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- Primarily in collaboration with
  - Steve McCormick, Tom Manteuffel, John Ruge, Marian Brezina at CU-Boulder, and Rob Falgout from CASC-LLNL.
  - James Brannick from Penn State University

## **Big Picture**

#### AMG is a nice algorithm

- Efficiently solves many problems
- Good algorithmic and parallel scalability
- Somewhat mature technology

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- Requires some expert knowledge
- Convergence isn't well understood

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#### When AMG works, it is often the best solver

# **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 difference/element models of elliptic systems
- Matrices are
  - sparse
  - symmetric
  - positive definite

Solving Ax = b

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

## **Algorithmic Goals**

Efficient and robust solver for heterogeneous models

Efficient: Optimal scalability, both algorithmic and parallel

- Cost of solve linearly proportional to number of unknowns
- Natural parallelism; most calculations should be data-local

Robust: Consistent performance with few parameters

- Predictable performance based on simple characteristics
- Not expert software; no magic parameters

# **Efficiency First**

Heterogeneity is an added complication, but not fundamental

Still need techniques to handle

- Large problem sizes
- Large condition numbers
- Multiscale structure of operator

Robustness without efficiency is EASY! Gaussian Elimination

# **Efficiency First**

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Still need techniques to handle

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Robustness without efficiency is EASY! Gaussian Elimination

- Start with an efficient solver for homogeneous models
  - Geometric multigrid
- Look for where robustness and heterogeneity play a role

- Want to improve approximation,  $x^{(0)}$ , to  $x = A^{-1}b$
- Residual,  $r^{(0)}$ , is a measure of the error

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

• Choose 
$$M^{-1}pprox A^{-1}$$

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

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

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Error propagation form:  $e^{(1)} = (I - M^{-1}A)e^{(0)}$  $e^{(2)} = (I - M^{-1}A)e^{(1)}$ 

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Error propagation form:  $e^{(1)} = (I - M^{-1}A)e^{(0)}$  $e^{(2)} = (I - M^{-1}A)^2 e^{(0)}$  $\vdots$  $e^{(n)} = (I - M^{-1}A)^n e^{(0)}$ 

## **Convergence of Stationary Iterations**



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# 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?

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- 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 easily represented using fewer degrees of freedom

• Sine series representation:

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

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• Discrete problems can only approximate certain modes

Coarse grids accurately represent low-frequency modes Natural complement to relaxation

# Complementarity

Use two complementary processes to efficiently damp all errors

**Relaxation:** Damp high-frequency error by stationary iteration

**Coarse-grid correction:** Eliminate low-frequency error by relaxation on coarse grids
# Complementarity

Use two complementary processes to efficiently damp all errors

**Relaxation:** Damp high-frequency error by stationary iteration

**Coarse-grid correction:** Eliminate low-frequency error by relaxation on coarse grids

Key realization: Solve for coarse-grid representation of error

• At any stage, error is reflected in residual:

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

• Don't transfer Ax = b to coarse grid, transfer Ae = r

#### **Multigrid Components** Relax: $x^{(1)} = x^{(0)} + D^{-1}r^{(0)}$

• Relaxation

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



- Transfer residual to coarse grid
- Compute *Rr*<sup>(1)</sup>



• Use coarse-grid correction to eliminate smooth errors

$$B_c x_c = Rr^{(1)}$$



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 Recursion!

Apply same methodology to solve coarse-grid problem

# Key to Success

Effective multigrid comes from complementarity

- Fixed relaxation effectively reduces certain types of error
- Coarse-grid correction must properly damp all complementary modes



# **Geometric Multigrid**

For homogeneous operators, relaxation is predictable

- Jacobi/Gauss-Seidel relaxation
- Regular coarsening
- Linear interpolation



#### Fully explained by local mode (Fourier) analysis

#### Limitations of Geometric Approach

Geometric multigrid requires several assumptions on

- Problem geometry
- Form of operator
- Performance of relaxation

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- Problem geometry
- Form of operator
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These assumptions may be difficult to satisfy

- Heterogeneous coefficients
- Unstructured geometry
- Time-dependence
- Monte-Carlo simulations

Try to generalize algorithm to allow for heterogeneous coefficients and unstructured grids

# **Multigrid Without Grids**

The essence of multigrid has nothing to do with grids!

