevel Modeling

- multilevel approximate solution must be cheaper than an optimal solution of the fine-grid problem (this is often violated by two-level or two-scale methods)
- we want large coarsening factors (i.e. 100 in each direction).
- we cannot rely on scale separation
- we want to control the trade-off between accuracy and cost
- we can leverage ideas and frameworks from multigrid solvers
- there is excellent potential for building algorithms with error estimation

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Multigrid

It's not just for solving equations anymore!

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Multigrid

It's not just for solving equations anymore!

It provides a framework for constructing multilevel multiscale simulations algorithms.

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The Residual or Defect Equation

Let u be the exact solution and $u^{(i)}$ be the current iterate.
The *error* associated with the current iterate:

$$e^{(i)} = u - u^{(i)}$$

The *residual* associated with the current iterate:

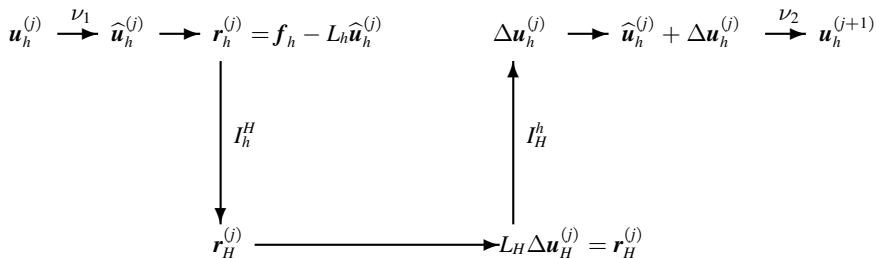$$r^{(i)} = f - Lu^{(i)} = Lu - Lu^{(i)} = L\left(u - u^{(i)}\right)$$

Combining these definitions we obtain the *residual equation*

$$Le^{(i)} = r^{(i)}$$

which will play a key role role in our development of the multigrid algorithm
(particularly approximations to it).

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Two Grid Iteration: Correction Scheme (CS)

Schematic of the two-grid CS iteration

$$u_h^{(j)} \xrightarrow{\nu_1} \widehat{u}_h^{(j)} \longrightarrow r_h^{(j)} = f_h - L_h\widehat{u}_h^{(j)} \qquad \Delta u_h^{(j)} \longrightarrow \widehat{u}_h^{(j)} + \Delta u_h^{(j)} \xrightarrow{\nu_2} u_h^{(j+1)}$$

$$\Big\downarrow I_h^H \qquad\qquad\qquad \Big\uparrow I_H^h$$

$$r_H^{(j)} \longrightarrow L_H \Delta u_H^{(j)} = r_H^{(j)}$$

The associated iteration matrix is

$$G_h^H = S_h^{\nu_2} K_h^H S_h^{\nu_1} \qquad \text{with} \qquad K_h^H = I_h - \left(I_H^h L_H^{-1} I_h^H \right) L_h$$

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The Nonlinear Residual Equation

Consider a nonlinear equation, $N(u) = f$. Let u be the exact solution and $u^{(i)}$ be the current iterate.

The *error* associated with the current iterate:

$$e^{(i)} = u - u^{(i)}$$

The *residual* associated with the current iterate:

$$r^{(i)} = f - N(u^{(i)}) = N(u) - N(u^{(i)})$$
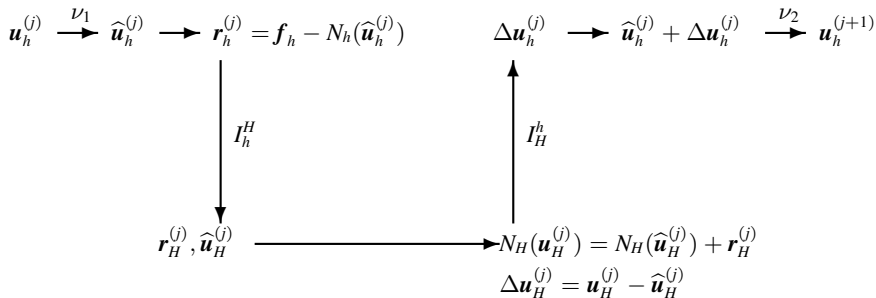
We can't combine these definitions as easily to obtain an equation relating the residual and the error, but we can write

$$r^{(i)} = N(u^{(i)} + e^{(i)}) - N(u^{(i)})$$

which will play a key role role in the development of the Full Approximation Scheme (FAS) multigrid algorithm.

