Variational Modeling Across Scales

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Heterogeneous Problems

What makes a problem *heterogeneous?*

- Large relative variation in material properties
- Abrupt changes in material properties
- Large variation in spatial scales

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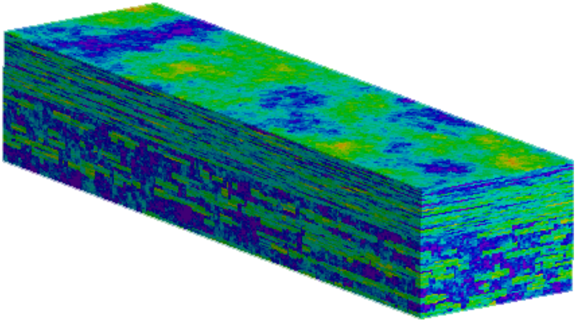
Why do we care?

- Many natural materials are heterogeneous
- Fine-scale variation affects macroscopic behavior
- Simulation of heterogeneous problems must resolve variation

Subsurface Flow

Rate of flow through a reservoir depends on its composition



- Porosity & Permeability vary on scales from mm upwards
- Domain is $\sim 700\text{m} \times 350\text{m} \times 50\text{m}$

From SPE Comparative Solution Project: www.spe.org/csp/

Darcy's Law

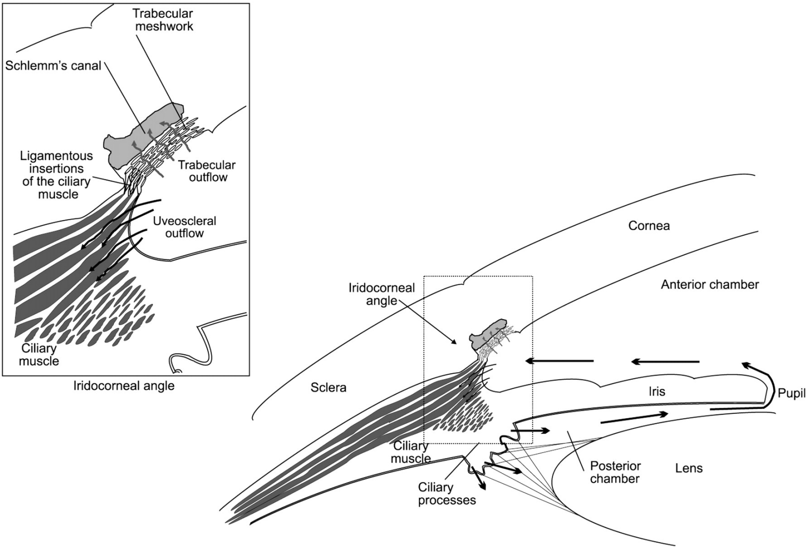
Model hydraulic head, h, of a fluid confined in a porous media

$$Q = -\mathcal{K}\nabla h$$

$$S_s \frac{\partial h}{\partial t} + \nabla \cdot Q = q$$

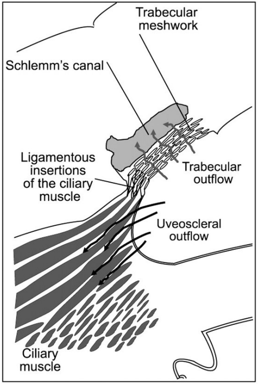
- Q denotes the Darcy-law flux
- q represents external sources or sinks of fluid
- Material properties
  - S_s = specific storage
  - $\mathcal{K}$ = hydraulic conductivity

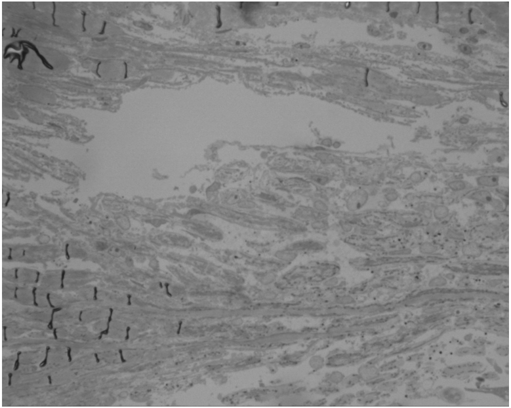
Ocular Flow



A. Llobet et al, *News Physiol. Sci.* **18**, pp 205-209, 2003.

Trabecular Meshwork





(left) A. Llobet et al, *News Physiol. Sci.* **18**, pp 205-209, 2003.
(right) Courtesy W.D. Stamer, U of Arizona & J.J. Heys, Arizona State U

Cardiac Bidomain Equations

Model intra- and extra-cellular potentials, ϕ_i and ϕ_e, in cardiac tissue:

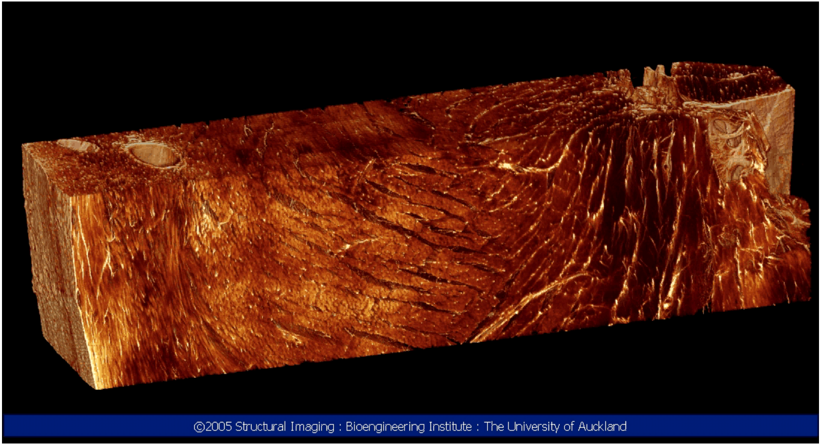
$$V_m = \phi_i - \phi_e$$

$$A_m C_m \frac{\partial V_m}{\partial t} - \nabla \cdot (\sigma_i \nabla V_m) = \nabla \cdot (\sigma_i \nabla \phi_e) - A_m I_{\text{ion}}$$

$$-\nabla \cdot ((\sigma_i + \sigma_e) \nabla \phi_e) = \nabla \cdot (\sigma_i \nabla V_m) + i_e(t)$$

- A_m is surface-to-volume ratio of the cell membrane
- C_m is the membrane capacitance per unit area
- I_{ion} represents ionic currents
- $i_e(t)$ represents extracellular current injections
- Material properties
  - σ_i = intracellular conductivity
  - σ_e = extracellular conductivity

Cardiac Tissue



Sample of rat left ventricular wall, dimensions are approximately $3.6 \times 0.8 \times 0.8$mm.

Courtesy T. Austin, Univ. Auckland

Elliptic Model Problem

A simpler model still displays same sensitivity to heterogeneity:

$$-\nabla \cdot (\mathcal{K} \nabla h) = q$$

- Implicit time stepping adds lower-order term
- Main terms in operator-splitting approach
- Assume $\mathcal{K} = \mathcal{K}(\mathbf{x})$, possibly tensor-valued

Develop approach for model problem, then extend to particular applications

Simulation Challenges

Even for model problem, simulation can be difficult

- If $\mathcal{K}(\mathbf{x})$ varies on a fine-enough scale, simulation may be intractable

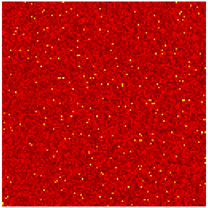
  Example: 1 km $\times$ 1 km $\times$ 1 km reservoir, sediment varies on mm-scale requires 10^{18} Degrees of Freedom

Two approaches:

- Average conductivity to scale where simulation is possible
- Take variation in $\mathcal{K}(\mathbf{x})$ into account in discretization

Effective Media

Given heterogeneous conductivity in a region, can we replace it by a homogeneous one without changing overall flow?



