Coarsening in Adaptive Algebraic Multigrid

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Target Applications

- Fluid flow in porous media
 - Highly heterogeneous media
 - Interested in global properties of the solution
- Coupled fluid-elastic systems
 - Multiple material regimes
 - Different models require very different treatment
- Lattice quantum chromodynamics
 - Highly heterogeneous operator
 - Randomized heterogeneity within Monte Carlo process

Target Discrete Models

Finite element models of elliptic formulations of PDEs

Matrices are

sparse

symmetric

positive definite

Solving Ax = b

Sparsity with large bandwidth means that direct methods are not effective for these problems

Stationary Iterative Methods

- Given some approximation, $x^{(0)}$, want to improve it
- Introduce residual, $r^{(0)} = b Ax^{(0)}$, as a measure of the error

•
$$r^{(0)} = b - Ax^{(0)} = Ax - Ax^{(0)} = A(x - x^{(0)})$$

Let
$$B^{-1}$$
 be an approximation to A^{-1}

Take
$$x^{(1)} = x^{(0)} + B^{-1}r^{(0)}$$

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

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Let
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$$x^{(1)} = x^{(0)} + B^{-1}r^{(0)}$$

Error propagation form: $e^{(n)} = (I - B^{-1}A)^n e^{(0)}$

Convergence of Stationary Iterative Methods



Convergence of Stationary Iterative Methods



Errors with small $B^{-1}A$ -Rayleigh Quotients are slowest to converge

Scalability

These methods fail when the problem size gets large enough!



Failing in a Structured Way

For all of these methods, low-energy modes of $B^{-1}A$ cause the most trouble

For simple-enough B, these are the same as (or close to) the low-energy modes of A

Can we use this to our advantage?



Random initial error



Error after 1 weighted Jacobi iteration



Error after 2 weighted Jacobi iterations



Error after 3 weighted Jacobi iterations



Error after 4 weighted Jacobi iterations



Error after 5 weighted Jacobi iterations



Error after 6 weighted Jacobi iterations



Error after 7 weighted Jacobi iterations



Error after 8 weighted Jacobi iterations



Error after 9 weighted Jacobi iterations



Error after 10 weighted Jacobi iterations

Complementarity

Error after a few weighted Jacobi iterations has structure

Instead of throwing out the method, look to complement its failings

How can we best correct error modes that are slow to be reduced by relaxation?

Complementarity

Error after a few weighted Jacobi iterations has structure

Instead of throwing out the method, look to complement its failings

How can we best correct error modes that are slow to be reduced by relaxation?

- Slow-to-converge errors are smooth
- Smooth vectors can be accurately represented using fewer degrees of freedom

Coarse Grids

Sine series representation:

$$f(x) = \sum_{k=1}^{\infty} c_k \sin(k\pi x)$$

Discrete problems can only approximate certain modes

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Coarse-Grid Correction

- Smooth vectors can be accurately represented using fewer degrees of freedom
- Idea: transfer job of resolving smooth components to a coarser grid version of the problem
- Need:
 - Complementary process for resolving smooth components of the error on the coarse grid
 - Way to combine the results of the two processes

Variational Coarsening

- Idea is to correct the approximation after relaxation, $x^{(1)}$, from a coarse-grid version of of the problem
- Need interpolation map, P, from coarse grid to fine grid

Corrected approximation will be $x^{(2)} = x^{(1)} + Px_c$

What is the best x_c for correction?

A-norm and A-inner product

- Asking for the best solution implies a metric
- Symmetric and positive-definite matrix, A, defines an inner product and a norm:

$$\langle x, y \rangle_A = y^T A x$$
 and $||x||_A^2 = x^T A x$

Best then means closest to the exact solution in norm

$$y^{\star} = \underset{y}{\operatorname{argmin}} \|x - y\|_{A}$$

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What is the best x_c for correction?

