Lawrence Livermore National Laboratory

Adaptive AMG for Diffusion Equations with Stochastic Coefficients

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Outline

Background
- Motivation
- Uncertainty

Solvers
- Spectral AMGe
- Adaptive AMGe

Numerical Experiments

Conclusions

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Motivation

Uncertainty Quantification in Subsurface Flow

- CO_2 Sequestration
- Contaminant Transport and Remediation
- Reservoir Performance Forecasting

Uncertainty in Conductivity Field

- Reasonable priors from geological assumptions
- Use available real world data (core samples, well data)
- Difficult to sample from posterior distribution

Model Problem

Steady State Single Phase Subsurface Slow:

$$\begin{aligned} \mathbf{q} + k\nabla p &= g \text{ in } D \subset \mathbb{R}^d, \;\; d = 1, 2, 3 \\ \nabla \cdot \mathbf{q} &= 0 \end{aligned}$$

subject to suitable B.C.'s

- p is the pressure head
- $\mathbf{q}$ is the Darcy flux
- k is the hydraulic conductivity field

Model Problem

Uncertainty in p and $\mathbf{q}$ is typically modeled by taking k to be a random field $k(x, \omega)$ on $D \times \Omega$.

The model problem can then be written as a 2nd-order elliptic problem with stochastic coefficients.

$$-\nabla \cdot (k(x, \omega) \nabla p(x, \omega)) \quad = \quad f(x) \text{ in } D \times \Omega$$

$k(x, \omega)$ is assumed to be log-normal with prior determined mean and covariance structure.

Model Problem

$k(x,\omega)$ is log-normal. $Y(x,\omega) := \log k(x,\omega)$ is normal.

Assumed covariance structure:

$$\mathbb{E}\left[Y(x,\cdot)\,Y(x',\cdot)\right] := C(x,x') = \sigma^2 \exp\left(-\sum_{i=1}^{d} \frac{|x_i - x_i'|^p}{\gamma_i^p}\right).$$

γ_i is the correlation length in the ith direction.

Small γ_i's indicate a highly heterogeneous material.

Uncertainty Quantification

Goal: Given prior assumptions about uncertainty in conductivity field, quantify uncertainty in the solution, $p(x, \omega)$.

Method - Monte Carlo Simulation: Generate many realizations of conductivity field. Solve deterministic PDE to obtain many realizations of the solution.

$$\mathbb{E}\left[Q\left(p; k\right)\right] = \frac{1}{N}\sum_{i=1}^{N} Q(p^{(i)}; k^{(i)})$$

where Q is some quantity of interest which depends on the solution.

Need to generate samples of $k(x, \omega)$.

Sampling from the Prior

Expand $Y(x,\omega)$ in a Karhunen-Loeve expansion (KLE):

$$Y(x,\omega) = \mathbb{E}[Y(x,\cdot)] + \sum_{k=1}^{\infty} \sqrt{\lambda_k}\phi_k(x)\,\xi_k(\omega)$$

where (λ_k, ϕ_k) satisfy

$$\int_D C(x,x')\,\phi_k(x')\,dx' = \lambda_k\phi_k(x) \qquad k = 1, 2, \ldots$$

and the ξ_k's are centered, uncorrelated random variables.

Truncate: $Y_M(x,\omega) = \mathbb{E}[Y(x,\cdot)] + \sum_{k=1}^{M} \sqrt{\lambda_k}\phi_k(x)\,\xi_k(\omega)$

Sampling from the Prior

Use truncated KLE to generate realizations of $k(x, \omega)$:

1. Generate $\xi_k^{(i)}$ from $\mathcal{N}(0,1)$, $k = 1, 2, \ldots, M$
2. Form $Y_M^{(i)}(x, \omega) = \mathbb{E}[Y(x, \cdot)] + \sum_{k=1}^{M} \sqrt{\lambda_k} \phi_k(x) \xi_k^{(i)}$
3. Set $k^{(i)}(x, \omega) = \exp\left[Y_M^{(i)}(x, \omega)\right]$

Note that the stochastic process describing k was constructed based solely on prior assumption.