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Two Grid Iteration: Full Approximation Scheme (FAS)

Schematic of the two-grid FAS iteration

$$\boldsymbol{u}_h^{(j)} \xrightarrow{\nu_1} \widehat{\boldsymbol{u}}_h^{(j)} \longrightarrow \boldsymbol{r}_h^{(j)} = \boldsymbol{f}_h - N_h(\widehat{\boldsymbol{u}}_h^{(j)}) \qquad \Delta\boldsymbol{u}_h^{(j)} \longrightarrow \widehat{\boldsymbol{u}}_h^{(j)} + \Delta\boldsymbol{u}_h^{(j)} \xrightarrow{\nu_2} \boldsymbol{u}_h^{(j+1)}$$

$$\Big\downarrow I_h^H \qquad\qquad\qquad \Big\uparrow I_H^h$$

$$\boldsymbol{r}_H^{(j)}, \widehat{\boldsymbol{u}}_H^{(j)} \longrightarrow N_H(\boldsymbol{u}_H^{(j)}) = N_H(\widehat{\boldsymbol{u}}_H^{(j)}) + \boldsymbol{r}_H^{(j)}$$
$$\Delta\boldsymbol{u}_H^{(j)} = \boldsymbol{u}_H^{(j)} - \widehat{\boldsymbol{u}}_H^{(j)}$$

Comments:

- If N is linear, then the FAS and CS iterates are identical
- The coarse-grid equation may be written,
  $$N_H(\boldsymbol{u}_H^{(j)}) = \boldsymbol{f}_H + \tau_h^H \qquad \text{with} \qquad \tau_h^H = N_H(I_h^H \widehat{\boldsymbol{u}}_h^{(j)}) - I_h^H N_h(\widehat{\boldsymbol{u}}_h^{(j)})$$

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Motivation for Multilevel Methods

Which scale is up, in the full approximation scheme (FAS)

"Instead of regarding the coarse grid as a device for accelerating convergence on the fine grid, we can view the fine grid as a device for calculating the correction, τ_h^H, to the coarse-grid equations."
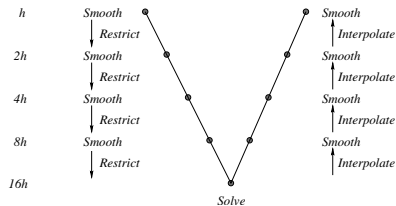
(Brandt, *Multigrid Techniques: 1984 Guide*)

W. L. Briggs, V. E. Henson, and S. F. McCormick, *A Multigrid Tutorial*, SIAM Books, 2000.
U. Trottenberg, C. Oosterlee, and A. Schuller, *Multigrid*, Academic Press, 2001.

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Schematic of Multigrid Cycles

Multigrid uses coarser resolutions recursively to obtain an approximation to the error at the finest resolution

Grid Spacing

h — Smooth / Restrict ... Smooth / Interpolate

2h — Smooth / Restrict ... Smooth / Interpolate

4h — Smooth / Restrict ... Smooth / Interpolate

8h — Smooth / Restrict ... Smooth / Interpolate

16h — Solve

W-cycle, recursion parameter $\gamma = 2$.
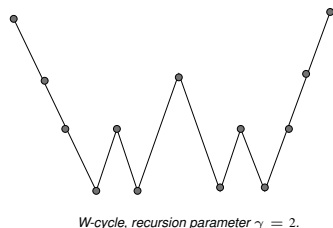
Convergence rate is independent of the grid resolution,
Solving Poisson problems on structured grids using a $V(1,1)$-cycle achieves a convergence rate of ≈ 0.05.
Solving diffusion problems with highly discontinuous coefficients using a $V(1,1)$-cycle achieves a convergence rate of $\approx 0.05 - 0.25$.

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Robust Multigrid on Structured Grids: BoxMG

Coarsening:

- selected *a priori*, e.g., standard or semi-coarsening

Smoothing:

- selected to complement the coarsening/interpolation
- standard coarsening: alternating line (2D), plane relaxation (3D)

Interpolation: I_{k-1}^k

- constructed from the discrete operator L_k
- approximately preserves the continuity of $\mathbf{u} \cdot \mathbf{n}$

Variational Coarse Grid Operator: $L_{k-1} = (I_{k-1}^k)^* L_k I_{k-1}^k$

- minimizes the error in the range of the interpolation

Restriction: $J_k^{k-1} = (I_{k-1}^k)^*$

- dictated by variational principle, and preserves symmetry of L_k

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Robust Multigrid on Unstructured Grids: AMG

Smoothing:

- selected *a priori*, e.g., point Gauss-Siedel

Coarsening:

- multipass selection designed to complement smoothing/interpolation
- heuristics relate stencil weights to algebraically smooth errors

Interpolation: I_{k-1}^k

- constructed from the discrete operator L_k
- based on chosen coarse grid and algebraically smooth errors

Variational Coarse Grid Operator: $L_{k-1} = (I_{k-1}^k)^* L_k I_{k-1}^k$

- minimizes the error in the range of the interpolation

Restriction: $J_k^{k-1} = (I_{k-1}^k)^*$

- dictated by variatinal principle, and preserves symmetry of L_k

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Is there an optimal coarse-grid operator?