Best means closest to the exact solution in norm

$$x_{c} = \underset{y_{c}}{\operatorname{argmin}} \|x - (x^{(1)} + Py_{c})\|_{A}$$

Best x_c satisfies $(P^T A P) x_c = P^T A (x - x^{(1)}) = P^T r^{(1)}$



Relax:
$$x^{(1)} = x^{(0)} + B^{-1}r^{(0)}$$

Relaxation

- Use a smoothing process (such as Jacobi or Gauss-Seidel) to eliminate oscillatory errors
- Remaining error satisfies $Ae^{(1)} = r^{(1)} = b Ax^{(1)}$



- Relaxation
- Restriction

Relax:
$$x^{(1)} = x^{(0)} + B^{-1}r^{(0)}$$

Restriction

- Transfer residual to coarse grid
- Compute $P^T r^{(1)}$



Use coarse-grid correction to eliminate smooth errors

Best correction, x_c , in terms of A-norm satisfies

$$P^T A P x_c = P^T r^{(1)}$$



Transfer correction to fine grid

Compute $x^{(2)} = x^{(1)} + Px_c$



Relax once again to remove oscillatory error introduced in coarse-grid correction



Direct solution of coarse-grid problem isn't practical
Two-grid cycle



Direct solution of coarse-grid problem isn't practical Use an iterative method!

Two-grid cycle



Recursion!

Apply same methodology to solve coarse-grid problem

The Multigrid V-cycle



Properties of Effective Cycles

Fast convergence

- Effective reduction of all error components
- On each level, coarse-grid correction must effectively reduce exactly those errors that are slow to be reduced by relaxation alone
- Hierarchy of coarse-grid operators resolves relevant physics at each scale
- Low iteration cost
 - Simple relaxation scheme (cheap computation of $B^{-1}r$ on all levels)
 - Sparse coarse-grid operators (cheap computation of residuals on all levels)
 - Sparse interpolation/restriction operations

What Haven't I Told You?

- How do we choose P?
 - Number of columns
 - Sparsity structure
 - Non-zero values
- Often consider these independently, but there are dependencies
- These choices must be informed by properties of relaxation

- For Poisson's equation, error left after relaxation is smooth
- Low-order geometric interpolation is accurate for smooth functions

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- For Poisson's equation, error left after relaxation is smooth
- Low-order geometric interpolation is accurate for smooth functions
- Linear interpolation works well for problems with smooth, isotropic coefficients when grid geometry is known
 - May not know grid geometry
 - Linear interpolation can make O(1) errors for problems with non-smooth coefficients

Linear interpolation can make O(1) errors for problems with non-smooth coefficients

Slowest to converge error for $\frac{d}{dx} \left(\sigma \frac{du}{dx} \right)$, for $\sigma = \begin{cases} 10^{-8} & x \le \frac{3}{8} \\ 1 & x > \frac{3}{8} \end{cases}$



Linear interpolation can make O(1) errors for problems with non-smooth coefficients

Slowest to converge error for $\frac{d}{dx} \left(\sigma \frac{du}{dx} \right)$, for $\sigma = \begin{cases} 10^{-8} & x \le \frac{3}{8} \\ 1 & x > \frac{3}{8} \end{cases}$





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- Linear interpolation can make O(1) errors for problems with non-smooth coefficients
- The abrupt change in character of slow-to-converge errors is reflected in matrix entries
- Idea: Use the entries in the matrix operator to help define interpolation

Algebraic Multigrid Interpolation

- Assume a partition into fine (F) and coarse (C) grid sets
- No geometric information used in defining interpolation
- Start with small-residual assumption that errors left after relaxation have small residuals: for $i \in F$,

 $(Ae)_i \approx 0$ $a_{ii}e_i = -\sum_{j \in F} a_{ij}e_j - \sum_{k \in C} a_{ik}e_k$

Use assumptions about slow-to-converge error to collapse connections to $j \in F$ onto $k \in C \cap \{k : a_{ik} \neq 0\}$

Calibrating Interpolation

What if we don't know what to assume about slow-to-converge errors?

Calibrating Interpolation

What if we don't know what to assume about slow-to-converge errors? Run relaxation to find out!

