Recent Advances in System Solvers

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Outline

- Introductory Remarks
- Linear Solvers
  - Context
  - MG/AMG
  - Adaptive AMG
- Nonlinear Systems
  - Context
  - Nested Iteration/Newton/Krylov/AMG
- Summary

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Theme song:

Everything is linear,

Linear Solvers

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Everything is linear,

...in its own way

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Take a simple Newton step,

Theme song:

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Take a simple Newton step,

and iterate from 1 *to* k*.*

Sung to the tune of "Everything is Beautiful" by Ray Stevens

Krylov Methods $\Leftrightarrow$ Polynomial Methods

$$A\underline{x} = \underline{b}$$

$\underline{x}_0$		initial guess
$\underline{x}_i$		iterate
$\underline{e}_i$	$= \underline{x} - \underline{x}_i$	error
$\underline{r}_i$	$= \underline{b} - A\underline{x}_i$	residual

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Error Equation: $p_i(0) = 1.0$

$$\underline{e}_i = p_i(A)e_0$$

$$\underline{r}_i = p_i(A)r_0$$

Polynomial Methods: Error Bounds

Jordan Decomposition

$$A = SJS^{-1}$$

Error Bound

$$\|e_i\| \leq \|S\| \|S^{-1}\| \|p_i(J)\|$$

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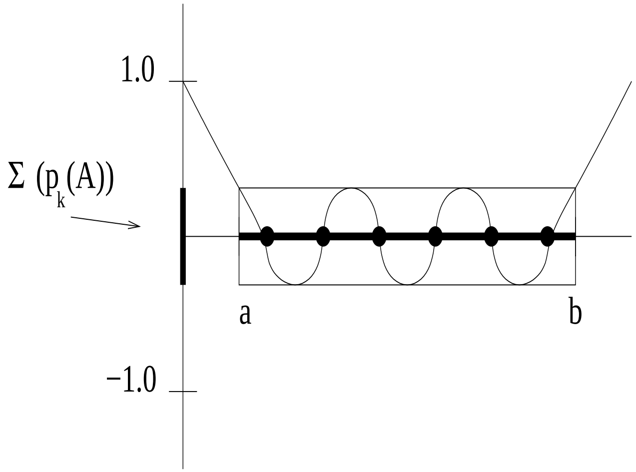

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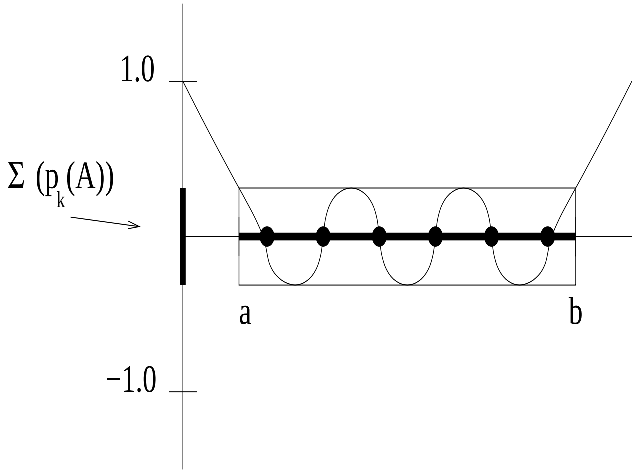

If condition of A is large, it is hard to make a polynomial small on all of the eigenvalues and still have $p_i(0) = 1$.

Preconditioning

$$C A \underline{x} = C \underline{b}$$

C – Any linear process

Choose C so that system with CA is easier to solve in some sense

For example, condition of CA is much smaller than that of A

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- $C = A^*$ — Normal Equations

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- $C = A^*$ Normal Equations
- $C =$ Multigrid V-cycle PCG-MG

Preconditoned Polynomial Methods

Preconditioning $\Leftrightarrow$ Matrix Splitting

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- Any linear process, C, can be used as a preconditioning
- Any preconditioning can accelerated by a polynomial method

Numerical PDEs

- In general, if A comes from a PDE, optimal preconditioning requires a Multilevel algorithm
  - Optimal $\Rightarrow$ condition of CA is independent of the mesh

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  - Optimal $\Rightarrow$ work grows linearly with the problem size

If you want to solve a problem with billions of unknowns on $128,000$ *processors, you will need a multilevel algorithm somewhere.*

Recent Developments

- A lot of recent activity in multilevel algorithms

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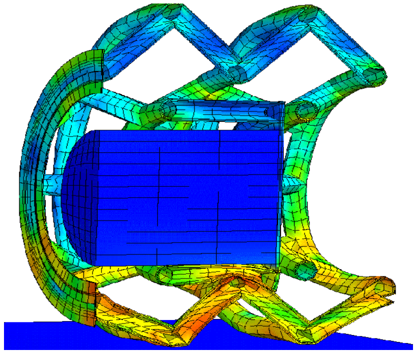


DYNA3D

Multigrid

Basic Components

- Simple relaxation or smoothing
  - Usually a matrix splitting or simple preconditioned one-step like damped Jacobi, Gauss/Sedel or block Gauss/Seidel
  - Resolves error in direction of eigenvectors with large eigenvalues
- Coarse-grid correction
  - Lower dimensional or simpler problem
  - Resolves error left by relaxation
- Recursion
  - Coarse-grid problem is solved by multigrid