Objective: Minimize the error in the range of the interpolation

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Is there an optimal coarse-grid operator?

Objective: Minimize the error in the range of the interpolation

Consider the equivalent variational formulation:

$$u^h = \min_{v \in \mathcal{H}} \left\{ \mathcal{L}\left[v\right] \equiv \frac{1}{2} v^T L_h v - v^T f_h \right\}$$

Let $\tilde{u}^h$ be an approximation obtained after smoothing, then the error $e^h \equiv u^h - \tilde{u}^h$ is smooth and is well approximated on a coaser grid.

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$$u^h = \min_{v \in \mathcal{H}} \left\{ \mathcal{L}\left[v\right] \equiv \frac{1}{2} v^T L_h v - v^T f_h \right\}$$

Let $\tilde{u}^h$ be an approximation obtained after smoothing, then the error $e^h \equiv u^h - \tilde{u}^h$ is smooth and is well approximated on a coaser grid. Substituting the interpolant, $u^h \approx \tilde{u}^h + I_{2h}^h e^{2h}$, into the functional

$$\mathcal{L}\left[u^h\right] = \left(\tilde{u}^h + I_{2h}^h e^{2h}\right)^T L_h \left(\tilde{u}^h + I_{2h}^h e^{2h}\right) - \left(\tilde{u}^h + I_{2h}^h e^{2h}\right)^T f_h$$

$$\frac{\partial \mathcal{L}}{\partial e^{2h}} = 0 \Rightarrow \left(I_{2h}^h\right)^T L_h I_{2h}^h e^{2h} = \left(I_{2h}^h\right)^T \left(b_h - L_h \tilde{u}^h\right)$$

This implies that the coarse-grid operator is given by

$$L_{2h} = \left(I_{2h}^h\right)^T L_h I_{2h}^h \quad \text{and} \quad f_{2h} = \left(I_{2h}^h\right)^T \left(f_h - L_h \tilde{u}^h\right)$$

A. Brandt, Multigrid Techiques: 1984 Guide with Applications to Fluid Dynamics, The Weizmann Institute of Applied Science, 1984.

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Multilevel Interpretation of Basis Functions

Consider a fine-scale bilinear FEM discretization on grid level k,

$$\left(L_k\right)_{ij} = e_j^T L_k e_i = \int_\Omega \left(\mathcal{K}(\boldsymbol{r}) \nabla \varphi_i^k, \nabla \varphi_j^k\right) d\Omega$$

Variational coarsening leads to

$$\left(L_{k-1}\right)_{ij} = \left(\left[I_k^{k-1}\right]^T L_k I_{k-1}^k\right)_{ij} = \left[I_k^{k-1} e_j^{k-1}\right]^T L_k \left[I_k^{k-1} e_i^{k-1}\right]$$

$$= \left(\sum_l p_{lj} e_l^k\right)^T L_k \left(\sum_m p_{mi} e_m^k\right)$$

$$= \int_\Omega \left(\mathcal{K}(\boldsymbol{r}) \nabla\left\{\sum_m p_{mi} \varphi_m^k\right\}, \nabla\left\{\sum_l p_{jl} \varphi_l^k\right\}\right) d\Omega$$

Thus we have a recursive definition of our multiscale basis function

$$\varphi_j^{k-1} = \sum_m p_{mi} \varphi_m^k$$

Grauschopf, T., M. Griebel, and H. Regler, *Appl. Numer. Math.*, **23**, pp. 63–96, 1997.