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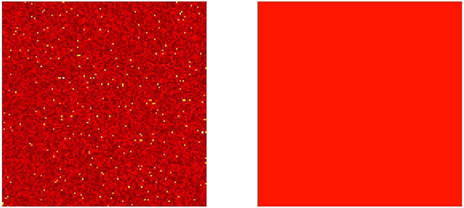
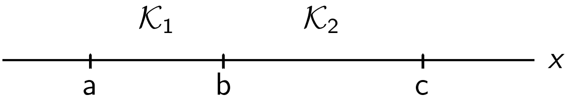


In general,

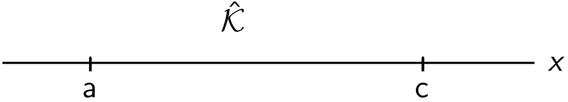
- depends on medium and physics
- depends on flow conditions
- no single average always works

Effective Conductivity in One Dimension

Is it possible to replace a heterogeneous cell,



with an effective (*homogenized*, or *equivalent*) cell,



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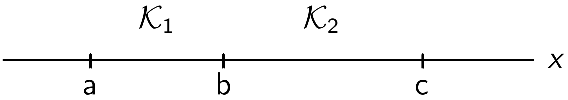

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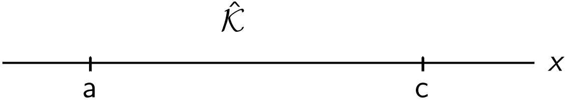

that doesn't perturb the solution outside $a < x < c$?

$$\hat{h}(a) = h(a), \qquad \hat{h}(c) = h(c)$$

$$\hat{Q}(a) = Q(a), \qquad \hat{Q}(c) = Q(c)$$

Harmonic Averages

One-dimensional model problem:

$$-\frac{\partial}{\partial x}\mathcal{K}\frac{\partial}{\partial x}h(x) = 0.$$

For constant $\mathcal{K}_1$ on $[a, b]$, integrating in x gives

$$\begin{bmatrix} h(b) \\ Q(b) \end{bmatrix} = \begin{bmatrix} 1 & -\frac{b-a}{\mathcal{K}_1} \\ 0 & 1 \end{bmatrix} \begin{bmatrix} h(a) \\ Q(a) \end{bmatrix} = M_a^b \begin{bmatrix} h(a) \\ Q(a) \end{bmatrix}.$$

For a heterogeneous media, then

$$\begin{bmatrix} h(c) \\ Q(c) \end{bmatrix} = M_b^c M_a^b \begin{bmatrix} h(a) \\ Q(a) \end{bmatrix} = \hat{M}_a^c \begin{bmatrix} h(a) \\ Q(a) \end{bmatrix}$$

If $\hat{M}_a^c = M_b^c M_a^b$, then $\hat{\mathcal{K}} = (c-a)\left(\frac{b-a}{\mathcal{K}_1} + \frac{c-b}{\mathcal{K}_2}\right)^{-1}$.

Effective Conductivities

- In 1D, harmonic average gives correct behaviour
- What about in more dimensions?

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Simple averages be arbitrarily bad!

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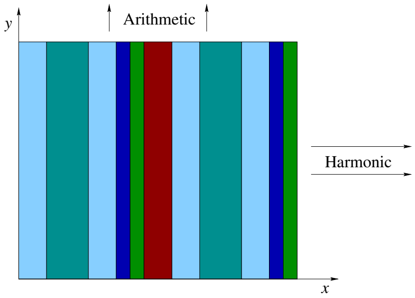
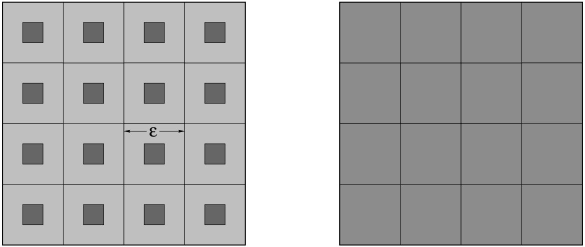
Depending on flow conditions:



Asymptotic Analysis



Let $\mathcal{K} = \mathcal{K}(\frac{\mathbf{x}}{\varepsilon})$, and consider

$$-\nabla \cdot \left(\mathcal{K}\left(\frac{\mathbf{x}}{\varepsilon}\right) \nabla h_\varepsilon \right) = q(\mathbf{x}).$$

A two-scale asymptotic analysis gives behavior as $\varepsilon \to 0$.

Homogenization

Effective conductivity depends on unit cell, Y, relative to $\frac{\mathbf{x}}{\varepsilon}$.

Define

$$a_\varepsilon(u,v) = \int_Y \left(\mathcal{K}\left(\frac{\mathbf{x}}{\varepsilon}\right) \nabla_\varepsilon u \right) \cdot \nabla_\varepsilon v,$$

then

$$\xi^T \hat{\mathcal{K}} \xi^T = \min_{\phi \in H_p^1(Y)} a_\varepsilon(h_\xi + \phi, h_\xi + \phi),$$

where

- $\xi = \nabla h_\xi$ is constant
- $H_p^1(Y)$ is the Sobolev space, $H^1(Y)$, with periodic boundary conditions

Weak Forms

Consider solution of

$$-\nabla \cdot \mathcal{K}(\mathbf{x})\nabla h(\mathbf{x}) = q(\mathbf{x})$$

Weak Forms

Consider solution of

$$(-\nabla \cdot \mathcal{K}(\mathbf{x}) \nabla h(\mathbf{x})) \, \varphi(\mathbf{x}) = \quad q(\mathbf{x}) \varphi(\mathbf{x})$$

Weak Forms

Consider solution of

$$\int_{\Omega} \left(-\nabla \cdot \mathcal{K}(\mathbf{x}) \nabla h(\mathbf{x})\right) \varphi(\mathbf{x}) = \int_{\Omega} q(\mathbf{x}) \varphi(\mathbf{x})$$

Weak Forms

Consider solution of

$$\int_{\Omega} (\mathcal{K}(\mathbf{x})\nabla h(\mathbf{x})) \cdot \nabla\varphi(\mathbf{x}) = \int_{\Omega} q(\mathbf{x})\varphi(\mathbf{x}) + \text{BCs}$$

Weak Forms

Consider solution of

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Define

$$a(u, v) = \int_\Omega (\mathcal{K}(\mathbf{x})\nabla u(\mathbf{x})) \cdot \nabla v(\mathbf{x})$$

Properties of $a(u, v)$:

- Defined for u (and v) such that $\int_\Omega \nabla u \cdot \nabla u < \infty$
- Positive Definite: $a(u, u) > 0$ for $u \neq 0$
- Symmetric: $a(u, v) = a(v, u)$,

Weak form defines an inner product and a norm on $H^1(\Omega)$

Subspace Minimization

Let h be the solution of

$$a(h, \varphi) = \int_\Omega q(\mathbf{x})\varphi(\mathbf{x}) + \text{BCs for all } \varphi \in H^1(\Omega).$$