Multigrid: example

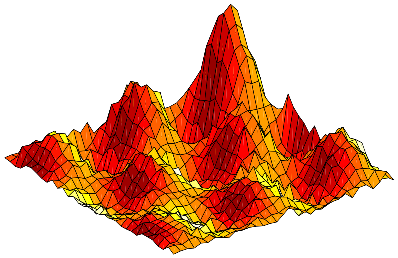
Example: discrete forms of second-order elliptic operators

$$-\nabla \cdot A \nabla u + cu = f$$

- Large eigenvalues are associated with high frequency eigenvectors
- Simple iterative methods leave error geometrically smooth
- Coarse grid problem is a version of fine grid problem

Multigrid: example

Given Error



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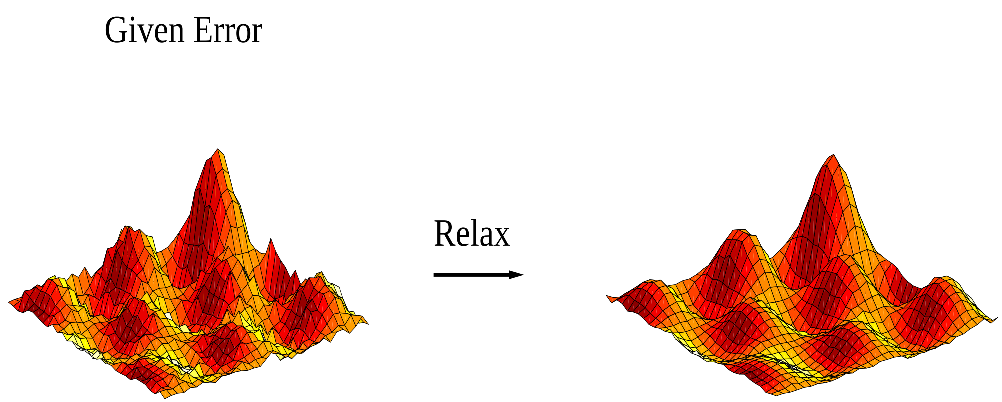

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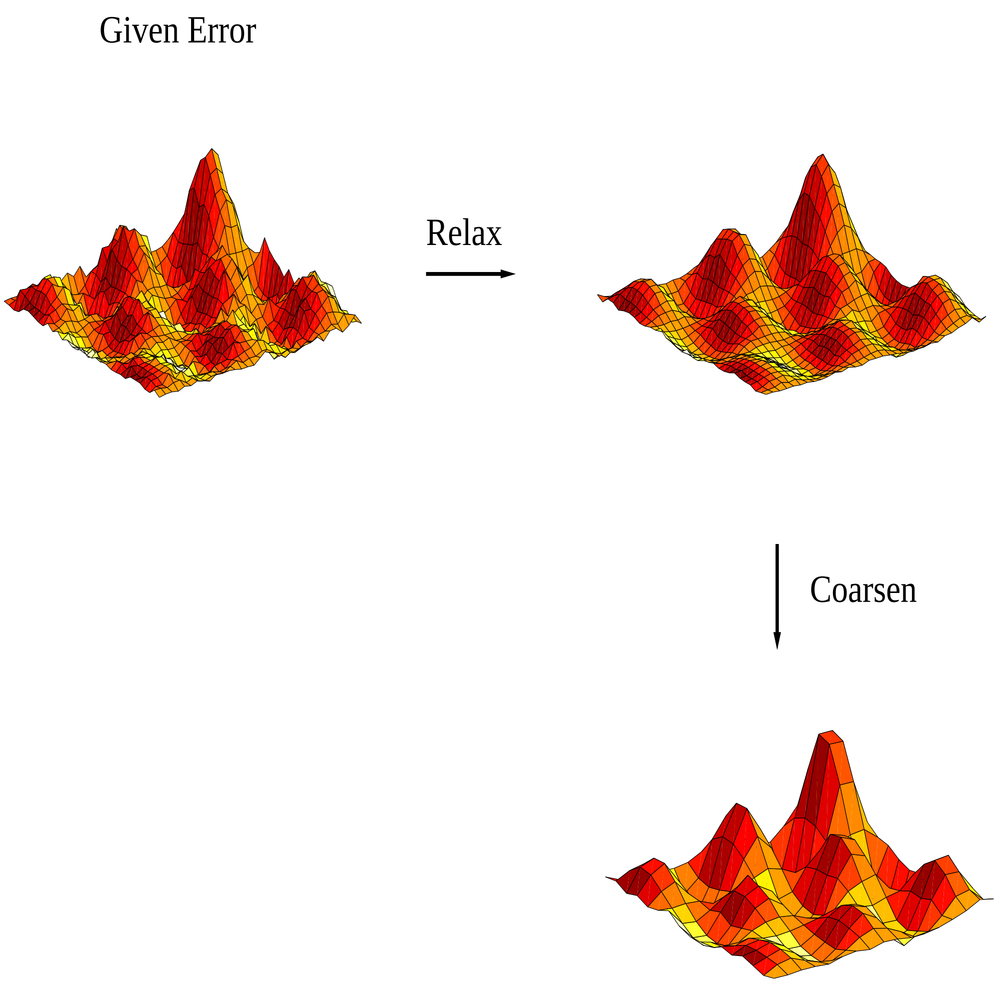