How can we incorporate real world data into the simulation?

Markov Chain Monte Carlo

Prior distribution, $P(k)$, based on KLE and geological assumption.

$P(k)$ is easy to sample from.

Suppose we want to condition samples on some data F.

Want to sample from posterior distribution, $P(k|F)$.

This is Difficult!

Markov Chain Monte Carlo

From Bayes Law: $P(k|F) \propto P(F|k)\, P(k)$.

Define likelihood function: $P(F|k) \propto \exp\left(-\frac{\|F-F_k\|^2}{\sigma_f^2}\right)$

Then $\pi\,(k) = P(k|F) \propto \exp\left(-\frac{\|F-F_k\|^2}{\sigma_f^2}\right) P\,(k)$

Metropolis-Hastings Algorithm:

1. At state k generate k' from transition probability $q\,(k'|k)$.
2. Accept k' as a sample with probability

$$\alpha\left(k, k'\right) \quad = \quad \min\left(1, \frac{\pi\,(k')\, q\,(k|k')}{\pi\,(k)\, q\,(k'|k)}\right)$$

Note: Each evaluation of $\pi\,(k)$ requires deterministic PDE solve!

Markov Chain Monte Carlo

How do we sample from transition probability $q\left(k'|k\right)$?

One method is to use a random walk.

k' is obtained from k by adding a uniform r.v. to each ξ_j

$$\xi_j' = \xi_j + \epsilon_j \quad \text{with } \epsilon_j \in \mathrm{U}\left[-\delta, \delta\right] \text{ for } \quad j = 1, 2, \ldots, M$$

The model problem is solved using the new conductivity field and k is either accepted or rejected.

May be hundreds of discarded proposals between each acceptance!

Must have efficient solvers to offset cost of discarded samples.

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General Multigrid

Discretize model problem using P1 finite elements over a triangularization $\mathcal{T}_h$ of D.

Represent conductivity field by piecewise constant functions over each element.