Given a subspace, $\mathcal{V} \subset H^1(\Omega)$, best solution in $\mathcal{V}$ is

$$h_\mathcal{V} = \operatorname*{argmin}_{v \in \mathcal{V}} a(h - v, h - v)$$

Minimizer must satisfy

$$a(h_\mathcal{V}, \varphi) = \int_\Omega q(\mathbf{x})\varphi(\mathbf{x}) + \text{BCs for all } \varphi \in \mathcal{V}$$

Basis Functions

Suppose $\mathcal{V} = \text{span}\{\phi_j(\mathbf{x})\}_{j=1}^n$, then $h_{\mathcal{V}}(\mathbf{x}) = \sum_{j=1}^n h_j \phi_j(\mathbf{x})$. Then,

$$\sum_{j=1}^{n} h_j a(\phi_j, \phi_i) = \int_\Omega q(\mathbf{x})\phi_i(\mathbf{x}) + \text{BCs}_i = q_i \text{ for all } i.$$

Writing $\mathbf{h} = (h_1, h_2, \ldots, h_n)^T$ and $\mathbf{q} = (q_1, q_2, \ldots, q_n)^T$, then

$$A\mathbf{h} = \mathbf{q},$$

where $A_{ij} = a(\phi_j, \phi_i)$.

Classical Finite Elements

Want to choose basis, $\{\phi_j\}_{j=1}^n$, so that

- $h_{\mathcal{V}}$ is a good approximation to h
- A and $\mathbf{q}$ are easy to calculate
- $A\mathbf{h} = \mathbf{q}$ is easy to solve

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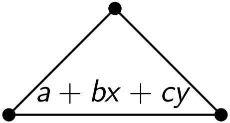
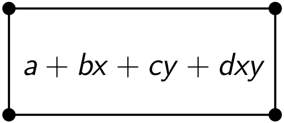
Typical choices:

- Piecewise linears on triangles and tetrahedra
- Piecewise bilinears on quadrilaterals
- Piecewise trilinears on hexahedra

Local bases on polyhedra, with as many degrees of freedom as nodes





Approximation Properties

- Take $\{\hat{\phi}_j\}_{j=1}^{\infty}$ to be an $a(\cdot,\cdot)$-orthogonal basis for H^1
- $\{\hat{\phi}_j\}_{j=1}^{n}$ is a basis for $\mathcal{V} \subset H^1$

Writing $h = \sum_{j=1}^{\infty} \hat{h}_j \hat{\phi}_j, \quad h_{\mathcal{V}} = \sum_{j=1}^{n} \hat{h}_j \hat{\phi}_j$

$$a(h - h_{\mathcal{V}}, h - h_{\mathcal{V}}) = \sum_{j=n+1}^{\infty} \hat{h}_j^2 a(\hat{\phi}_j, \hat{\phi}_j)$$

Want the projection of h onto $\mathcal{V}^{\perp}$ to be small in the $a(\cdot,\cdot)$-norm

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Want the projection of h onto $\mathcal{V}^{\perp}$ to be small in the $a(\cdot,\cdot)$-norm

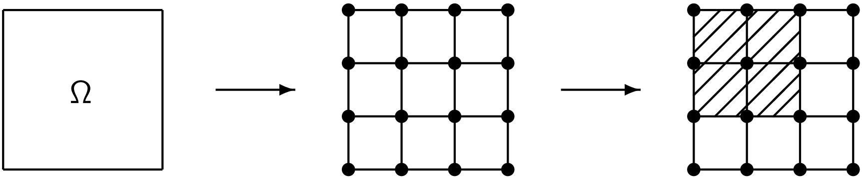
For a general q (+ BCs), $\hat{h}_j = \frac{\int_\Omega q\hat{\phi}_j}{a(\hat{\phi}_j,\hat{\phi}_j)}$

- Important to capture modes where $\frac{\int_\Omega q\hat{\phi}_j}{a(\hat{\phi}_j,\hat{\phi}_j)}$ is large
- Important to capture functions where $\frac{a(\varphi,\varphi)}{\langle\varphi,\varphi\rangle}$ is small

Multiscale Finite Element Method

Compute nodal basis of modes where $\frac{a(\varphi,\varphi)}{\langle\varphi,\varphi\rangle}$ is small

- Given Ω, partition into elements on scale for computation
- For each node, choose non-zero support over neighboring elements



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- Nodal basis implies $\phi_i(\mathbf{x}_j) = \delta_{ij}$
- Take $\phi_i(\mathbf{x}) = 0$ on boundary of its support

Can $\phi_i = \text{argmin}\{\frac{a(\varphi,\varphi)}{\langle\varphi,\varphi\rangle} : \varphi(\mathbf{x}_j) = \delta_{ij}, \varphi(\mathbf{x}) = 0 \text{ on } \partial\Omega_i\}$?

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I don't know.

MSFEM ignores the denominator

- define ϕ_i piecewise on each element
- fix boundary conditions and solve $a(\phi_i, \varphi) = 0$ on interior

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Artificial Boundary Conditions

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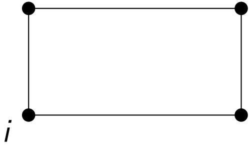

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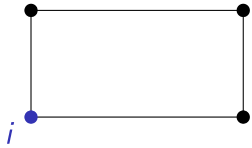

- Fix $\phi_i(\mathbf{x}_i) = 1$

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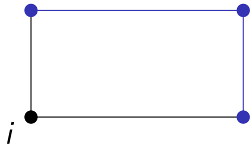

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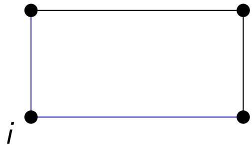

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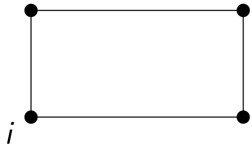

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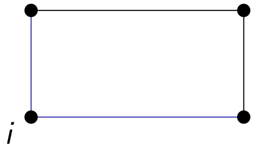


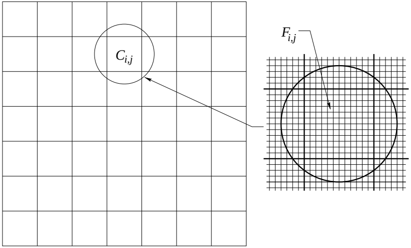
- Fix $\phi_i(\mathbf{x}_i) = 1$
- Set $\phi_i(\mathbf{x}) = 0$ on $\partial\Omega_i$
- **Impose boundary conditions on remaining edges**
- Solve $a(\phi_i, \varphi) = 0$ in interior

Exact boundary conditions aren't known

- use linear
- solve one-dimensional problem along edge

Computational Cost of MSFEM

For each node of each element, need to compute basis function



- constant permeability tensor given on each fine-scale cell $F_{i,j}$
- choose computational scale, $C_{i,j}$
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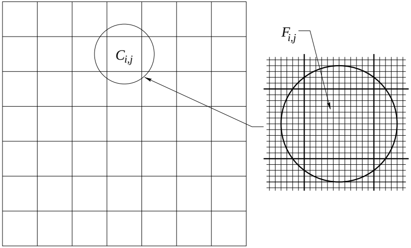

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We had three goals for our basis:

- good approximation
- **easy to calculate A and $\mathbf{q}$**
- easy to solve $A\mathbf{p} = \mathbf{q}$

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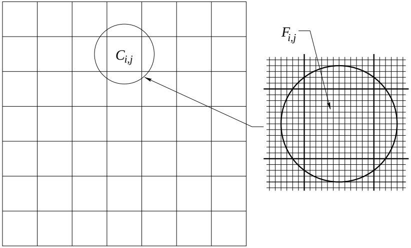

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We had three goals for our basis:

- good approximation
- **easy to calculate A and q**
- easy to solve $A\mathbf{p} = \mathbf{q}$

What is the cost of finding four basis functions over each element, compared to solving fine-scale equations?