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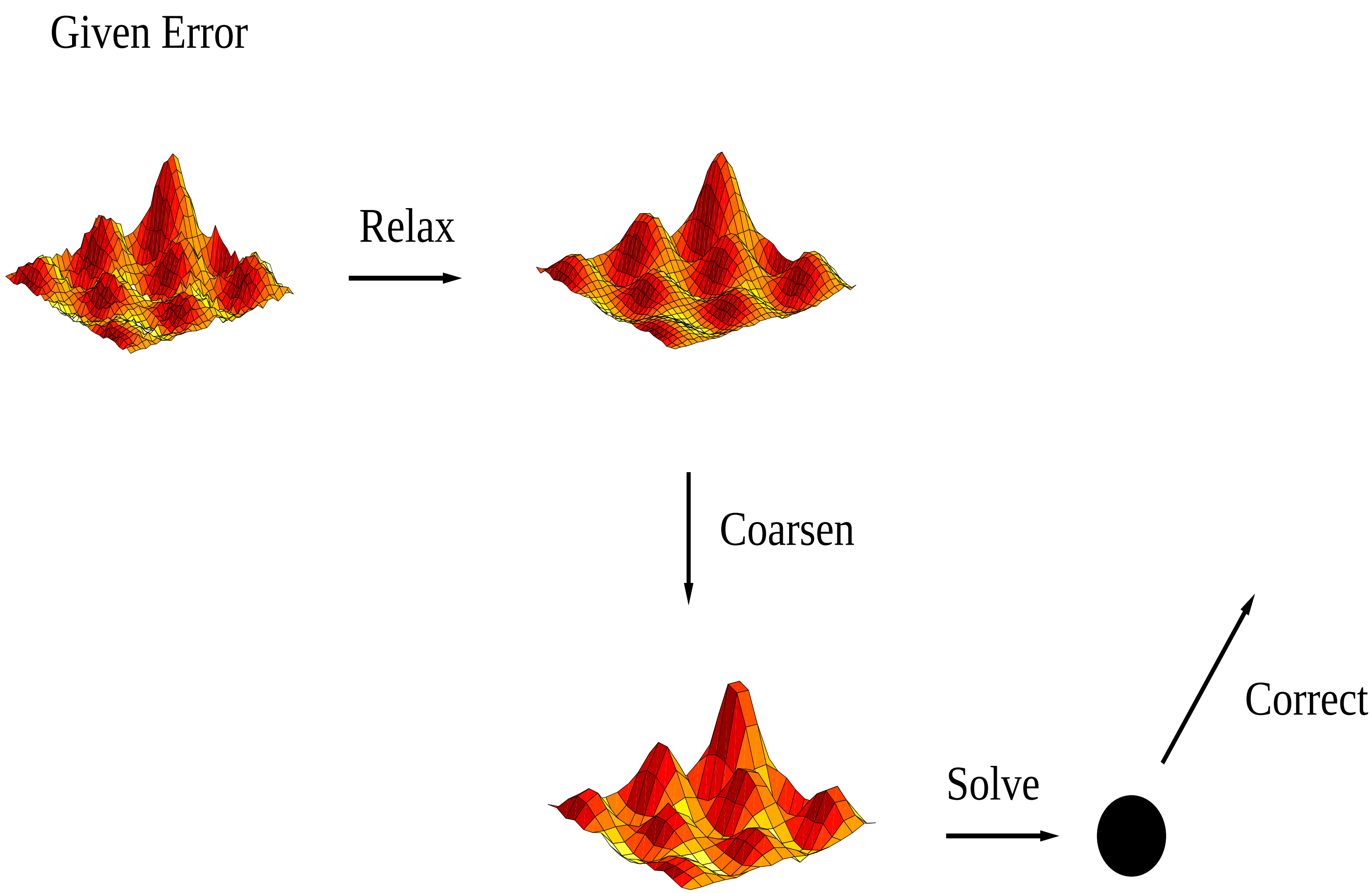

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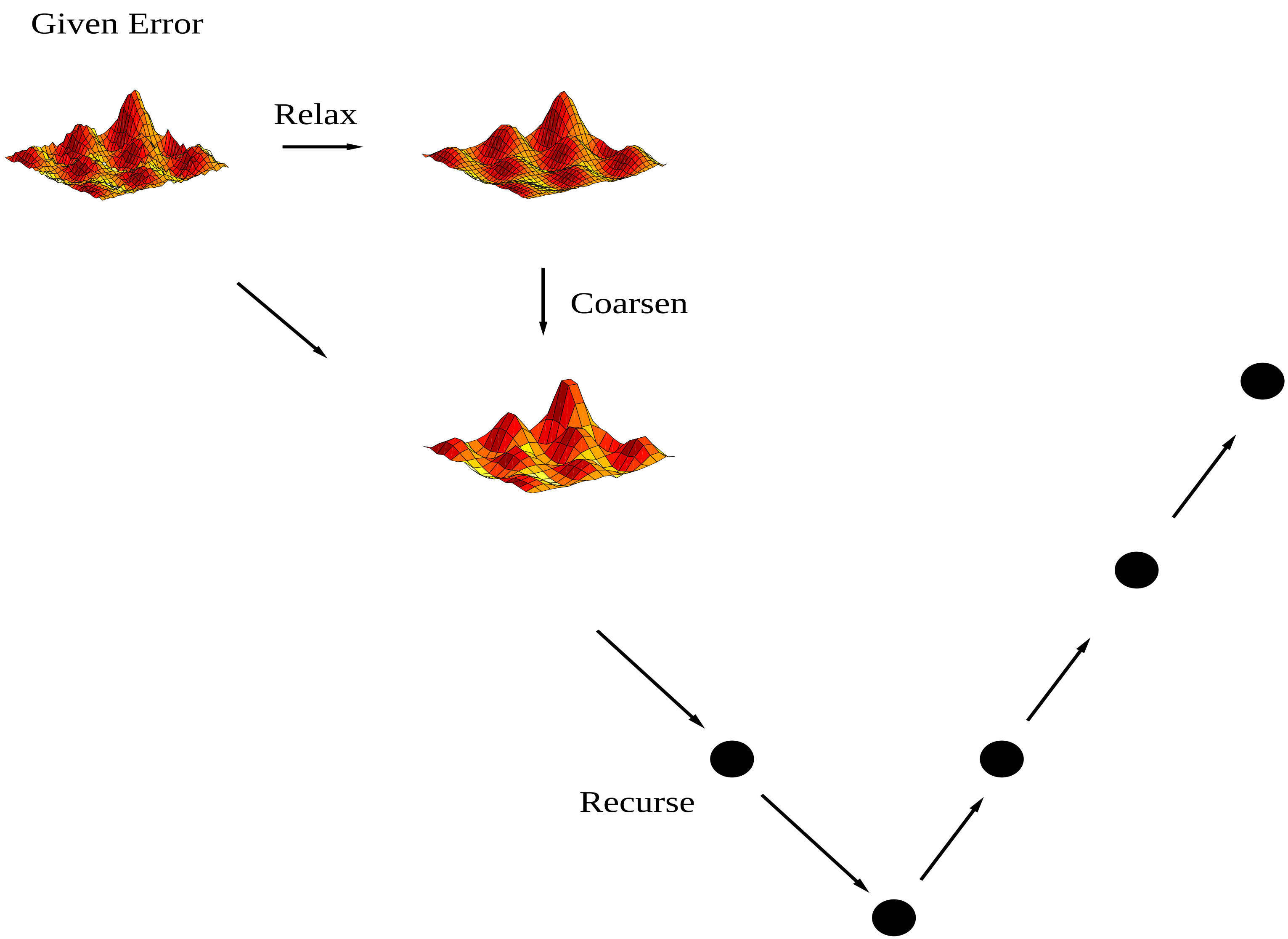