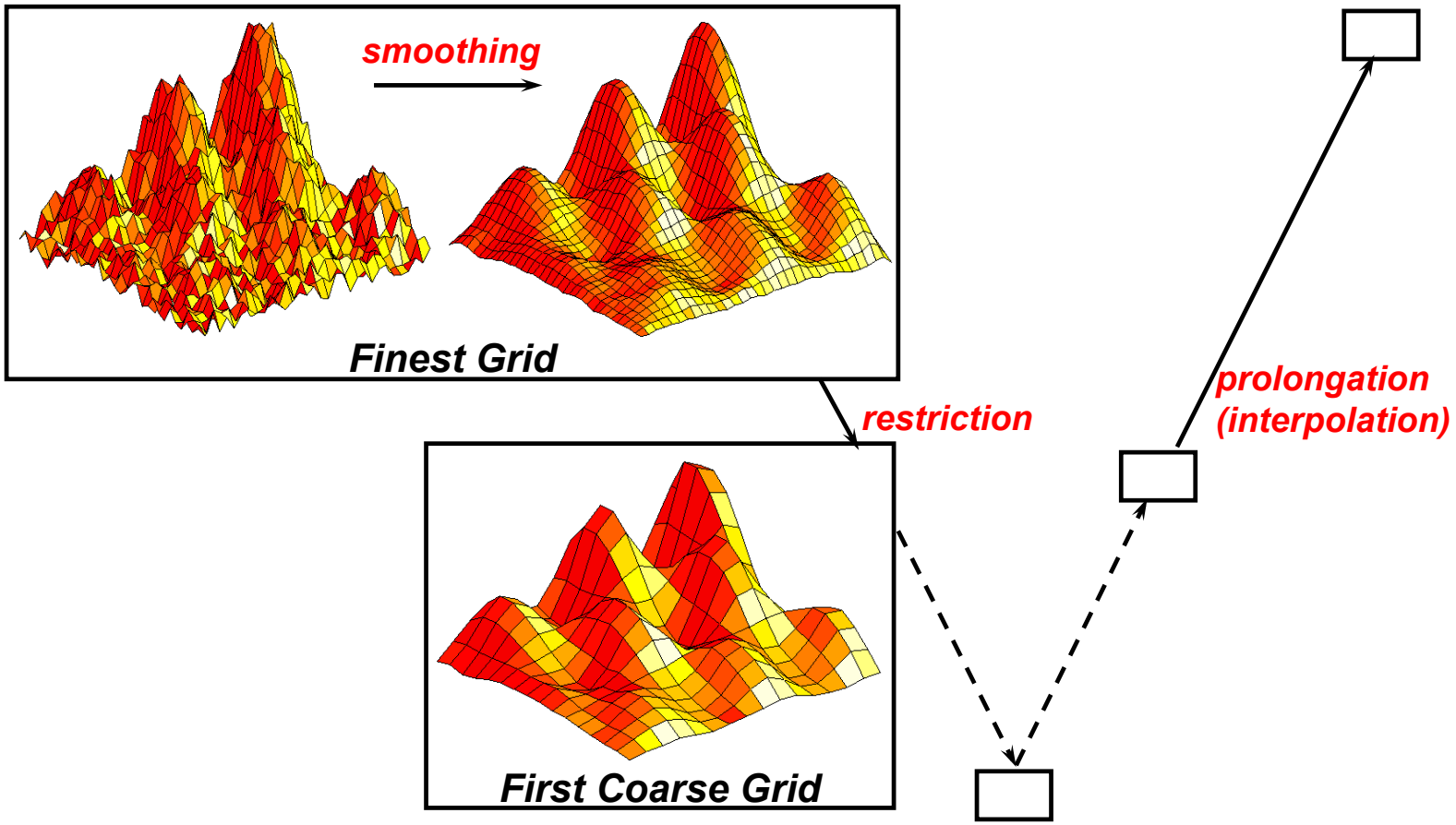
Must solve linear system of equations $A(k)x = b$ for many realizations of conductivity field k.

For very rough k the solution of even one system may be difficult.

MCMC means k and k' are in some sense close (random walk).

Goal: Build solver for $A(k)$ that also works for $A(k')$.