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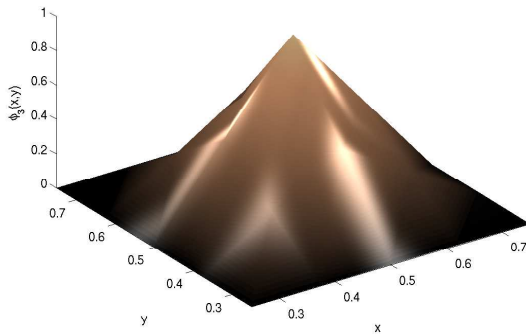Variational Coarsening and Multilevel Basis Functions

Multilevel Basis Functions

An approximation to the influence of fine-scale structure is efficiently generated through variational coarsening and stored in the interpolation weights:
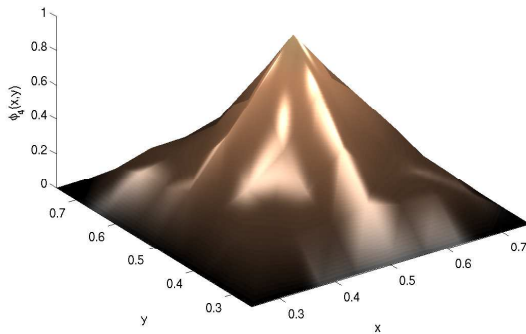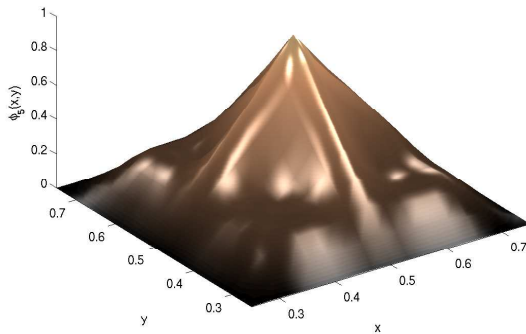

A tiling with a simple periodic inclusion: inclusions have $K = 10^3$, the background has $K = 1$.

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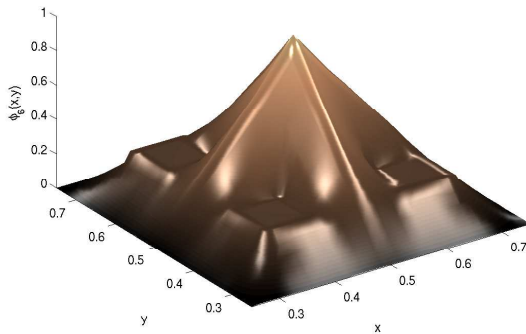

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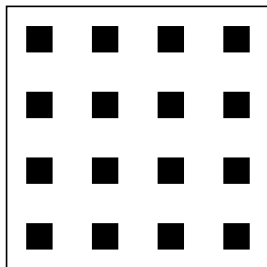Multilevel Modeling
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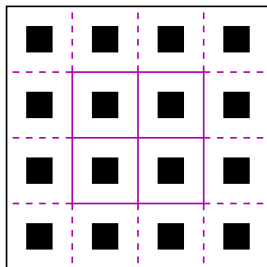
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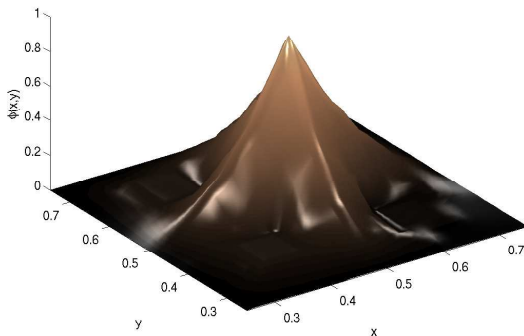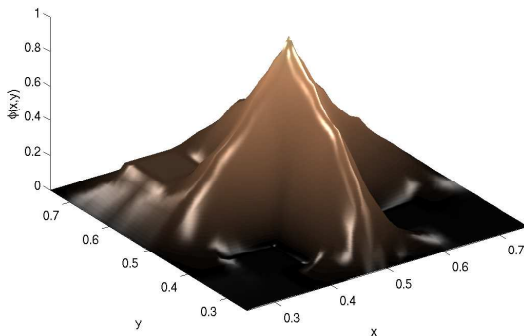
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Adaptive Algebraic Multigrid αAMG

Motivation:

- we may not know *a priori* how to characterize algebraically smooth error
- assumptions made in the operator-induced interpolation of BoxMG and AMG may be inconsistent with the actual algebraically smooth error

Components of αAMG:

- first, consider the fine level.
- use relaxation on the homogeneous problem to expose the local character of algebraic smoothness
- use this information to define interpolation through a local collapsing of the operator that fits this prototypical algebraically smooth error
- use galerkin coarsening to define the coarse-grid operator
- apply these ideas recursively to construct a complete hierarchy of components

M. Brezina, R. Falgout, S. MacLachlan, et al., Adaptive Algebraic Multigrid, SIAM J. Sci. Comp., 27, pp. 1261–1286, 2006.