Basic Components (again)

Multigrid algorithm is determined by

- Relaxation
- Interpolation from coarse grid to fine grid (P)
- Restriction from fine grid to coarse grid (R)
- Coarse-grid operator (A_c)

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- Relaxation
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In variational MG,

$$A_c = RA_fP$$

Multigrid Flavors

- Geometric Multigrid (GMG)
- Algebraic Multigrid (AMG)

Multigrid Flavors

Geometric multigrid (GMG)

- Coarse-grid problem is geometrically determined
- It is usually a smaller version of the fine grid problem
- Interpolation and restriction usually determined by the operator

Multigrid Flavors

Algebraic Multigrid (AMG)

- Directly address the matrix A without presumed knowledge of
  - Geometry
  - Operator

Multigrid Flavors

Algebraic Multigrid (AMG)

- Directly address the matrix A without presumed knowledge of
- Assume simple relaxation
  - For example, Damped Jacobi, Gauss/Seidel

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- Directly address the matrix A without presumed knowledge of
- Assume simple relaxation
- Coarse-grid problem is chosen to resolve the “Algebraicaly smooth” error
  - Defined to be the error that relaxation does not resolve

Multigrid Flavors

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- The coarse-grid operator is formed variationally ($A_c = RA_fP$)

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- Geometric Multigrid (GMG)
- Algebraic Multigrid (AMG)
  - AMG
  - Smoothed Aggregation (SA)
  - Adaptive AMG (αAMG, αSA)

AMG Principles

AMG is characterized by choice of the Coarse Grid, Interpolation, P, and Restriction, R.

For simplification, assume A symmetric and $R = P^t$

AMG Principles

Divide degrees of freedom into the Coarse DOF and Fine DOF

$$A = \begin{bmatrix} A_{ff} & A_{fc} \\ A_{cf} & A_{cc} \end{bmatrix}$$

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$$||A\underline{e}|| << ||\underline{e}||$$

error in direction of large eigenvalues has been reduced

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After relaxation

$$\begin{aligned} AP\underline{e}_c &= \underline{r} \\ P^t AP\underline{e}_c &= P^t \underline{r} \\ A_c \underline{e}_c &= \underline{r}_c \end{aligned}$$

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A_c is the Schur Complement

$$A_c = A_{cc} - A_{cf} A_{ff}^{-1} A_{fc}$$

A_c is Dense

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Problem: A_{ff}^{-1} is Dense $\Rightarrow A_c$ is Dense

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Solution: Sparse Approximation of A_{ff}^{-1}

- $A_{ff}^{-1} \longrightarrow D_{ff}^{-1}$ Diagonal of A_{ff}
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For example: simple iteration on $A_{ff} = D_{ff} - B_{ff}$

$$A_{ff}^{-1} \to (I + D_{ff}^{-1} B_{ff}) D_{ff}^{-1}$$

Iterated Interpolation, Long Range Interpolation, Compatible Relaxation

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Are any of these any good?

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Interpolation must approximate an eigenvector up to the same accuracy as the size of the corresponding eigenvalue

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Two-grid Convergence Factor

$$\rho \leq 1 - O(\frac{1}{C})$$

Measure can be enforced locally

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for some parameter θ. (e.g. θ = .25)

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New, more general, definitions of strength derived from local approximation of A^{-1}

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Strength of connection fundamental in choosing the coarse grid

AMG Alphabet Soup

AMG	Classical AMG (84)
SA	Soothed Aggregation (96)
AMGe	finite element AMG (01)
AMG$\not{e}$	element free AMGe (02)
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Adaptive Algorithms

AMG	adaptive AMG (84)
BAMG	Bootstrap AMG (01)
αSA	adaptive Soothed Aggregation (04)
CR	Compatible Relaxation (04)
αAMG	adaptive AMG (06)
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  - Developed by Brandt/McCormick/Ruge (84)
  - Implemented by Ruge/Stuben (85)