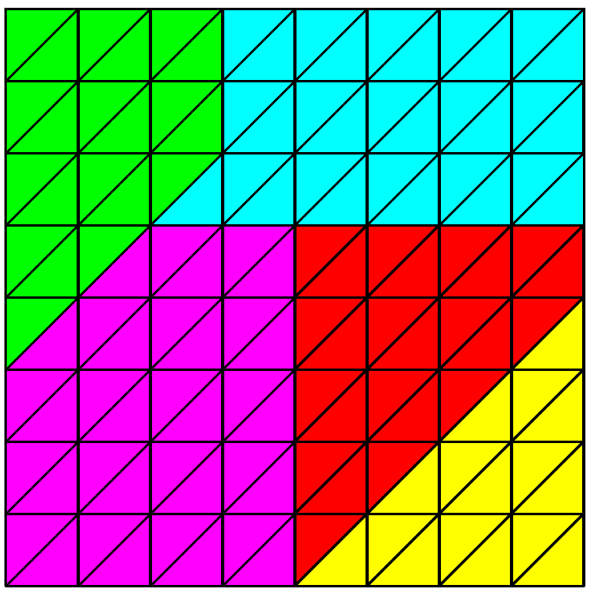
General Multigrid

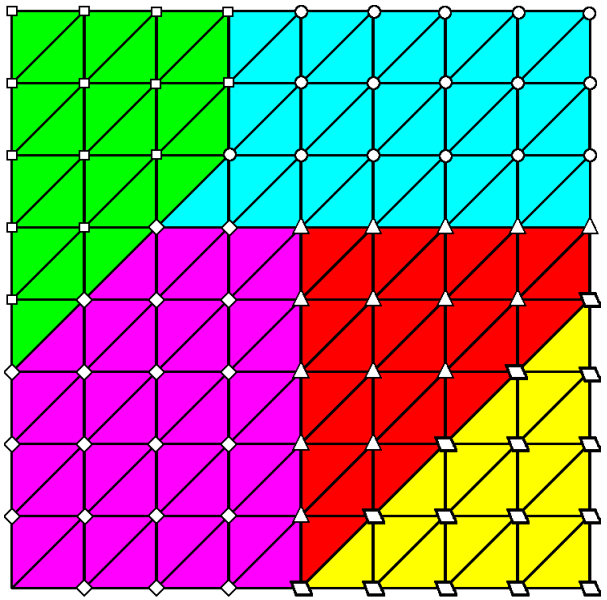


Two-Level Spectral AMGe - Interpolation

Partition $\mathcal{T}_h$ into set of agglomerated elements $\{T\}$.

Let $\{\mathcal{A}\} = \{\mathcal{A}_r\}_{r=1}^{n_c}$ be a corresponding set of aggregates such that each $\mathcal{A}$ is contained in a unique T.





Two-Level Spectral AMGe - Interpolation

Assemble the local stiffness matrices A_T for each T.

Solve the local generalized eigenvalue problem for each T:

$$A_T \mathbf{q}_k = \lambda_k D_T \mathbf{q}_k, \qquad k = 1, \ldots, n_T$$

For a given tolerance $\theta \in (0, 1]$ select the first $m_T \leq n_T$ eigenvectors such that

$$\lambda_k \leq \theta \lambda_{\max} \text{ and } \lambda_{k+1} \geq \theta \lambda_{\max}$$

Restrict local vectors to each aggregate $\mathcal{A}$ and orthogonalize

$$\left\{ \mathbf{p}_1^{\mathcal{A}}, \mathbf{p}_2^{\mathcal{A}}, \ldots, \mathbf{p}_{m_T'}^{\mathcal{A}} \right\}$$

Two-Level Spectral AMGe - Interpolation

Local tentative interpolant is then $\overline{P}_{\mathcal{A}} = \left[\mathbf{p}_1^{\mathcal{A}}, \mathbf{p}_2^{\mathcal{A}}, \ldots, \mathbf{p}_{m'_T}^{\mathcal{A}}\right]$

Global tentative interpolant is

$$\overline{P} = \begin{bmatrix} \overline{P}_{\mathcal{A}_1} & 0 & & 0 \\ 0 & \overline{P}_{\mathcal{A}_2} & & 0 \\ 0 & 0 & \ddots & \vdots \\ 0 & 0 & \ldots & \overline{P}_{\mathcal{A}_{n_c}} \end{bmatrix}.$$

The final interpolant is obtained by pre-multiplying $\overline{P}$ by a suitably chosen smoother:

$$P = \left(I - D^{-1}A\right)\overline{P}$$

Two-Level Spectral AMGe - Relaxation

We choose polynomial smoothers for their good parallelization properties.

Let $p_\nu(t) = \prod_{j=1}^{\nu} \left(1 - \frac{t}{\tau_j}\right)$. Note $p_\nu(0) = 1$ and $p_\nu(\tau_j) = 0$

Define $M^{-1} = \left[I - p_\nu\left(D^{-1}A\right)\right] A^{-1}$

Since $p_\nu(0) = 1$ we have $p_\nu(t) = 1 - t q_{\nu-1}(t)$ and so

$$M^{-1} = q_{\nu-1}\left(D^{-1}A\right) D^{-1}$$

Note: M^{-1} does not depend on A^{-1} and is sym if A and D are.