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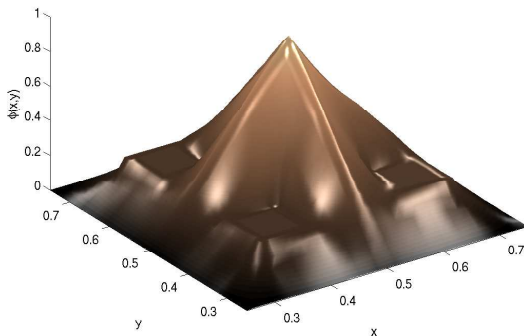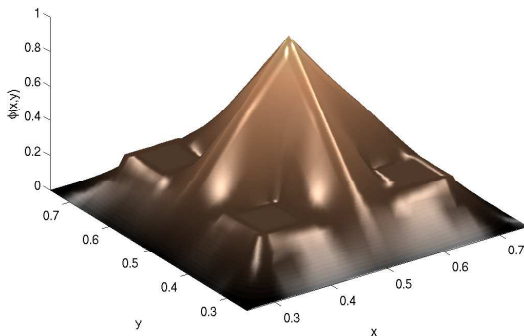
Adaptive Generation of Basis functions

An approximation to the influence of fine-scale structure is efficiently generated through variational coarsening and stored in the interpolation weights:

A tiling with a simple periodic inclusion: inclusions have $K = 10^3$, the background has $K = 1$.

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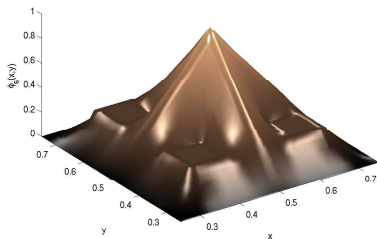
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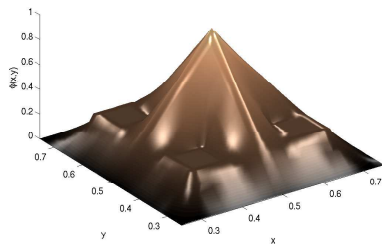

The multilevel basis function at $(\frac{1}{2}, \frac{1}{2})$ after one αAMG cycle: $\rho = 0.973$.

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An approximation to the influence of fine-scale structure is efficiently generated through variational coarsening and stored in the interpolation weights:

The multilevel basis function at $(\frac{1}{2}, \frac{1}{2})$ after two αAMG cycle: $\rho = 0.851$.

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An approximation to the influence of fine-scale structure is efficiently generated through variational coarsening and stored in the interpolation weights:

The multilevel basis function at $(\frac{1}{2}, \frac{1}{2})$ after three αAMG cycle: $\rho = 0.375$.

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The multilevel basis function at $(\frac{1}{2}, \frac{1}{2})$ after four αAMG cycle: $\rho = 0.100$.

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Similarity of BoxMG and αAMG Basis Functions

Both algorithms exibit similar convergence rates and use very similar basis functions.

BoxMG multiscale basis function.

αAMG multiscale basis function.

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Multilevel Upscaling: Single Phase Flow
Multilevel Mimetic Multiscale (M^3): Two-Phase Flow

A Truly Multilevel Upscaling (MLUPS) Algorithm

MLUPS uses the components of robust multigrid methods to:

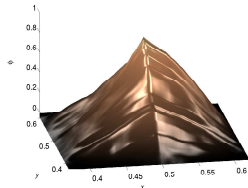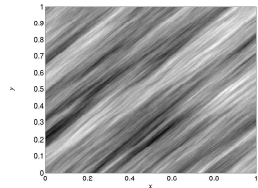1. construct a complete hierarchy of coarse-scale discrete models
2. compute multiscale basis functions efficiently
   (i.e., no fine-scale linear solves on coarse-scale patches)
3. provide a flexible methodology to achieve the desired accuracy
   efficiently (i.e., moving towards a flexible FAS methodology).

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A Truly Multilevel Upscaling (MLUPS) Algorithm

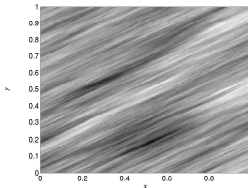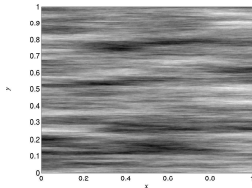*MLUPS uses the components of robust multigrid methods to:*

1. construct a complete hierarchy of coarse-scale discrete models
2. compute multiscale basis functions efficiently
   (i.e., no fine-scale linear solves on coarse-scale patches)
3. provide a flexible methodology to achieve the desired accuracy
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Multilevel Upscaling: Single Phase Flow
Multilevel Mimetic Multiscale (M^3): Two-Phase Flow

A Truly Multilevel Upscaling (MLUPS) Algorithm

MLUPS uses the components of robust multigrid methods to:

1. construct a complete hierarchy of coarse-scale discrete models
2. compute multiscale basis functions efficiently
   (i.e., no fine-scale linear solves on coarse-scale patches)
3. provide a flexible methodology to achieve the desired accuracy
   efficiently (i.e., moving towards a flexible FAS methodology).