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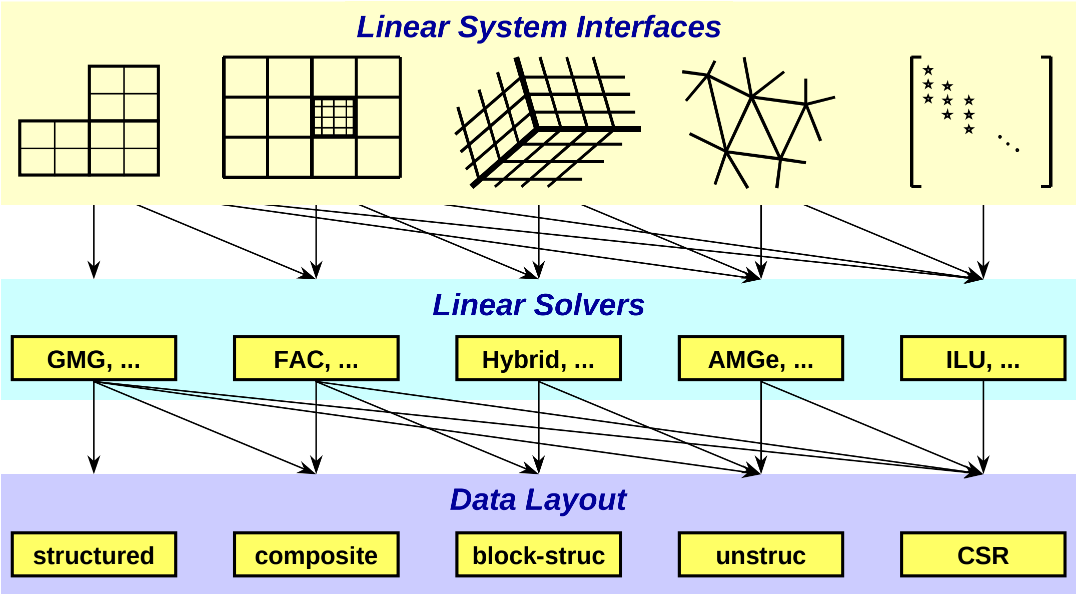

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- Based on M-matrix principles

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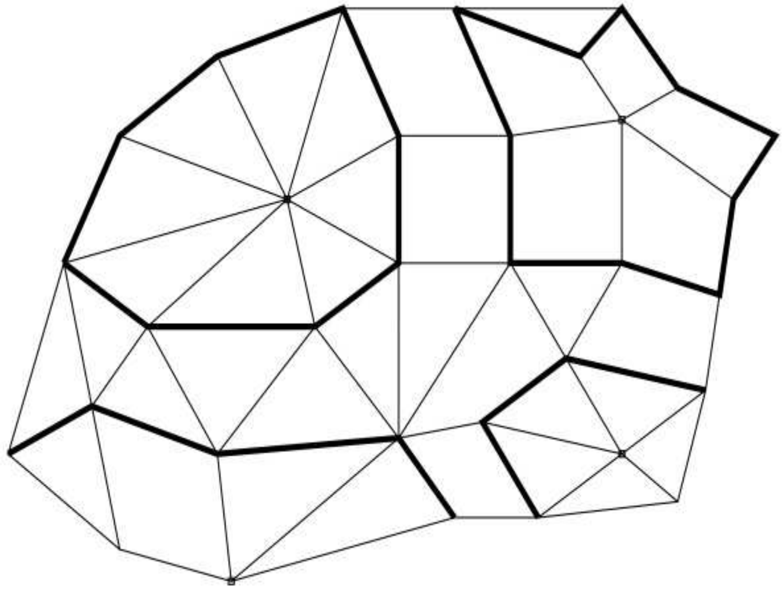
- Divide the Graph of A into disjoint aggregates, $\{\mathcal{A}_i\}$
- Associate one (or more) coarse-level DOF with each aggregate
- Construct a tentative interpolation matrix, $\hat{P}$, by chopping up the near null-space vector(s)

Smoothed Aggregation: Interpolation

Null-space vector: $\underline{v} = (v_1, v_2, \ldots, v_n)^t$

$$\hat{P} = \begin{bmatrix} v_1 & & \\ \vdots & & \\ v_{n_{f_1}} & & \\ & v_{n_2} & \\ & \vdots & \\ & v_{n_{f_2}} & \\ & & v_{n_c} \\ & & \vdots \\ & & v_{n_{f_c}} \end{bmatrix}$$



Note: $\underline{v}$ is in Range(P)

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Recurse

Smoothed Aggregation

$$A_c = P^t A P = \hat{P}^t (I - \alpha A) A (I - \alpha A) \hat{P}$$

- Reduces the condition of A_c
- Maintains good approximation of null-space vector, $\underline{v}$
  - Null-space, $\underline{v}$, still in the range of P
  - Other near null-space vectors still well approximated by P
- Yields aggressive coarsening

Multiple Null Space Vectors

Accommodate multiple (near) null-space vectors, $V = [\underline{v}_1, \ldots, \underline{v}_k]$

$$V_j = \begin{bmatrix} v_{1n_j} & \cdot & v_{kn_j} \\ \vdots & & \vdots \\ v_{1n_{f_j}} & \cdot & v_{kn_{f_j}} \end{bmatrix}$$

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$$\hat{P}^t \hat{P} = I$$

Smooth $\hat{P}$

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- *Amenable to parallel implementation*
- *Conceptionally straightforward*

SA and AMG

Compare SA to AMG

- SA constructs P column by column
- AMG constructs P row by row
- Both attempt to accurately interpolate algebraically smooth vectors
- Both try to reduce the complexity (number of nonzeros) of the coarse-grid operator