Complementarity is key:

- Fix choice of relaxation
- For any A, some errors are slow to converge
- These errors must be corrected some other way

A. Brandt, S. McCormick, J. Ruge, in *Sparsity and Its Applications*, 1984 J. Ruge and K. Stüben, in *Multigrid Methods*, 1987 Improving and Understanding Algebraic Multigrid Convergence- p.18

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Coarse-grid correction:

$$x \leftarrow x + PB_c^{-1}Rr$$
  
 $e \leftarrow e - PB_c^{-1}Rr$ 

A. Brandt, S. McCormick, J. Ruge, in *Sparsity and Its Applications*, 1984 J. Ruge and K. Stüben, in *Multigrid Methods*, 1987

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#### Variational Coarsening

Coarse-grid correction,

$$I - PB_c^{-1}RA,$$

can only correct errors in the range of P

Choosing  $R = P^T$  and  $B_c = P^T A P$  exactly eliminates errors in this space.

Complementarity is key:

- Errors reduced by relaxation and coarse-grid correction
- Errors that relaxation reduces slowly must be in range(P)

R. Nicolaides, Math. Comp. 1977, 31:892-906

Improving and Understanding Algebraic Multigrid Convergence- p.19

• 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  $\sigma = \begin{cases} 10^{-8} & x \leq \frac{3}{8} \\ 1 & x > \frac{3}{8} \end{cases}$ 



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

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



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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



- 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

# Algebraically Smooth Error

# Slow to converge errors of relaxation replace smooth modes within $\mathsf{AMG}$

Design interpolation to accurately represent these modes

- Assume these errors give small residuals, Aepprox 0
- Expand residual equation:

$$a_{ii}e_i = -\sum_{j\in C}a_{ij}e_j - \sum_{k\notin C}a_{ik}e_k$$

• Use assumption on character of these errors to eliminate connections to  $k \notin C$ 

A. Brandt, S. McCormick, J. Ruge, in *Sparsity and Its Applications*, 1984 J. Ruge and K. Stüben, in *Multigrid Methods*, 1987

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## **Graph-based coarsening**

Goal: Choose coarse-grid nodes to allow easy elimination of fine-fine connections

- Filter to eliminate small matrix entries
- Create graph of filtered matrix
- Greedy algorithm to choose maximal independent subset

Maximal independent subset ensures

- every fine-fine connection is "close" to a coarse-grid point
- coarse grid is small, but not too small

A. Brandt, S. McCormick, J. Ruge, in *Sparsity and Its Applications*, 1984 J. Ruge and K. Stüben, in *Multigrid Methods*, 1987 Improving and Understanding Algebraic Multigrid Convergence- p.22

#### AMG working well

Bilinear finite element discretizations of  $abla\cdot\mathcal{K}
abla p$ 

- Problem 1:  $\mathcal{K} = 1$ , Dirichlet BCs
- Problem 2:  $\mathcal{K} = 1$ , Neumann BCs
- Problem 3:  $\mathcal{K}(x) = \begin{cases} 10^{-8} & x \in [\frac{1}{3}, \frac{2}{3}]^2, \\ 1 & \text{otherwise.} \end{cases}$
- Problem 4:  $\mathcal{K}(x) = 10^{-8}$  on 20% of elements, chosen randomly,  $\mathcal{K} = 1$  elsewhere