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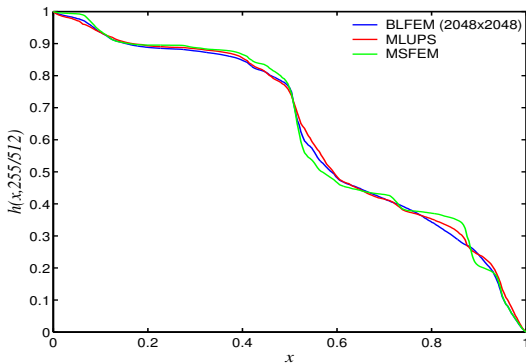
MLUPS Basis Functions for Anisotropic Media

GSLIB recipe for generating realizations of the conductivity:

- A principle axis of statistical anisotropy between 0 and 90 degrees.
- $log_{10}(\mathcal{K}(\boldsymbol{r}))$ is normally distributed with mean zero and variance 4
- correlation lengths of 0.8 and 0.04.

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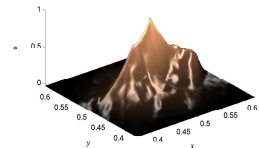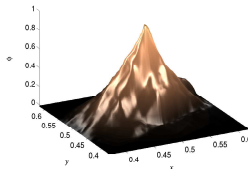
Cross-Sections of the Fine-Scale Pressure

- anisotropy oriented at $30°$
- pressure upscaled from a 256×256 grid to an 8×8 grid
- note abrupt deviations in the MSFEM solution around $x = \frac{3}{4}$ and $x = \frac{7}{8}$

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Two-Phase Flow

The flow of two immiscible and incompressible fluids (e.g., oil and water) that fill the pore space of a porous medium, may be described by,

$$\nabla \cdot \mathbf{u} = Q(\mathbf{r}) = q_w(\mathbf{r}) + q_o(\mathbf{r})$$
$$\mathbf{u} = -\mathcal{K}(\mathbf{r})\lambda\left(S_w\right)\nabla p$$
$$\phi\frac{\partial S_w}{\partial t} + \nabla \cdot \left(f_w\left(S_w\right)\mathbf{u}\right) = q_w(\mathbf{r})$$

where we have used $S_w + S_o = 1$, and assumed that the porosity, ϕ, is constant. We are ignoring gravity and capillary effects (i.e., $p_o = p_w = p$) and have used the following definitions:

$$\lambda(S_w) = \lambda_w(S_w) + \lambda_o(1 - S_w) \qquad \text{total mobility}$$
$$f_w(S_w) = \lambda_w/\lambda \qquad \text{fractional flow rate}$$

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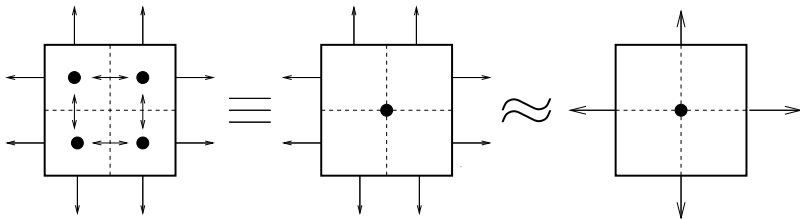Multilevel Mimetic Multiscale (M^3): Two-Phase Flow

Schematic of M^3 Concept

Problem:

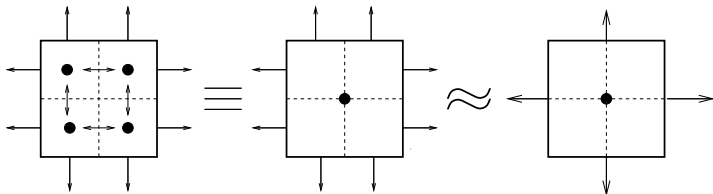- In an IMPES formulation, solving for pressure dominates the computation.