- Run relaxation on Ax = 0 with a random initial guess
- This exposes the local character of slow-to-converge errors
- Use resulting vector as a prototype of errors to be corrected by interpolation within algebraic multigrid

Adaptive Multigrid

Automatic probing of relaxation and algebraic coarsening

- Given matrix A, Relaxation operation $B^{-1}r$
- Iterate on homogeneous problem, Ax = 0, with a random initial guess
- Create interpolation such that prototype of slow-to-converge error is in its range
- Create coarse-grid problem and recurse

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Relaxation can be anything

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Relaxation can be anything, even the multigrid method itself!

Allows for iterative improvement of a poorly performing multigrid cycle

Adaptive Cycling

- Suppose we probe relaxation, design the best interpolation we know how, and the resulting MG cycle still doesn't work.
 - Interpolation was based on a single prototype of slow-to-converge errors
 - May not have enough information to complement all slow-to-converge modes
 - How can we identify a new prototype, distinct from the previous?

Apply the adaptive principles to the multigrid method itself

Controlling Adaptation

Two possible sources of slow adaptive MG convergence

- Prototype is a bad representative error
- Prototype is good, but there is distinct slow-to-converge error
- Want a measure to distinguish cause of bad performance

Use estimates of $||I - B^{-1}A||$ to measure both performance and quality of prototype sets

Estimate $||B^{-1}A||$ using Rayleigh Quotients

Algorithm Overview

• while $||I - B_{MG}^{-1}A||_{est}$ is large

• if $||I - B_{rel}^{-1}A||_{est}$ is increasing

iterate on Ax = 0 with "relaxation", $x \leftarrow (I - B_{rel}^{-1}A)x$

 \blacksquare recalibrate interpolation based on new x

recompute coarse-grid operator

restrict x to coarse grid and cycle there

- interpolate further improved x after coarse-grid cycle
- else

Replace "relaxation" with multigrid cycle: $B_{rel} \leftarrow B_{MG}$

Testing Adaptation

2-D Finite Element Shifted Laplacian, Dirichlet BCs, 512×512 grid

$$-\Delta u - 2\pi^2 (1 - 2^{-15})u = 0$$

■ $\lambda_{\min} = 6.64 \times 10^{-4}$, random $x^{(0)}$

Iteration	$\ I - B_{rel}^{-1}A\ _{est}$	$\ I - B_{MG}^{-1}A\ _{est}$		
1	0.87	0.9999998		
2	0.996	0.999985		
3	0.99988	0.9996		
4	0.999997	0.986		
5	0.99999993	0.622		
6	0.999999997	0.078		
7	0.999999998	0.071		

Linear Elasticity

Model displacement, u, of an elastic body under external forces

$$-\mu\Delta u - (\lambda + \mu)\nabla\nabla \cdot u = f$$

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)} \quad \text{and} \quad \mu = \frac{E}{2(1+\nu)}$$

Fix $\nu = 0.32$ (steel)

- Let *E* vary between 1 (nylon/polypro) and 10^{σ} (100 = titanium, 1000 = diamond)
- Know properties of slow-to-converge errors for small σ

Numerical Results: Linear Elasticity

	Fixed			Adaptive			
σ	$\ I - B_{MG}^{-1}A\ $	Iterations	CPU (s)	$\ I - B_{MG}^{-1}A\ $	Iterations	CPU (s)	
2	0.1146	9	25.99	0.2141	12	267.72	
3	0.2466	14	35.68	0.3095	16	275.62	
4	0.3948	20	49.99	0.4040	21	289.39	
5	0.5545	32	73.63	0.4966	27	381.16	

3D cube, 201,720 degrees of freedom, exponential distribution of ${\it E}$

Lattice Quantum Chromodynamics

- Modelling strong interactions between fermions (quarks) on a lattice
- Goal: Solve $H(u, \rho)f = b$, for multiple fermionic source vectors, b, at each step of a Monte Carlo simulation
- Difficulty: u is a complex unitary field defined on the lattice edges, with phases chosen randomly based on system temperature parameter, β
- H is naturally Hermitian, but indefinite, so solve normal equations
- As \(\rho\) approaches a critical value, \(H^*H\) becomes singular (at any temperature)
- Structure of low-energy modes strongly depends on *u*
 - When $\beta \to \infty$, $u \to 1$, H^*H looks like a second-order discrete differential operator
 - For each state, new characterization of low-energy modes