	128  imes 128	256  imes 256	$512 \times 512$	1024  imes 1024	
Problem 1	0.115	0.124	0.131	0.137	
Problem 2	0.069	0.070	0.071	0.071	
Problem 3	0.122	0.130	0.136	0.141	
Problem 4	0.212	0.233	0.290	0.375	

Asymptotic AMG V-cycle convergence factors

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#### AMG working badly

Same matrices, but symmetrically diagonally scaled by matrix,  $\boldsymbol{D},$  where

 $d_{ii} = 10^{5r_i}$ 

for  $\{r_i\}$  uniformly distributed on [0, 1]

	128  imes 128	256  imes 256	$512 \times 512$	1024  imes 1024	
Problem 1r	0.997	0.996	0.996	0.996	
Problem 2r	0.993	0.993	0.993	0.992	
Problem 3r	0.997	0.996	0.996	0.996	
Problem 4r	0.996	0.996	0.996	0.995	

Asymptotic AMG V-cycle convergence factors

#### **Calibrating Interpolation**

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

A. Brandt and D. Ron, in *Multilevel Optimization in VLSICAD*, 2003 M. Brezina et al., SISC 2004, **25**:1896-1920; SISC 2006, **27**:1261-1286 Improving and Understanding Algebraic Multigrid Convergence- p.25

### **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

A. Brandt and D. Ron, in *Multilevel Optimization in VLSICAD*, 2003 M. Brezina et al., SISC 2004, **25**:1896-1920; SISC 2006, **27**:1261-1286 Improving and Understanding Algebraic Multigrid Convergence- p.25

# **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 AMG-style interpolation such that prototype of slow-to-converge error is in its range
- Create coarse-grid problem and recurse

M. Brezina et al., SISC 2004, **25**:1896-1920; SISC 2006, **27**:1261-1286 Improving and Understanding Algebraic Multigrid Convergence- p.26

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Relaxation can be anything

M. Brezina et al., SISC 2004, 25:1896-1920; SISC 2006, 27:1261-1286

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# **Adaptive Multigrid**

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Relaxation can be anything, even the multigrid method itself!

• Allows for iterative improvement of a poorly performing multigrid cycle

M. Brezina et al., SISC 2004, 25:1896-1920; SISC 2006, 27:1261-1286 Improving and Understanding Algebraic Multigrid Convergence- p.26

# **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  $\lambda_{\min}(B^{-1}A)$  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",  $x \leftarrow (I B_{rel}^{-1}A)x$
    - 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,  $512 \times 512$  grid

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

• 
$$\lambda_{\min} = 6.64 imes 10^{-4}$$
, 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

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

•  $\mu$ ,  $\lambda$  are Lamé coefficients, defined as

$$\lambda = rac{E
u}{(1+
u)(1-2
u)}$$
 and  $\mu = rac{E}{2(1+
u)}$ 

- Fix Poisson ratio,  $\nu = 0.32$  (steel)
- Let Young modulus, *E*, vary between 1 (nylon/polypro) and 10<sup>σ</sup> (100 = titanium, 1000 = diamond)
- Know properties of slow-to-converge errors for small  $\sigma$

#### Numerical Results: Linear Elasticity

3D cube, 201,720 DOFs, exponential distribution of E

	Standard SA			Adaptive SA		
σ	$ ho_{MG}$	ltns	CPU (s)	$ ho_{MG}$	ltns	CPU (s)
2	0.115	9	26.0	0.214	12	267.7
3	0.247	14	35.7	0.310	16	275.6
4	0.395	20	50.0	0.404	21	289.4
5	0.556	32	73.6	0.497	27	381.2

M. Brezina et al., SISC 2004, 25:1896-1920

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#### Lattice Quantum Chromodynamics

- Modelling interactions between fermions on a lattice
- Goal: Solve  $H(u, \rho)f = b$ , for multiple source vectors, b, at each step of a Monte Carlo simulation
- Difficulty: u is a complex unitary field defined on lattice edges, phases chosen randomly based on parameter,  $\beta$
- *H* is Hermitian, but indefinite, so solve normal equations
- As  $\rho$  approaches a critical value,  $H^*H$  becomes singular (for any  $\beta$ )
- 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