Multigrid: Relaxation on $A\mathbf{x} = \mathbf{b}$

- Want to improve approximation, $\mathbf{x}^{(0)}$
- Introduce residual, $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)} = A(\mathbf{x} - \mathbf{x}^{(0)})$
- Take $\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \omega\mathbf{r}^{(0)}$, for $\omega \approx \frac{1}{\|A\|}$

Error propagation form: $\mathbf{e}^{(1)} = (I - \omega A)\ \mathbf{e}^{(0)}$

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Error propagation form: $\mathbf{e}^{(n)} = (I - \omega A)^n \mathbf{e}^{(0)}$

This iteration converges slowly, but its **failure is structured**

- Eigenvectors of small eigenvalues of A are slow to change
- Can we use this to our advantage?

Multigrid: Subspace Correction

Dominant error after relaxation lies in a subspace

What if we could resolve this error by another process that acted only on the subspace**?**

Need

- complementary process
- way to combine its results with relaxation

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- way to combine its results with relaxation

Want a map from the subspace to the whole space.

Interpolation!

Multigrid: Variational Coarsening

- Have $\mathbf{x}^{(1)}$, approximation after relaxation
- Let P be map from any subspace to whole space
- Corrected approximation will be $\mathbf{x}^{(2)} = \mathbf{x}^{(1)} + P\mathbf{x}_c$

What is the best $\mathbf{x}_c$ for correction?

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What is the best $\mathbf{x}_c$ for correction?

Symmetric and positive-definite matrix, A, defines an inner product and a norm:

$$\langle \mathbf{x}, \mathbf{y} \rangle_A = \mathbf{y}^T A \mathbf{x} \quad \text{and} \quad \|\mathbf{x}\|_A^2 = \mathbf{x}^T A \mathbf{x}$$

Best then means closest to the exact solution in norm:

$$\mathbf{y}^\star = \operatorname*{argmin}_{\mathbf{y}} \|\mathbf{x} - \mathbf{y}\|_A$$

Multigrid: Variational Coarsening

- Have $\mathbf{x}^{(1)}$, approximation after relaxation
- Let P be map from any subspace to whole space
- Corrected approximation will be $\mathbf{x}^{(2)} = \mathbf{x}^{(1)} + P\mathbf{x}_c$

What is the best $\mathbf{x}_c$ for correction?

Closest approximation to $\mathbf{x}$ after correction given by

$$\mathbf{x}_c = \underset{\mathbf{y}_c}{\operatorname{argmin}} \|\mathbf{x} - (\mathbf{x}^{(1)} + P\mathbf{y}_c)\|_A$$

Best $\mathbf{x}_c$ satisfies $(P^T AP)\mathbf{x}_c = P^T A(\mathbf{x} - \mathbf{x}^{(1)}) = P^T \mathbf{r}^{(1)}$

Multigrid: the V-Cycle

Multigrid Components

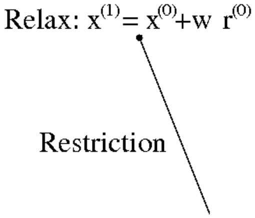
Relax: $x^{(1)} = x^{(0)} + w\ r^{(0)}$

- Relaxation

- Use a relaxation process (such as Jacobi or Gauss-Seidel) to damp errors
- Remaining error satisfies $A\mathbf{e}^{(1)} = \mathbf{r}^{(1)} = \mathbf{b} - A\mathbf{x}^{(1)}$

Multigrid: the V-Cycle

Multigrid Components



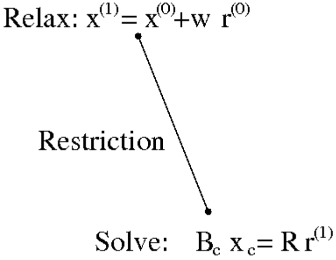
- Relaxation
- Restriction

- Transfer residual to subspace
- Compute $P^T \mathbf{r}^{(1)}$

Multigrid: the V-Cycle

Multigrid Components

- Relaxation
- Restriction
- Subspace Correction



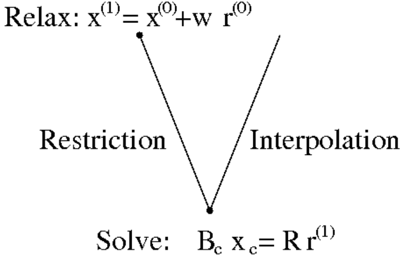
- Use subspace correction to eliminate dominating errors
- Best correction, $\mathbf{x}_c$, in terms of A-norm satisfies

$$P^T A P \mathbf{x}_c = P^T \mathbf{r}^{(1)}$$

Multigrid: the V-Cycle

Multigrid Components

- Relaxation
- Restriction
- Subspace Correction
- Interpolation

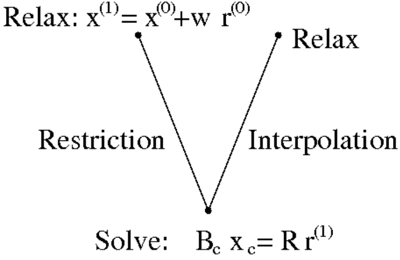


- Transfer correction to fine scale
- Compute $\mathbf{x}^{(2)} = \mathbf{x}^{(1)} + P\mathbf{x}_c$

Multigrid: the V-Cycle

Multigrid Components

- Relaxation
- Restriction
- Subspace Correction
- Interpolation
- Relaxation

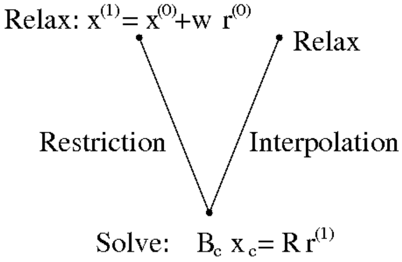


- Relax once again to damp errors introduced in subspace correction

Multigrid: the V-Cycle

Multigrid Components

- Relaxation
- Restriction
- Subspace Correction
- Interpolation
- Relaxation



Direct solution of coarse-grid problem isn't practical

Recursion!

Apply same methodology to solve coarse-grid problem

Multigrid: Operator-Induced Interpolation

Success of multigrid iteration depends on how well the range of P captures the slow-to-converge modes of relaxation

- For simple relaxation, slow-to-converge modes are close to **eigenvectors of A with small eigenvalues**
- Knowing structure of A (or continuum problem that generated it) allows effective choice of P

For $-\nabla \cdot \mathcal{K} \nabla h$, Black Box MG reduces error in the A-norm

- by a factor bounded less than 1 per iteration
- at a cost per iteration proportional to the size of A

J.E. Dendy, Jr., *J. Comput. Phys.*, **48**, pp. 366-386, 1982.

MSFEM and Optimal Solvers

For scalar elliptic PDEs, discretized by standard finite elements, **multigrid is an optimal solver**.

- Error-reduction factor bounded independent of matrix size
- Iteration cost is bounded proportional to matrix size

In essence, solving a problem with $2n$ degrees of freedom takes twice as long as solving one with n degrees of freedom.