Numerical Results: Lattice QCD

	Diagonal-PCG				AdaptiveMG-PCG			
$\rho-\rho_{\rm Cr}$	0.3	0.1	0.05	0.01	0.3	0.1	0.05	0.01
$\beta = 2$	0.85	0.94	0.96	0.99	0.31	0.31	0.31	0.33
$\beta = 3$	0.86	0.93	0.97	0.98	0.31	0.40	0.42	0.42
$\beta = 5$	0.83	0.92	0.96	0.99	0.28	0.29	0.31	0.31

 128×128 periodic lattice, average residual reduction per iteration

Adaptive MG setup time:13.7 secondsAdaptive MG-PCG solve time:0.8 secondsDiagonal-PCG solve time:4.7 seconds

Choosing Coarse Grids

Difficult to say what best coarse grid is

- Want enough coarse-grid points so that interpolation is accurate for all slow-to-converge errors
- Want significantly fewer coarse-grid points than fine-grid points
- Interpolation designed to complement failings of relaxation
 - Coarse-grid selection must make this possible

Maximal Independent Sets

- Want local interpolation operators
- Idea: Coarsen so that every fine-grid node has at least one coarse-grid neighbour

Problem: not all connections are equal

Really want every fine-grid node to be somehow strongly coupled to at least one coarse-grid node

Strong Connections - AMG

Classical AMG defines the strong connections for each node based directly on the matrix entries:

$$S_i = \left\{ j : -a_{ij} \ge \theta \max_{k \neq i} \{-a_{ik}\} \right\}$$

Based on properties of finite difference discretizations

Diagonally dominant M-matrices

Weaknesses

Definition of strong connections based on "nice" M-matrix properties

Breaks down if near null space of A is far from the constant

Diagonal rescaling,

$$A \to DAD$$

Finite element anisotropy,

$$-u_{xx} - \epsilon u_{yy} \rightarrow \frac{1}{6} \begin{bmatrix} (-1-\epsilon) & (2-4\epsilon) & (-1-\epsilon) \\ (-4+2\epsilon) & (8+8\epsilon) & (-4+2\epsilon) \\ (-1-\epsilon) & (2-4\epsilon) & (-1-\epsilon) \end{bmatrix}$$

Even for simple problems, size of a_{ij} may not reflect true connection between *i* and *j*

What are Strong Connections?

Point i strongly depends on point j if

- a change in the right-hand side at point j significantly changes the solution at point i.
- a change in the residual at point j significantly changes the error at point i
- Good coarse-grid correction depends on identifying strong connections
 - Interpolation to i is most effective from points that it strongly depends on
 - Corrections from weakly connected points have little effect on the error at i

Inverse-based Strength

For the discrete linear system, Ax = b, the inverse relates changes in b to changes in x

$$x = (A)^{-1} b$$

If a change in b_j causes a significant change in x_i , then $(A)_{ij}^{-1}$ must be large relative to other values of $(A)_{ik}^{-1}$



Columns of inverse of Isotropic and Anisotropic Poisson Operators

Measures of Strong Connections

- Strength of dependence of *i* on *j* depends on size of $(A)_{ij}^{-1}$
- How should we measure this size, relative to $(A)_{ik}^{-1}$?

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• How should we measure this size, relative to $(A)_{ik}^{-1}$?

 $L^{2} \text{ measure: } (A)_{ij}^{-1} \ge \theta \max_{k \neq i} \left\{ (A)_{ik}^{-1} \right\}$ Energy measure: Let $G_{j}^{(i)} = (A)_{ij}^{-1}, S_{ij} = \frac{\|G^{(i)} - G_{j}^{(i)}e^{(j)}\|_{A}}{\|G^{(i)}\|_{A}}$



Strength measures for Isotropic and Anisotropic Poisson Operators
Can we get useful, local approximations to $(A)_{ij}^{-1}$ and, thus, S_{ij} ?

Apply (localized) relaxation to $AG^{(i)} = e^{(i)}$

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Approximate S_{ij} after 1 weighted Jacobi Relaxation for Isotropic and Anisotropic Poisson Operators

Can we get useful, local approximations to $(A)_{ij}^{-1}$ and, thus, S_{ij} ?