Two-Level Spectral AMGe - Algorithm

TL - Algorithm

1. Define initial guess x
2. Pre-smoothing: $x = x + M^{-1}(b - Ax)$
3. Restrict residual: $r_c = P^T(b - Ax)$
4. Coarse solve: $x_c = \left(P^T A P\right)^{-1} r_c$
5. Correct current iterate: $x = x + P x_c$
6. Post-smoothing: $x = x + M^{-1}(b - Ax)$

Assuming symmetric A and D and a zero initial guess, we can write

$$b \mapsto B_{TG}^{-1} b = x_{TG}$$

where $B_{TG}^{-1} = M^{-1} + \left(I - M^{-1}A\right) P \left(P^T A P\right)^{-1} P^T \left(I - AM^{-1}\right)$

Adaptive AMGe

Have B_{TG} based on matrix A, $\{T\}$, $\{\mathcal{A}\}$, and $\{\mathbf{q}_k^{(T)}\}$

Want to use B_{TG} to solve problems involving $A' := A\left(k'\right)$

Test: Replace A with A' in TL-Algorithm and iterate on $A'x = 0$:

$$x_k = \left(I - B_{TG}^{-1} A'\right) x_{k-1}$$

Monitor $\|x_k\|_{A'} \to 0$. If convergence is good retain B_{TG}

Otherwise, take $x^{bad} = x_k$ and restrict it to AEs, x_T^{bad}

Adaptive AMGe

Solve the new local generalized eigenvalue problem for each T:

$$A'_T \mathbf{z}_k = \mu_k D'_T \mathbf{z}_k, \qquad k = 1, \ldots, m'_T + 1$$

in the subspace $\mathrm{Span}\{\mathbf{q}_1^T, \ldots \mathbf{q}_{m'_T}^T, x^{bad}\}$. Choose $\mathbf{z}_k$'s satisfying

$$\mu_k \leq \theta' \mu_{\max} \text{ and } \mu_{k+1} \geq \theta' \mu_{\max}$$

Restrict local vectors to each aggregate $\mathcal{A}$ and orthogonalize

$$\left\{ \mathbf{p}_1^{\mathcal{A}}, \mathbf{p}_2^{\mathcal{A}}, \ldots, \mathbf{p}_{m''_T}^{\mathcal{A}} \right\}$$

Construct global P as before to obtain B'_{TG}. Repeat as needed.

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$$
\begin{aligned}
-\nabla \cdot \left(k\left(x,\omega\right)\nabla p\left(x,\omega\right)\right) &= 1 \text{ in } \left[0,1\right]^2 \times \Omega \\
p &= 1 \text{ on } \left\{x_1 = 0\right\} \times \Omega \\
p &= 0 \text{ on } \left\{x_1 = 1\right\} \times \Omega \\
\nabla p \cdot \mathbf{n} &= 0 \text{ on } \left\{x_2 = 0, x_2 = 1\right\} \times \Omega
\end{aligned}
$$

$k\left(x,\omega\right)$ is chosen from a log-normal prior with zero mean and

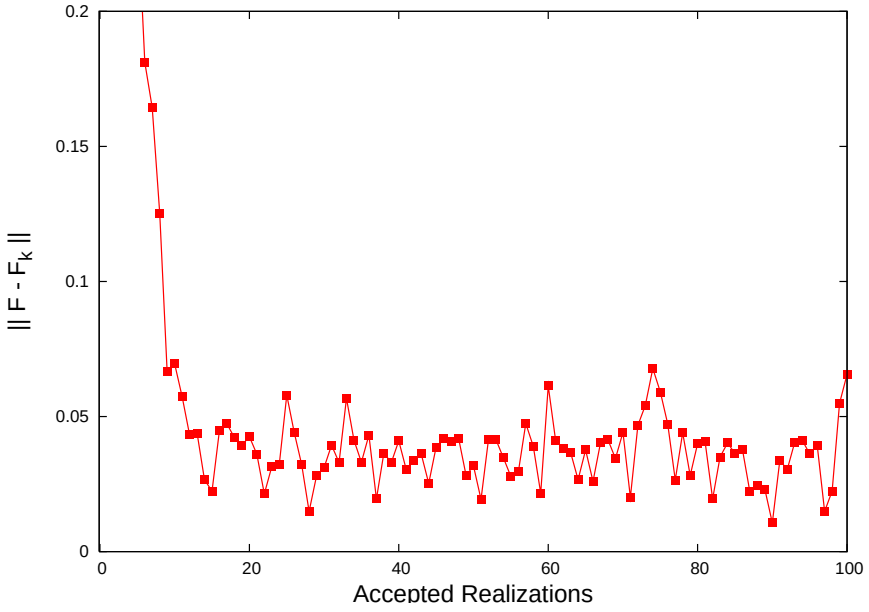
$$
C\left(x,x'\right) = \left(5\right)^2 \exp\left(-\frac{\left|x_1 - x_1'\right|}{0.1} - \frac{\left|x_2 - x_2'\right|}{0.4}\right).
$$