For MSFEM:

- Each basis function requires fine-scale solve over each element in its support
- Total cost is proportional to number of fine-scale nodes
- **Same as cost of solving fine-scale problem itself!**

Multigrid and Approximation

Optimal approximation properties rely on representing functions where $\frac{a(\varphi,\varphi)}{\langle\varphi,\varphi\rangle}$ is small

Operator-Induced Interpolation, P,

- chosen based on discrete operator
- must accurately represent modes where $\frac{\mathbf{x}^T A\mathbf{x}}{\mathbf{x}^T\mathbf{x}}$ is small

Variational coarsening

- restricts A to range of interpolation
- explicitly constructs coarse-scale discrete model, $A_c = P^T AP$

Modes needed for good approximation properties are also needed for good multigrid performance

Implicit Basis Functions

Fine-scale finite-element discretization:

$$A_{ij} = \mathbf{e}_j^T A \mathbf{e}_i = \int_\Omega (\mathcal{K}(\mathbf{x}) \nabla \phi_j) \cdot \nabla \phi_i$$

Variational coarsening gives coarse-grid operator,

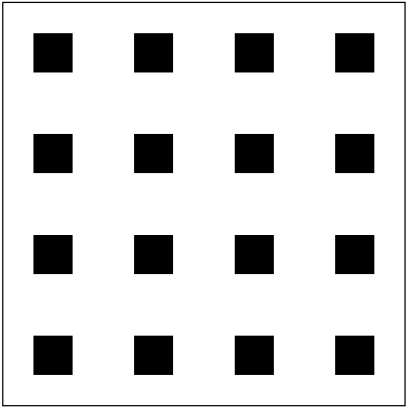
$$\begin{aligned}(A_c)_{ij} &= (P^T A P)_{ij} = (P\hat{\mathbf{e}}_j)^T A (P\hat{\mathbf{e}}_i) \\ &= \int_\Omega \left(\mathcal{K}(\mathbf{x}) \nabla \left(\sum_k p_{kj} \phi_k \right) \right) \cdot \nabla \left(\sum_l p_{li} \phi_l \right) \\ &= \int_\Omega \left(\mathcal{K}(\mathbf{x}) \nabla \hat{\phi}_j \right) \cdot \nabla \hat{\phi}_i\end{aligned}$$

Variational coarsening **implicitly defines basis functions** on coarse scale, $\hat{\phi}_i = \sum_l p_{li} \phi_l$.

T. Grauschopf, M. Griebel, & H. Regler, *Appl. Numer. Math.*, **23**, 1997

Multigrid Basis Functions

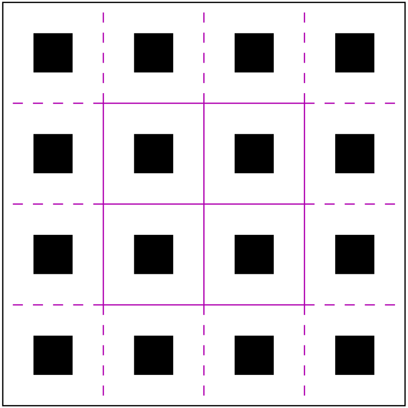
Variational multigrid defines a multiscale finite element basis



Periodic tiling of inclusion problem: $\mathcal{K} = 1000$ in inclusions, $\mathcal{K} = 1$ in background

Multigrid Basis Functions

Variational multigrid defines a multiscale finite element basis



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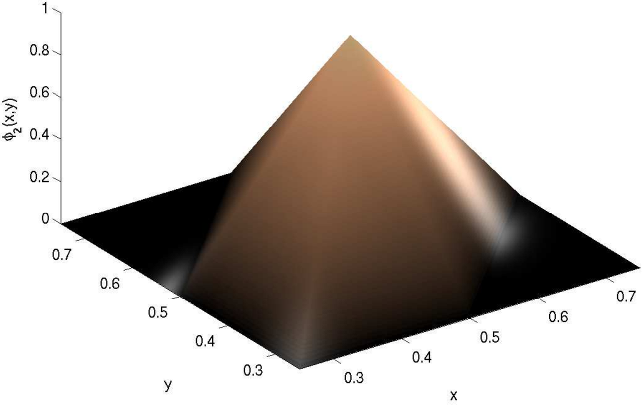
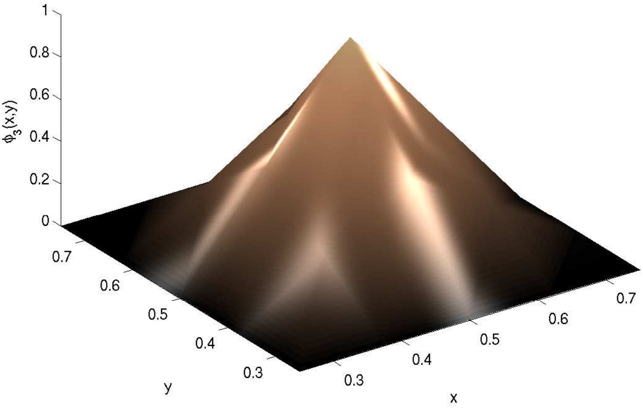


Bilinear basis function on coarse scale

Multigrid Basis Functions

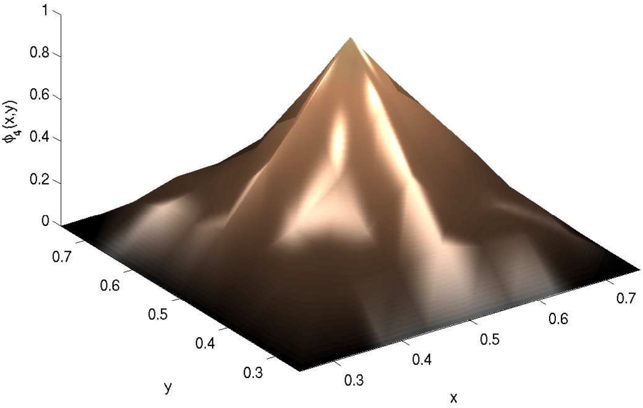
Variational multigrid defines a multiscale finite element basis



Basis function accounting for coarsest 2 scales

Multigrid Basis Functions

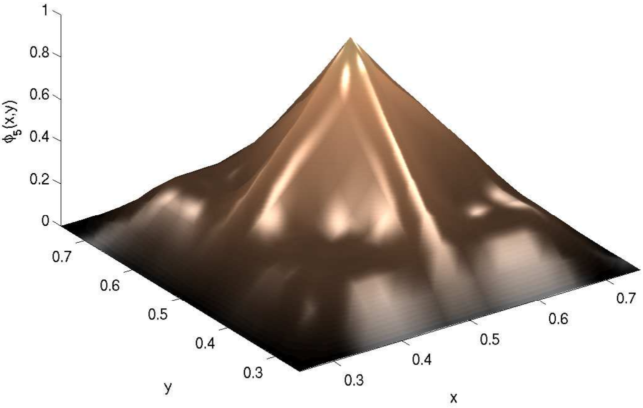
Variational multigrid defines a multiscale finite element basis