Objectives:

- Reduce this computational burden without significantly compromising the influence of fine-scale heterogeneous structure.
- develop a flexible multilevel process (i.e., use recursion)

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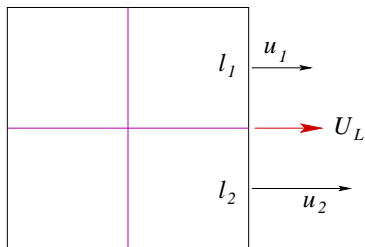Multilevel Mimetic Multiscale (M^3): Two-Phase Flow

Reduction of the Internal Degrees of Freedom

Yu.A.Kuznetsov,*Mixed finite element method for diffusion equations on polygonal meshes with mixed cells, J.Numer.Math., 14(4),2006,pp.305-315*

- block transformations eliminate internal degrees of freedom
- transformations involve computing the inverse of two matrices, of size n_i, and n_c. This favors coarsening by a small factor (e.g., 2) recursively over coarsening by a large factor all at once.
- by design the new pressure unknown is the weighted (integral) average of the fine-scale pressure unknowns
- if reaction terms exist, average reaction rate is preserved.

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Conservative Flux Coarsening

1. local mass conservation on all levels

$$U_L(|\ell_1| + |\ell_2|) = u_1|\ell_1| + u_2|\ell_2|.$$

2. preserve the form of the discretization on all levels

To interpolate coarse-scale fluxes, we let α be the ratio of fine-grid fluxes:

$$\alpha = \begin{cases} \frac{u_1}{u_2}, & u_2 \neq 0, \\ 1, & \text{otherwise.} \end{cases} \quad \Rightarrow \quad \left[\begin{array}{c} u_1 \\ u_2 \end{array} \right] = \mathbf{Q}_L U_L.$$

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Approximating α

Objectives:

- must be less expensive than solving the fine-scale problem
- accuracy should correlate with computational cost
- incorporate global information as needed

Proposed Algorithms:

- develop local approximations based on local medium properties
- solve local problems (e.g., Arnes version of MsMFEM)
- leverage robustness and efficiency of variational coarsening in AMG
  - setup fine-scale Lagrange multiplier system
  - solve using PCG preconditioned with AMG V(1,1) cycles to weak tolerance in L_2 norm of relative residual.

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Two-Phase Flow Specifications

We define the the relative permeability curves as,

$$k_{rw}(S) = (S^*)^2 \qquad k_{ro}(S) = (1 - S^*)^2 \qquad S^* = \frac{S - S_{wc}}{1 - S_{wc} - S_{or}},$$

where S_{wc} is the critical saturation, and S_{or} is the residual saturation.

- $S_{wc} = S_{or} = 0.1$.
- initial saturation, $S(t = 0) = S_{wc} = 0.1$
- phase viscosities, $\mu_w = 1$ and $\mu_o = 4$
- porosity of the medium, $\phi = 0.2$
- *no-flow* boundary conditions
- flow is driven by source/sink terms
- time is measured in Pore Volume Injected (PVI).

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Quantities of Interest

- breakthrough time of water at the production wells
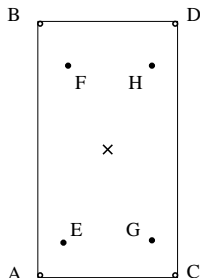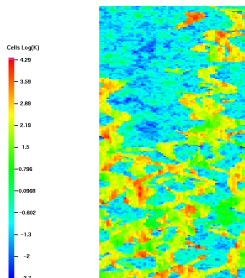- saturation of water at the production wells
- water cut,

$$\frac{q_w}{q_w + q_o}$$

- relative error in saturation
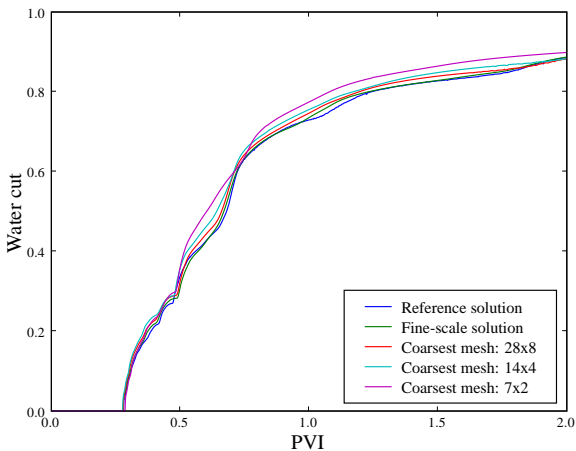
$$\delta_S(t) = \frac{|S_r(t) - S(t)|}{S_r(t)}$$

where $S_r(t)$ denotes the reference saturation, which is computed using standard IMPES approach on a twice refined grid.