Apply (localized) relaxation to $AG^{(i)} = e^{(i)}$



Approximate S_{ij} after 2 weighted Jacobi Relaxation for Isotropic and Anisotropic Poisson Operators

Can we get useful, local approximations to $(A)_{ij}^{-1}$ and, thus, S_{ij} ?

Apply (localized) relaxation to $AG^{(i)} = e^{(i)}$



Approximate S_{ij} after 3 weighted Jacobi Relaxation for Isotropic and Anisotropic Poisson Operators

Can we get useful, local approximations to $(A)_{ij}^{-1}$ and, thus, S_{ij} ?

Apply (localized) relaxation to $AG^{(i)} = e^{(i)}$



Approximate S_{ij} after 4 weighted Jacobi Relaxation for Isotropic and Anisotropic Poisson Operators

Can we get useful, local approximations to $(A)_{ij}^{-1}$ and, thus, S_{ij} ?

Apply (localized) relaxation to $AG^{(i)} = e^{(i)}$



Approximate S_{ij} after 5 weighted Jacobi Relaxation for Isotropic and Anisotropic Poisson Operators

Choosing C

For point *i*, $\{S_{ij}\}$ are now measures of strengths of connection

• We now say *i* strongly depends on *j* if $(A)_{ij} \neq 0$ and

$$S_{ij} - 1 \ge \theta \max_{k \ne i} \left\{ S_{ik} - 1 \right\}$$

For now, $\theta = 0.25$ seems to work fine

Coarse grid selection now accomplished by taking a maximal independent subset of the graph of strong connections

 $-u_{xx} - u_{yy} = f$, Dirichlet BCs

- 32×32 bilinear finite element grid
- **2** Steps Weighted Jacobi to determine S_{ij}



 $-u_{xx} - 0.01u_{yy} = f$, Dirichlet BCs

- 32×32 bilinear finite element grid
- **2** Steps Weighted Jacobi to determine S_i



 $-u_{xx} - u_{yy} = f$, Dirichlet BCs

■ 32×32 bilinear finite element grid, $A \rightarrow DAD$, $d_{ii} = 10^{5r_i}$

2 Steps Weighted Jacobi to determine S_i



 $-u_{xx} - 0.01u_{yy} = f$, Dirichlet BCs

■ 32×32 bilinear finite element grid, $A \rightarrow DAD$, $d_{ii} = 10^{5r_i}$

2 Steps Weighted Jacobi to determine S_i



Algorithm

- Given *A*,*b*
- Relax ν_0 times on $A\mathbf{x} = \mathbf{0}$ with a random initial guess
- On each level
 - Determine local strong connections by μ relaxations on $A\mathbf{G}^{(i)} = \mathbf{I}^{(i)}$
 - Choose coarse grid by colouring algorithm
 - Relax ν_1 times on $A\mathbf{x} = \mathbf{0}$ to improve representation of algebraically smooth error
 - Form interpolation, P, based on \mathbf{x}
 - Compute $A_c = P^T A P$, inject $\mathbf{x}_c = (\mathbf{x})_c$
- Examples have fixed $\nu_0 = \nu_1 = 15$, $\mu = 2$

Numerical Results

Convergence	Factors	of Resulting	V(1,1)	Cycles
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grid	Laplace	Scaled Laplace	Anisotropic	Scaled Anisotropic
32×32	0.06	0.06	0.10	0.10
64×64	0.07	0.07	0.10	0.10
128×128	0.07	0.07	0.10	0.10
256×256	0.07	0.07	0.10	0.10
512×512	0.07	0.07	0.10	0.10

Good convergence factors, but setup cost is now high

Compatible Relaxation

Heuristics seem to work well and can be made robust

Alternative: choose coarse grids so that we know that interpolation can be chosen to complement relaxation

Theory of Compatible Relaxation says that if relaxation on the fine-grid submatrix is fast to converge, then there is an interpolation operator which yields a multigrid method with small convergence factor

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Fine-grid relaxation: $I - \omega B_{ff}^{-1} A_{ff}$ is efficient if