Basis function accounting for coarsest 3 scales

Multigrid Basis Functions

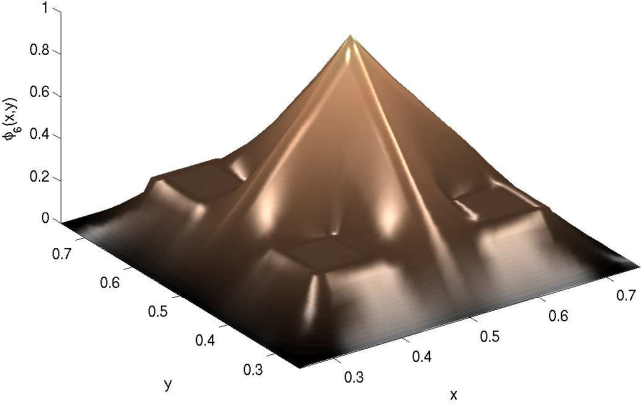
Variational multigrid defines a multiscale finite element basis



Basis function accounting for coarsest 4 scales

Multigrid Basis Functions

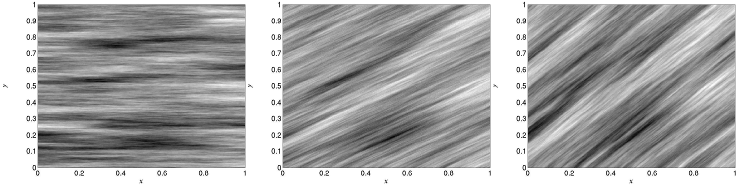
Variational multigrid defines a multiscale finite element basis



Basis function accounting for all scales

Geostatistical Media

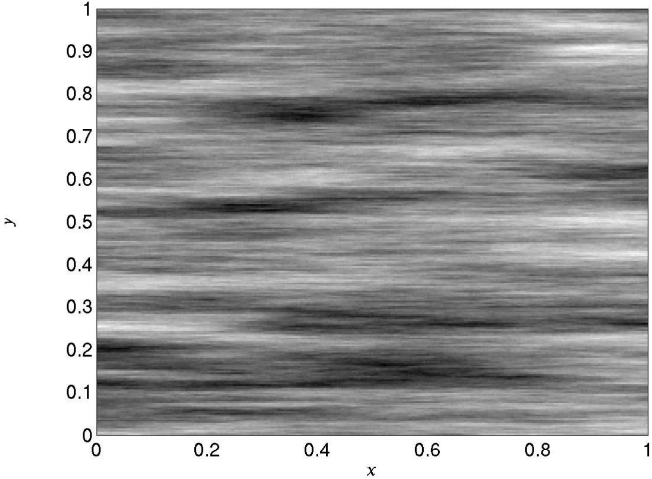
- Principle axis of statistical anisotropy chosen
- Correlation length of 0.8 along axis, 0.04 across axis
- $\log_{10}(\mathcal{K})$ normally distributed with mean 0, variance 4



C. Deutsch and A. Journal, *GSLIB, geostatistical software library*, 1998

Multigrid Basis Functions

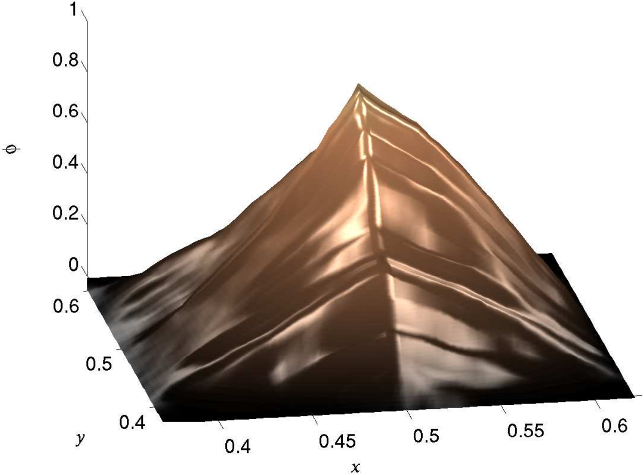
Variational multigrid defines a multiscale finite element basis



Permeability field for 0 degrees

Multigrid Basis Functions

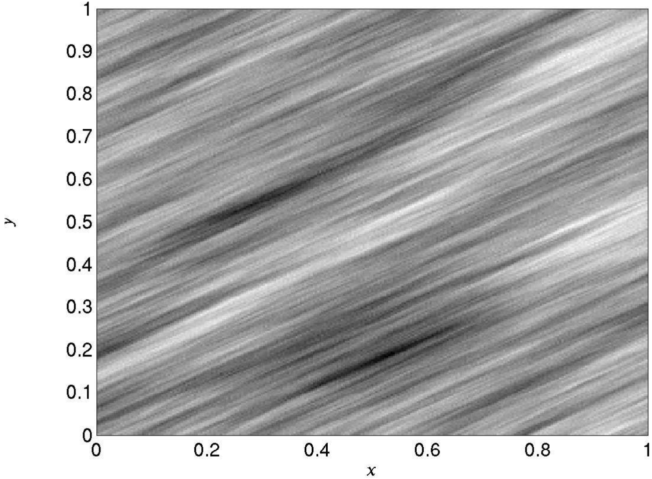
Variational multigrid defines a multiscale finite element basis



Basis for node at $(\frac{1}{2}, \frac{1}{2})$ for 0 degrees

Multigrid Basis Functions

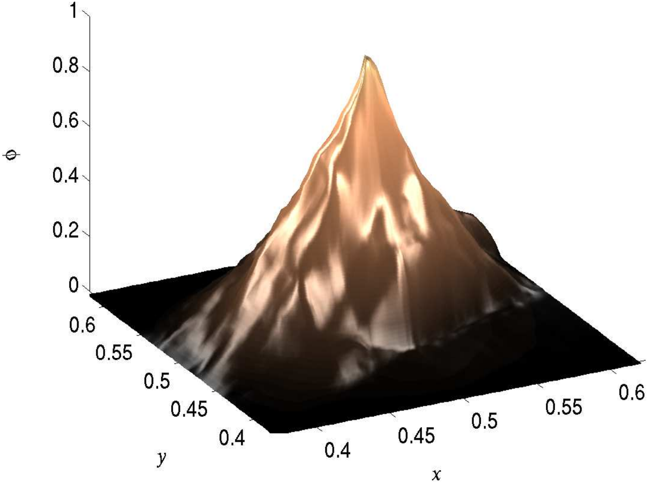
Variational multigrid defines a multiscale finite element basis



Permeability field for 30 degrees

Multigrid Basis Functions

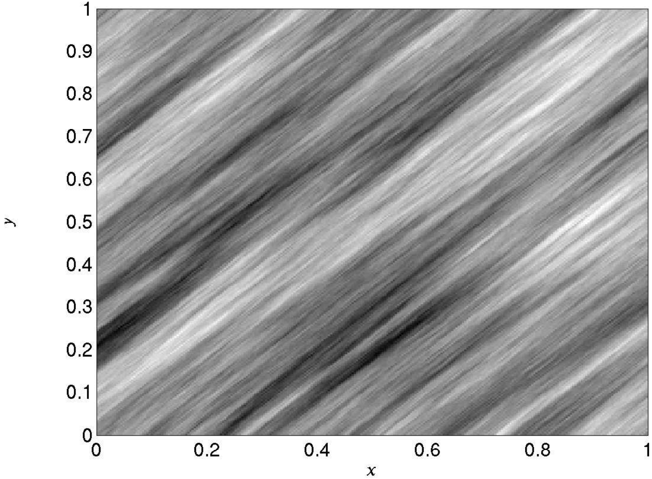
Variational multigrid defines a multiscale finite element basis