AMG Alphabet Soup

AMG	Classical AMG (84)
SA	Soothed Aggregation (96)
AMGe	finite element AMG (01)
AMG$\cancel{e}$	element free AMGe (02)
ρAMGe	spectral AMGe (03)

Adaptive Algorithms

AMG	adaptive AMG (84)
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αSA	adaptive Soothed Aggregation (04)
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AMG Gang

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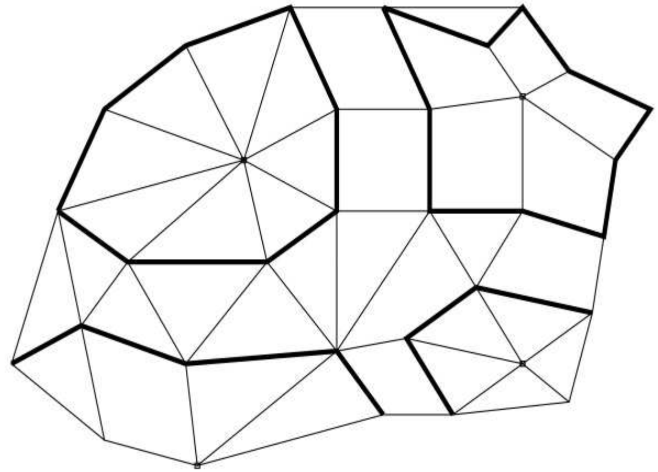
Finite element AMG (04)

- Uses local stiffness matrices
- Aggregates elements like SA
- Uses local null-space to determine local interpolation properties



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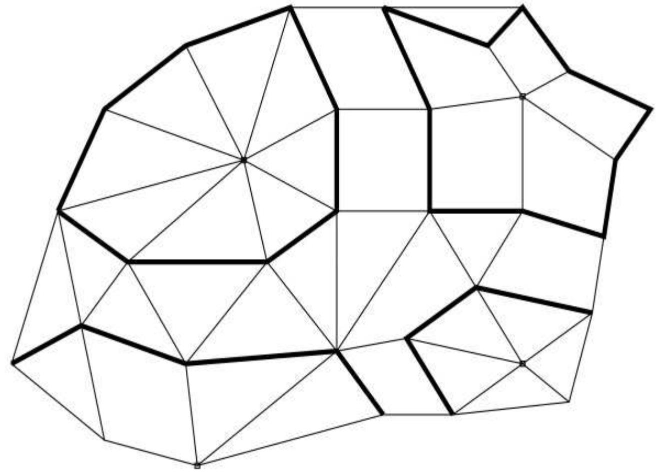
- Aggregates elements like SA
- Uses local null-space to determine local interpolation properties
- Effective for
  - Anisotropic Problems
  - Systems PDEs



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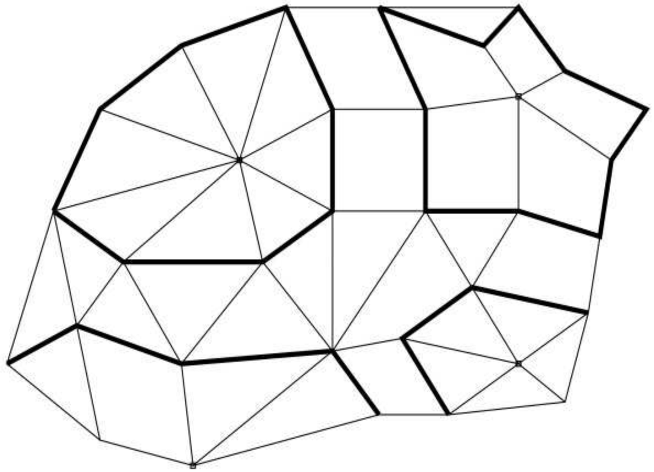

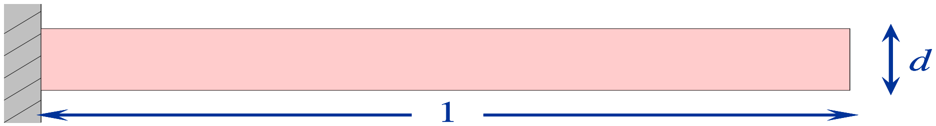

	AMG	AMGe
ρ	.98	.26

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- Based on local stiffness matrices like AMGe
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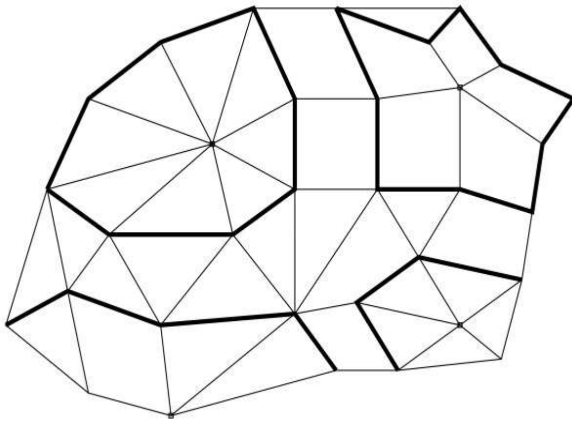

Spectral AMGe

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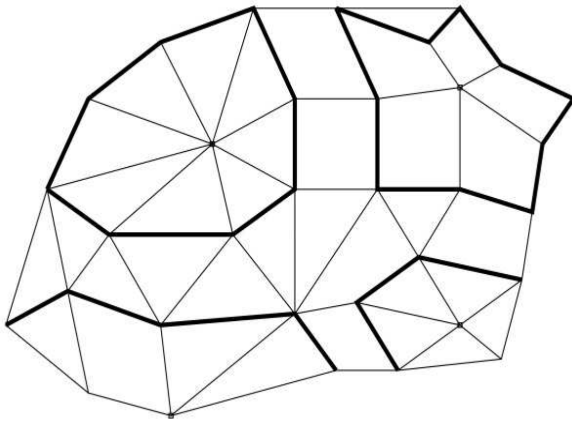
Spectral AMGe (02)