2D Dirac-Wilson normal equations

 $128 \times 128$  periodic lattice

average residual reduction per iteration AdaptiveMG-PCG Diagonal-PCG 0.05 0.01 0.3 0.1 0.05 0.01 0.3 0.1 $\rho - \rho_{\rm cr}$  $\beta = 2$ 0.85 0.94 0.96 0.99 0.31 0.31 0.310.33 = 30.86 0.93 0.97 0.98 0.31 0.40 0.42 0.42 0.83 0.99 0.28 0.31 0.31 = 50.92 0.96 0.29

> Adaptive MG setup time: Adaptive MG-PCG solve time: 0.8 seconds Diagonal-PCG solve time:

13.7 seconds 4.7 seconds

J. Brannick et al., Proc. DD16, 2007

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# Why does it work?

In principle, adaptive AMG is obvious:

- Fix relaxation, coarse-grid correction must complement
- Find out how relaxation fails, then build appropriate hierarchy
- In practice, difficult to analyse
  - Adaptive AMG interpolation depends nonlinearly on prototype
  - Very dependent on coarse/fine partition

# Simplifying AMG

Analyse simpler algorithm than full-blown AMG

- Ignore partition (assume properties of partition)
- Linearise dependence of adaptivity on prototype
- Directly link relaxation and interpolation

Start with partitioned matrix,

$$A = \left[ egin{array}{cc} A_{ff} & A_{fc} \ A_{cf} & A_{cc} \end{array} 
ight],$$

derive and analyse AMG variant, then adaptivity
#### **Reduction-Based AMG**

Suppose we can partition the grid,  $\Omega = F \cup C$ , so that

$$x_f^T M_{ff} x_f \leq x_f^T A_{ff} x_f \leq \lambda_{\max} x_f^T M_{ff} x_f$$

and that  $\begin{bmatrix} M_{ff} & -A_{fc} \\ -A_{cf} & A_{cc} \end{bmatrix}$  is positive semi-definite. Choose **Relaxation:**  $I - \frac{2}{1+\lambda_{max}} \begin{bmatrix} M_{ff}^{-1} & 0 \\ 0 & 0 \end{bmatrix} A$ 

**Coarse-grid correction:** variational with  $P = \begin{bmatrix} M_{ff}^{-1}A_{fc} \\ I \end{bmatrix}$ 

Then

$$\rho_{\mathsf{MG}} \leq \left(1 - \left(\frac{2}{\lambda_{\mathsf{max}} + 1}\right)^2\right)^{\frac{1}{2}}$$

M. Ries, U. Trottenberg, G. Winter, J. Lin. Alg. Applic., 1983 S. MacLachlan, T. Manteuffel, S. McCormick, Numer. Linear Algebra Appl. 2006.

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#### **Additive Multigrid**

Theory for additive preconditioners has similar conditions.

Let  
• 
$$B = \begin{bmatrix} I & 0 \\ -A_{cf}M_{ff}^{-1}I \end{bmatrix} \begin{bmatrix} M_{ff} & 0 \\ 0 & S \end{bmatrix} \begin{bmatrix} I & -M_{ff}^{-1}A_{fc} \end{bmatrix}$$
  
•  $\begin{bmatrix} M_{ff} & -A_{fc} \\ -A_{cf} & A_{cc} \end{bmatrix}$  be positive semi-definite  
•  $x_{f}^{T}M_{ff}x_{f} \leq \lambda_{\min}x_{f}^{T}M_{ff}x_{f} \leq x_{f}^{T}A_{ff}x_{f} \leq \lambda_{\max}x_{f}^{T}M_{ff}x_{f}$   
•  $\nu_{\min}x_{c}^{T}Sx_{c} \leq x_{c}^{T}(A_{cc} - A_{cf}A_{ff}^{-1}A_{fc})x_{c} \leq \nu_{\max}x_{c}^{T}Sx_{c}$   
Then,

$$\kappa(B^{-rac{1}{2}}AB^{-rac{1}{2}}) \leq \left(1+\sqrt{1-rac{1}{\lambda_{\max}}}
ight)^2 rac{\lambda_{\max}^2 
u_{\max}}{\min(
u_{\min},\lambda_{\min})}.$$