Basis for node at $(\frac{1}{2}, \frac{1}{2})$ for 30 degrees

Multigrid Basis Functions

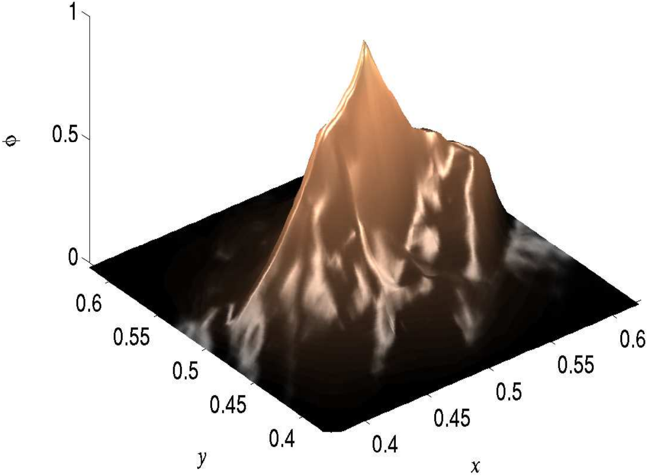
Variational multigrid defines a multiscale finite element basis



Permeability field for 45 degrees

Multigrid Basis Functions

Variational multigrid defines a multiscale finite element basis



Basis for node at $(\frac{1}{2}, \frac{1}{2})$ for 45 degrees

Implicit Upscaling

Multigrid coarse-scale operators represent consistently upscaled models

- Equivalent to finite element discretization with implicit basis functions
- Accurately represent small-Rayleigh quotient modes
- Require no fine-scale solution to form coarse-scale model
- Are easily solved using multigrid

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Multigrid coarse-scale operators represent consistently upscaled models

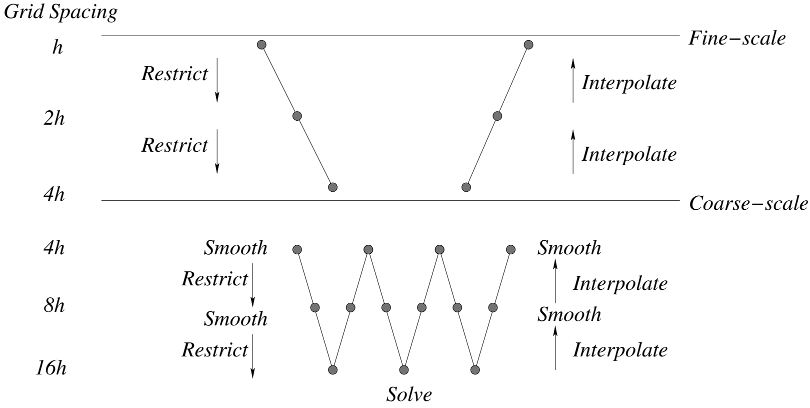
- Equivalent to finite element discretization with implicit basis functions
- Accurately represent small-Rayleigh quotient modes
- Require no fine-scale solution to form coarse-scale model
- Are easily solved using multigrid

Algorithm:

- Form fine-scale discrete model
- Use operator-induced variational coarsening to create coarse-scale models
- Restrict sources and boundary conditions to chosen computational scale
- Solve model on chosen scale
- Interpolate solution to fine scale

The Multilevel Upscaling Algorithm

From a multigrid point of view, this is just not smoothing on scales finer than the coarse (computational) scale



Adaptivity

MLUPS framework is a natural setting for adaptivity

Variational multigrid approach

- creates a hierarchy of models at different scales
- naturally restricts A-norm to coarse scales
- allows for coarse-scale error estimation
- allows for local improvement on scales finer than chosen coarse scale

Nonlinear multigrid (FAS) framework gives flexible framework for error estimation and control

Test problems

Two-dimensional geostatistical media

- Chosen axis of statistical anisotropy
- Correlation lengths of 0.8 along axis, 0.04 across axis
- $\log_{10}(\mathcal{K})$ normally distributed with mean 0, variance of 4

Boundary Conditions

- mean uniform flow driven by imposed Dirichlet boundaries
- $h(0, y) = 1$, $h(1, y) = 0$
- Homogeneous Neumann boundaries on top and bottom

Test problems

$\mathcal{K}$ chosen to be piecewise constant on 256×256 mesh

Four algorithms:

- Bilinear finite elements on 256×256 mesh
- MSFEM with coarse scale of 8×8 elements
- MLUPS with coarse scale of 8×8 elements
- MLUPSa with coarse scale of 8×8 elements
  - MLUPSa is MLUPS with relaxation on all finer scales in final interpolation

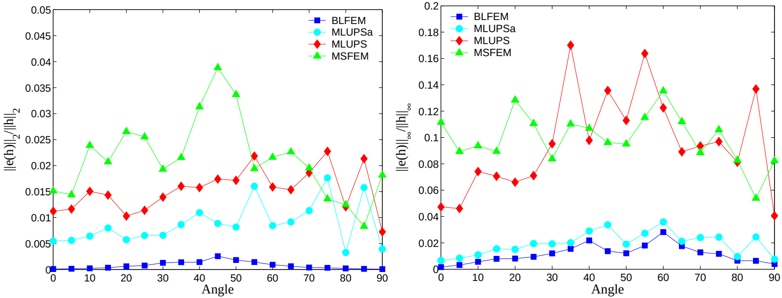
Accuracy measured versus solution of problem on 2048×2048 grid.

Errors in Fine-Scale Pressures

Errors are measured in discrete vector norms:

$$\|e(h)\|_2 = \left(\frac{1}{N} \sum_{i=1}^{N} e(h)_i^2 \right)^{\frac{1}{2}}, \qquad \|e(h)\|_\infty = \max_i |e(h)_i|,$$

evaluated at each node on the 2048×2048 mesh.

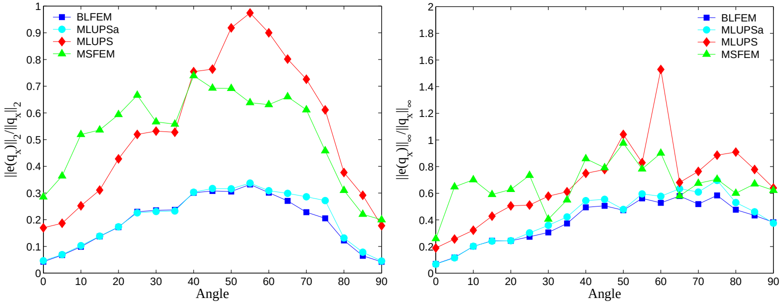


Errors in Fine-Scale Flux

Errors measured component-wise in discrete vector norms:

$$\|e(\mathbf{Q}\cdot\hat{\mathbf{x}})\|_2 = \left(\frac{1}{N}\sum_{i=1}^{N} e(\mathbf{Q}\cdot\hat{\mathbf{x}})_i^2\right)^{\frac{1}{2}}, \ \|e(\mathbf{Q}\cdot\hat{\mathbf{x}})\|_\infty = \max_i |e(\mathbf{Q}\cdot\hat{\mathbf{x}})_i|,$$

evaluated at cell-centers of the 2048×2048 mesh.



Errors in Fine-Scale Flux

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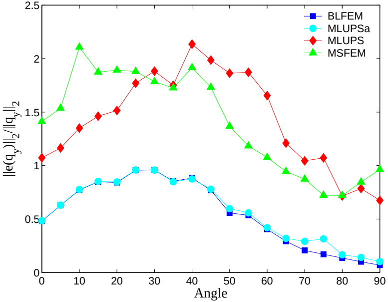
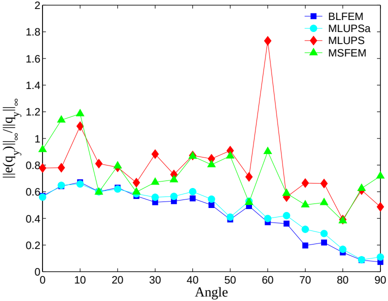




What's wrong with the fluxes?