 $c_1 \langle B_{ff} x_f, x_f \rangle \le \langle A_{ff} x_f, x_f \rangle \le c_2 \langle B_{ff} x_f, x_f \rangle$

for reasonable c_1, c_2

Under right assumptions, can show multigrid convergence is bounded less than 1, with bound dependent on $\frac{c_2}{c_1}$

Satisfying the Theory

Want to turn these results into a practical algorithm

- Idea: Choose partition so that we know fine-grid relaxation converges quickly
- Weighted Jacobi relaxation on A_{ff} converges quickly when A_{ff} is diagonally dominant

We can guarantee good 2-level convergence factors by choosing A_{ff} to be diagonally-dominant

NP-completeness

Define θ -dominance of A_{ff} as

$$a_{ii} \ge \theta \sum_{j \in F} |a_{ij}|$$

• Know theory can be satisfied as long as A_{ff} is θ -dominant

So, choose A_{ff} to be the largest submatrix of A that is θ -dominant

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So, choose A_{ff} to be the largest submatrix of A that is θ -dominant

This is an NP-complete problem

Greedy Algorithm Approach

• Want an O(n) coarse-grid selection algorithm, not an NP-complete one

- Initialize all points to be in U; F, C to be empty
- For each point *i*, compute diagonal dominance measure

$$\hat{\theta}_i = \frac{|a_{ii}|}{\sum_{j \in F \cup U} |a_{ij}|}$$

If $\hat{\theta}_i \geq \theta$, put *i* into *F*, remove it from *U*

- While U is non-empty
 - Find $j = \underset{i \in U}{\operatorname{argmin}} \hat{\theta}_i$
 - **Remove** j from U, put it in C
 - For each neighbouring point *i* of *j*, update $\hat{\theta}_i$

If $\hat{\theta}_i \geq \theta$, put *i* into *F*, remove it from *U*

Test Problems

Test problems based on finite element discretizations of $-\nabla \cdot K(x, y) \nabla p(x, y)$

Laplace equation, K(x, y) = 1

Smooth coefficient, $K(x, y) = 10^{-8} + 10(x^2 + y^2)$

Randomly chosen coefficient, $K(x, y) = 10^{-8}$ on 20% of the cells, chosen randomly, K(x, y) = 1 otherwise

Anisotropic coefficient, $K(x, y) = \begin{bmatrix} 1 & 0 \\ 0 & 0.01 \end{bmatrix}$

Algorithm:

- Greedy algorithm to select coarse grids
- Classical AMG to define interpolation
- Usual AMG-V(1,1) cycles with Gauss-Seidel relaxation

Multilevel AMG results

Coefficient	Grid	c_A	$t_{\sf setup}$	$t_{\sf solve}$	# iters.	ρ
K(x,y) = 1	512×512	1.33	1.3	0.7	5	0.13
	1024×1024	1.33	5.1	2.5	5	0.14
	2048×2048	1.33	21.9	10.5	5	0.14
smooth $K(x, y)$	512×512	1.33	1.3	0.6	5	0.13
	1024×1024	1.33	5.1	2.5	5	0.14
	2048×2048	1.33	21.7	10.4	5	0.14
random $K(x, y)$	512×512	2.06	2.3	1.2	6	0.35
	1024×1024	2.08	9.6	4.8	6	0.40
	2048×2048	2.10	41.0	19.8	6	0.46
anisotropic $K(x, y)$	512×512	2.39	1.5	1.0	5	0.13
	1024×1024	2.41	6.2	4.1	5	0.20
	2048×2048	2.43	25.8	17.7	5	0.20

Summary

- Single-level iterative methods slow to resolve low-energy modes of $B^{-1}A$
- Structure of these modes allows definition of efficient multigrid solvers
- If slow-to-converge error cannot be characterized beforehand, adaptive multigrid techniques can recover good performance at cost of extra setup
- Better heuristics allow more robust coarse-grid selection, but cost questions are important
- Theoretically motivated coarsening gives encouraging results
 - Competitive algorithmic cost
 - Good experimental results
 - Robustness and parallelism questions

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