O. Axelsson, Iterative Solution Methods, 1994

Y. Saad and B. Suchomel, Numer. Linear Algebra Appl. 2002, 9:359-378

Y. Notay, Numer. Linear Algebra Appl. 2005, 12:419-451

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#### Adaptive AMGr

• Key to success in AMGr is spectral equivalence

$$x_f^T M_{\mathrm{ff}} x_f \leq x_f^T A_{\mathrm{ff}} x_f \leq \lambda_{\max} x_f^T M_{\mathrm{ff}} x_f$$

• Control cycle cost by controlling sparsity in  $M_{\rm ff}$ Adaptive AMGr:

- Fix sparsity of  $M_{ff}$ ; e.g., take  $M_{ff}$  to be diagonal
- Adaptively choose entries in  $M_{\rm ff}$  to ensure equivalence
  - Upper bound is easy (Gerschgorin)
  - Lower bound is difficult (algebraic smoothness)

S. MacLachlan, T. Manteuffel, S. McCormick, Numer. Linear Algebra Appl. 2006.

## Adaptive setup algorithm

Adaptive stage in AMGr aims to compute lowest energy mode

- Multigrid approximation property says interpolation must be very accurate for this mode
- Good match needed for good spectral equivalence

Setup Algorithm:

- **1.** Relax on Ax = 0
- **2.** Define *P* such that  $Px_c = x$
- **3.** Compute  $x^{(\text{new})} = P(\operatorname{argmin}_{y_c} RQ(Py_c))$ .

S. MacLachlan, T. Manteuffel, S. McCormick, Numer. Linear Algebra Appl. 2006.

## Adaptive Convergence

Adaptive iteration is nonlinear, so global theory is complicated

- Special case:  $n_c = 2$ , uniform global convergence
  - Convergence dependent on initial guess
- General case:

Suppose  $A_{fc} \neq 0$ ,  $A_{ff}$  dominated by diagonal  $M_{ff}$ , SPSD A has one-dimensional null space, r.

Define  $\Lambda$  such that  $\Lambda^{-1}A_{fc}x_f = A_{ff}^{-1}A_{fc}x_f$ , use  $P = \begin{bmatrix} \Lambda^{-1}A_{fc} \\ I \end{bmatrix}$  plus exact coarse-grid RQ minimization.

Then adaptive setup map is a contraction in a neighbourhood of x = r.

S. MacLachlan, T. Manteuffel, S. McCormick, Numer. Linear Algebra Appl. 2006.

# Summary

- Effective multigrid arises by complementing relaxation with appropriate coarse-grid correction
- For simple problems, use simple corrections
- When details are complicated or unknown, AMG often helps
- AMG implicitly assumes certain properties of relaxation
- When these assumptions are wrong, adaptive AMG can restore good performance
- Good performance for difficult problems
- AMGr is a new theoretical framework
  - simpler than AMG
  - allows analysis of adaptive process

## **Current directions**

- AMGr is nice, but it isn't AMG
  - Extend AMGr-type theory to AMG itself, or closer variants
- Use insight from AMGr to improve coarsening/relaxation in AMG
  - Adaptive AMG focuses on interpolation, but theory gives other good insights
- Apply and tune adaptive AMG for specific applications
  - QCD application challenges even best adaptive solvers
- Bring adaptive and algebraic ideas back to simpler multigrid solvers
  - Can we get the benefits without the costs?