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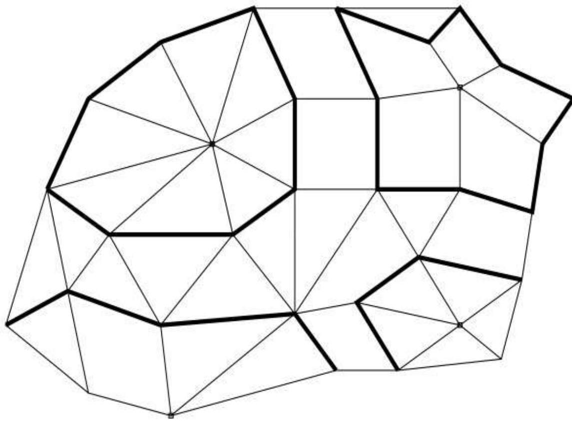
Spectral AMGe

ρAMGe | Spectral AMGe (02)



- Based on local stiffness matrices like AMGe
- Aggregates elements like SA
- Creates local columns in interpolation matrix based on local null-space
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- Effective when global null-space vectors not available, but local stiffness matrices are available

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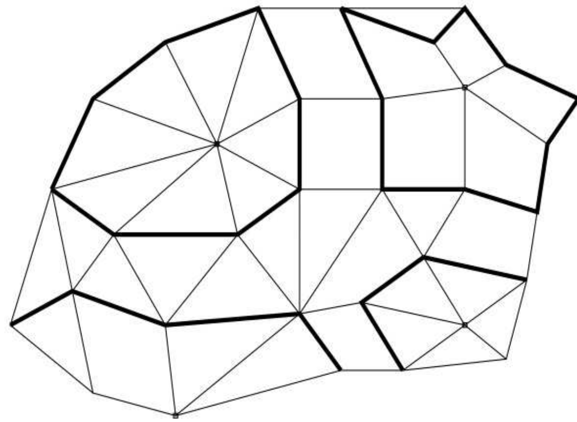

- Based on principles of AMGe
- Aggregates elements like SA
- Creates local stiffness matrices from neighboring elements

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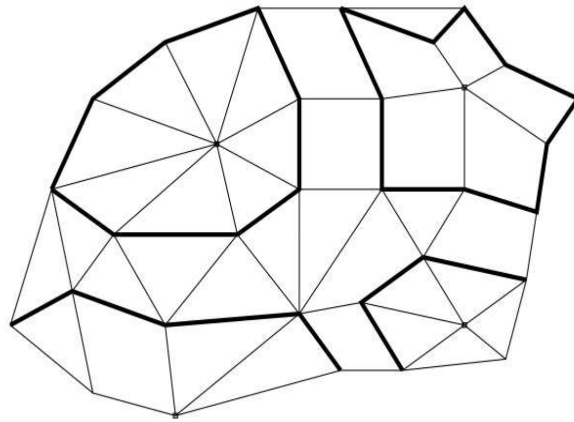

- Effective when local stiffness matrices are not available

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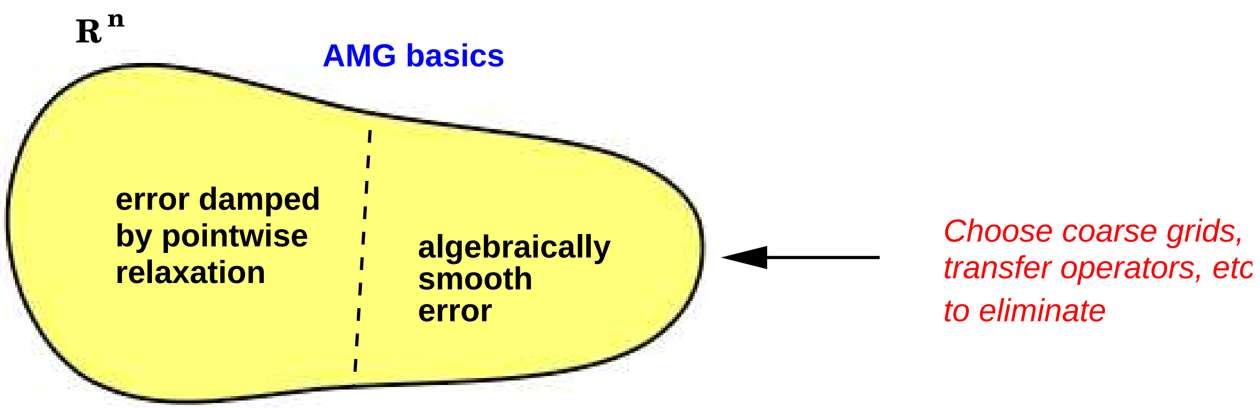
- The coarse-grid problem must capture all modes not effectively reduced by relaxation