Problem is inherent in second-order form FEM

$$-\nabla \cdot \mathcal{K} \nabla h = q$$

Compute h, then numerically differentiate to get $\mathbf{Q} = -\mathcal{K}\nabla h$

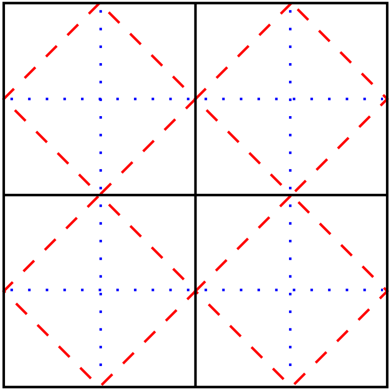
- Not explicitly enforcing conservation of mass on grid elements
- Problem already exists for fine scale, not helped by upscaling

Good pressure solutions $\not\Rightarrow$ Good flux solutions

Flux Post-Processing

Cordes and Kinzelbach consider post-processing for locally conservative fluxes in homogeneous medium

- Refine mesh
- Consider dual mesh

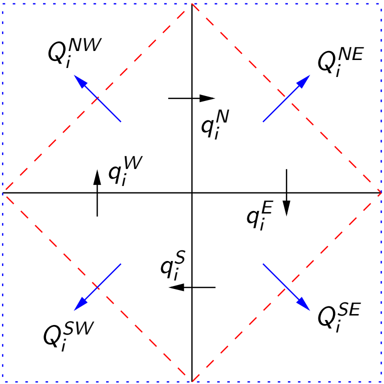


C. Cordes & W. Kinzelbach, *Water Resour. Res.*, **28**, 1992

Flux Post-Processing

Cordes and Kinzelbach consider post-processing for locally conservative fluxes in homogeneous medium

- Refine mesh
- Consider dual mesh
- Integrate FEM flux to define flux on dual-mesh edges
- Apply conservation of mass to compute fluxes on refined mesh



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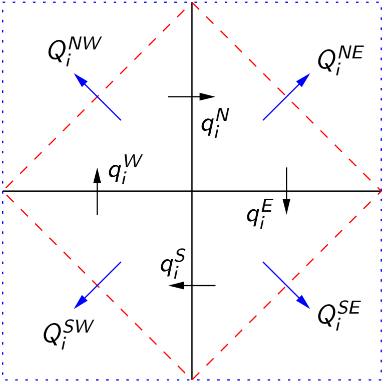


Need irrotationality constraint to make system well-posed

C. Cordes & W. Kinzelbach, *Water Resour. Res.*, **28**, 1992

The Heterogeneous Case

Irrotationality based on

$$\oint_\gamma \nabla h \cdot ds = 0$$

When $\mathcal{K} = 1$, $\mathbf{Q} = -\nabla h$

$\rightarrow$ easy to relate irrotationality and fluxes

For variable, tensor $\mathcal{K}$, write $\nabla h = -\mathcal{K}^{-1}\mathbf{Q}$, giving

$$a_N q_i^N + a_W q_i^W + a_S q_i^S + a_E q_i^E = 0$$

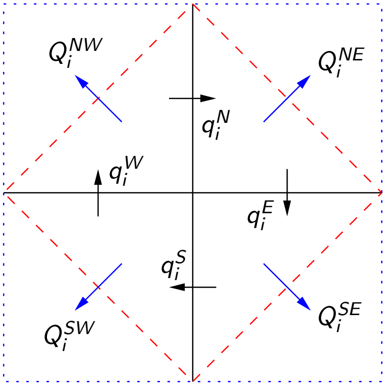
for

$$a_N = \{\mathcal{K}_{NE}^{-1}\}_{11} - \{\mathcal{K}_{NE}^{-1}\}_{12} + \{\mathcal{K}_{NW}^{-1}\}_{11} + \{\mathcal{K}_{NW}^{-1}\}_{12},$$

etc.

Relationship to Raviart-Thomas FEM

- Dual-cell flux problem looks locally like Darcy flow
- Use Raviart-Thomas mixed finite elements to gain local conservation of mass
- Local pressure Schur Complement to replace irrotationality equations



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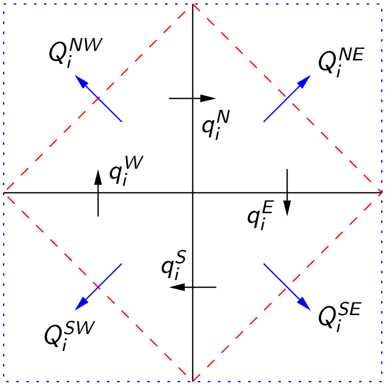
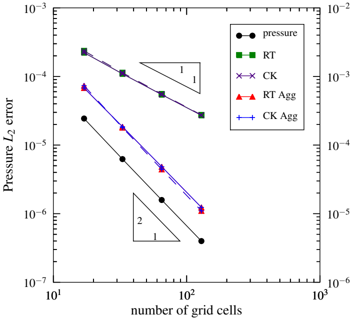
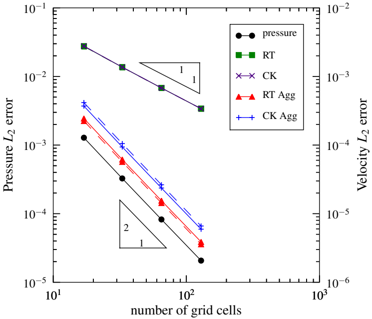


Differs from irrotationality only when non-zero source terms

Locally Conservative Fluxes

Two analytic test problems





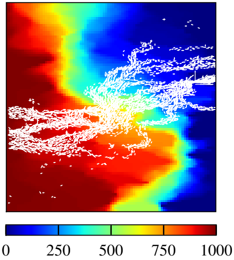
$$\mathcal{K} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

$$\mathcal{K}(x,y) = \begin{cases} 100 & x < 1/2 \\ 1 & x > 1/2 \end{cases}$$

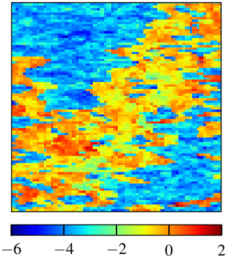
Locally Conservative Fluxes

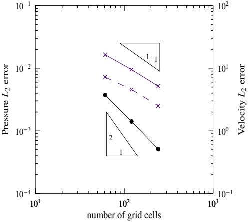
Slice from SPE Benchmark Problem

pressure and flux



log(permeability)





Summary

- Accurate simulation relies on resolving heterogeneities in media
- Coefficient upscaling only valid in special cases
- Variational principles allow accurate upscaling of model
- MSFEM approach accurate, but expensive
- Operator-induced multigrid also captures necessary modes
- Multilevel Upscaling (MLUPS) approach accurate, 15 times cheaper than MSFEM
- Local postprocessing can recover locally conservative fluxes

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S.P. MacLachlan & J.D. Moulton, *Water Resour. Res.*, **42**, 2006
`neumann.math.tufts.edu/~scott/research/multiscale.pdf`
E.T. Coon, S.P. MacLachlan & J.D. Moulton, 2009
`neumann.math.tufts.edu/~scott/research/conservative.pdf`