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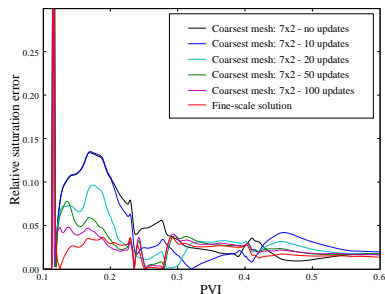Multilevel Mimetic Multiscale (M^3): Two-Phase Flow
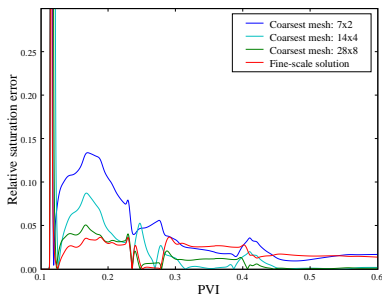
SPE 10 Layer 68

- The left image shows the permeability field of layer 68 SPE 10th Compartive Solution Project.
- The schematic on the right shows the locations of the injector well ($\times$) and producer wells A, B, C, and D ($\circ$).
- Details of the flow at the macro-edges ($\bullet$) located at points, E, F, G, and H are monitored.

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Breakthrough curves (watercut)

Water-cut curves for total coarsening factors 8, 16, and 32 at producer B.

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Relative Error in Saturation

Relative error in saturation at producer A for no updates and different coarsenings (left) and with different number of updates with the coarsest-mesh 2×7 macro-cells. The convergence tolerance is $\varepsilon = 0.01$.
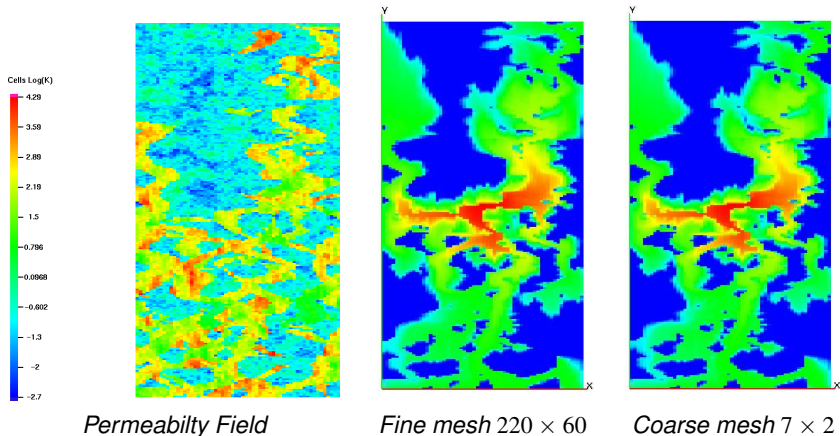
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Time Evolution of α
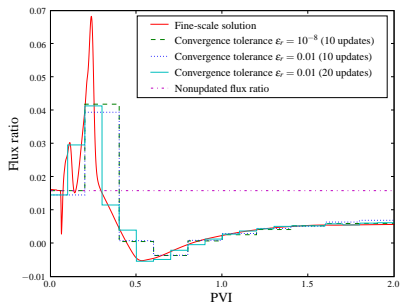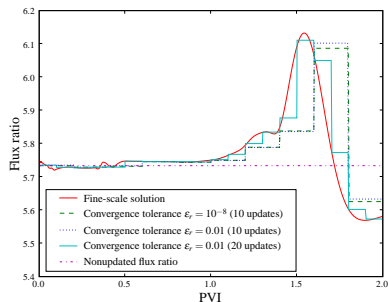
The comparison of the flux ratios obtained with different update strategies at points G and H.

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Viewgraph Norm

Water saturation at $t = 0.3$ PVI.

Permeabilty Field   *Fine mesh* 220×60 *Coarse mesh* 7×2

Conclusions

1. **Robust Multigrid Solvers**
   - FAS provides a flexible framework for multiscale simulation.
   - potential for error estimation and control
   - αAMG and αSA based AMG have promise for treating systems of multiphysics PDEs.

2. **Multilevel Upscaling**
   - basis functions are similar to MsFEM, but construction in MLUPS is ≈ 15 times faster and generates a complete hierarchy.
   - Homogenized/upscaled/effective coefficients and models may be recovered at coarser scales.

3. **Multilevel Multiscale Mimetic M^3**
   - leverages a robust variational multigrid (AMG) to estimate flux ratio
   - local mass conservation on all levels
   - offers great flexibility in balancing accuracy and efficiency
   - with large coarsening factors speedup is approximately 80 times in pressure solve, and approximately 8 times overall.

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