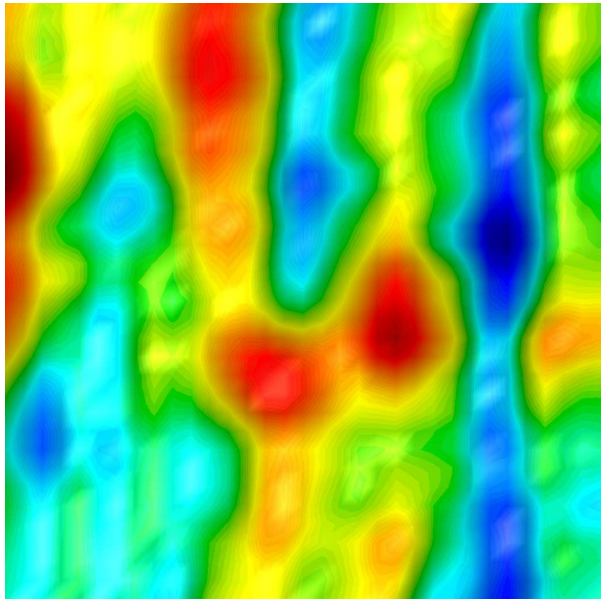
The first 500 terms in the KL-expansion are used.

Model Problem

Metropolis-Hastings MCMC is used to condition the conductivity samples on flow data at 4 points in the domain.

The transition probability $q\left(k'|k\right)$ is defined by a random walk drawn from $\mathcal{U}\left[-\delta,\delta\right]$.





Solver Performance

At each Metropolis-Hasting step, the TL-Algorithm is used as a stationary iteration to solve the resulting linear system.

A degree 4 polynomial smoother is used along with an initial spectral threshold parameter of $\theta = 0.01$.

A target convergence rate of $\rho = 0.5$ is defined and re-adaptation automatically occurs if the performance falls below this threshold.

The solver stops when the relative residual has decreased by a factor of 10^{-8}.

The MCMC algorithm is run for 10K iterations.

Solver Performance

The table shows the performance of the adaptive TL-Algorithm as well as the non-adaptive TL-Algorithm and standard Geometric Multigrid. The fine grid contained 16K degrees of freedom partitioned into 100 agglomerated elements.

δ	MG	TL-Alg.	αTL-Alg.	Adaptations Required
0.5	$.91/4$	$.52/35$	$.24/35$	124
1.0	$.92/4$	$.65/30$	$.26/30$	670

Values reported are the average convergence rate and the average coarsening factor between the fine and coarse grids averaged over 10K MCMC iterations.

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- We've presented an adaptive two-level AMGe method that can used to solve linear systems originating from 2nd-order elliptic PDE with stochastic coefficients.
- The resulting method can be re-used when the new system is in some sense *close* to the original.
- When the new system greatly differs from the original, re-adaption can be preformed quickly and efficiently.

Future Work

- Extend the two-level method to multilevel via recursion.
- Use the coarse spaces generated by the method to compute upscaled approximations of the fine-grid dynamics.
- Applications in the deterministic regime e.g. solution of nonlinear PDE.

Acknowledgments and References

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