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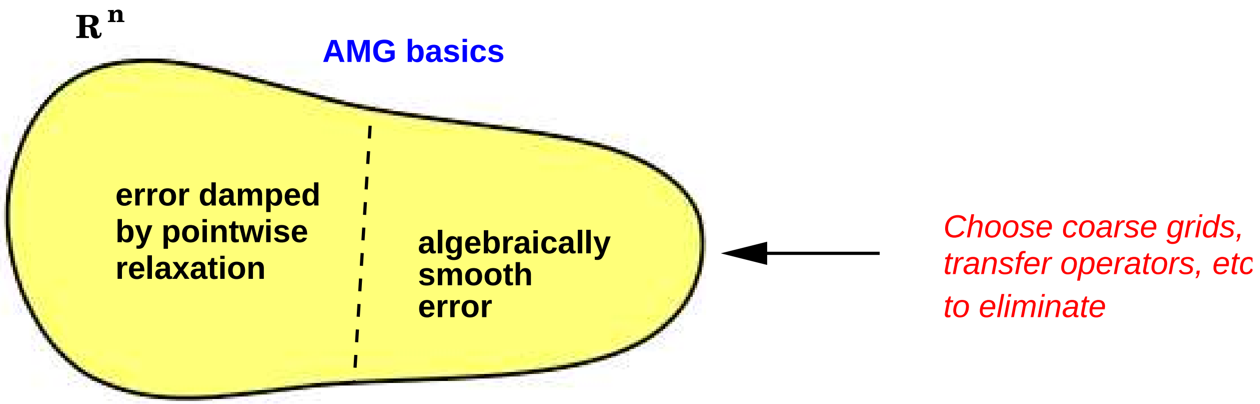
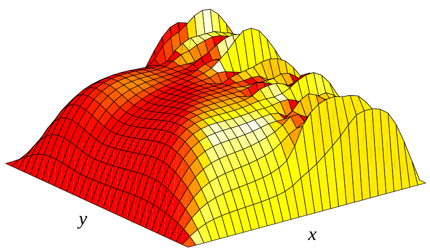
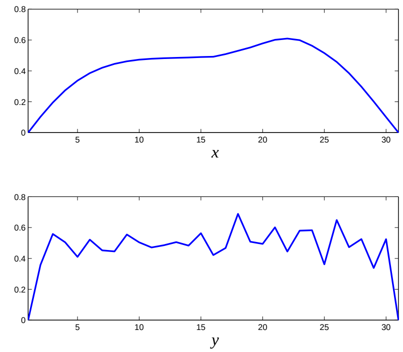


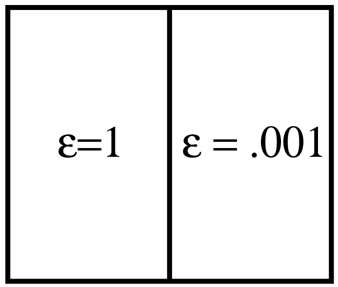
- Algebraically smooth vectors are not necessarily geometrically smooth

Algebraically smooth error can be oscillatory

- Error after seven Gauss/Seidel iterations on $-u_{xx} - \epsilon u_{yy} = f$







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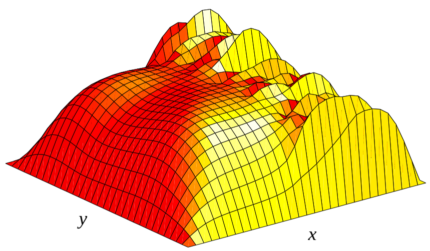
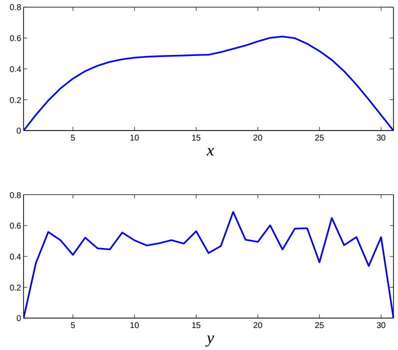
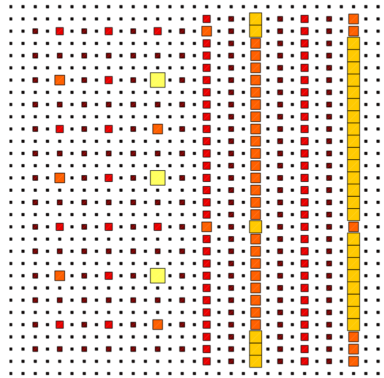




- Adaptive AMG can “follow physics”



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- Adjust AMG components to capture this error
- Do no harm: make sure change does not awaken previously reduced errors
- Do as much of the work as possible on the coarser grids
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Adaptive Smoothed Aggregation

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- Construct new coarse interpolation, P, and coarse-grid operator, A_c

Adaptive Smoothed Aggregation

Current approximation to the Null-space vector: $\underline{v} = (v_1, v_2, \ldots, v_n)^t$

$$\hat{P} = \begin{bmatrix} v_1 & & \\ \vdots & & \\ v_{n_{f_1}} & & \\ & v_{n_2} & \\ & \vdots & \\ & v_{n_{f_2}} & \\ & & v_{n_c} \\ & & \vdots \\ & & v_{n_{f_c}} \end{bmatrix}$$

Normalize

$$\hat{P}^t \hat{P} = I$$

Smooth $\hat{P}$

$$P = (I - \alpha A)\hat{P}$$

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Recurse

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Adaptive Flavors

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All depend on determining a local representation of algebraically smooth vectors

αAMG and αAMGr

Perfect Interpolation

$$A = \begin{bmatrix} A_{ff} & A_{fc} \\ A_{cf} & A_{cc} \end{bmatrix} \qquad P = \begin{bmatrix} -A_{ff}^{-1} A_{fc} \\ I \end{bmatrix}$$

αAMG and αAMGr

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Choose diagonal matrix Δ_{ff}

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CR

Livne(04), Brannick(05)

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- Principle: Coarse grid is adequate if A_{ff} is well conditioned

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- Principle: Coarse grid is adequate if A_{ff} is well conditioned
- Use simple relaxation on A_{ff}, together with a greedy independent set algorithm, to choose coarse grid

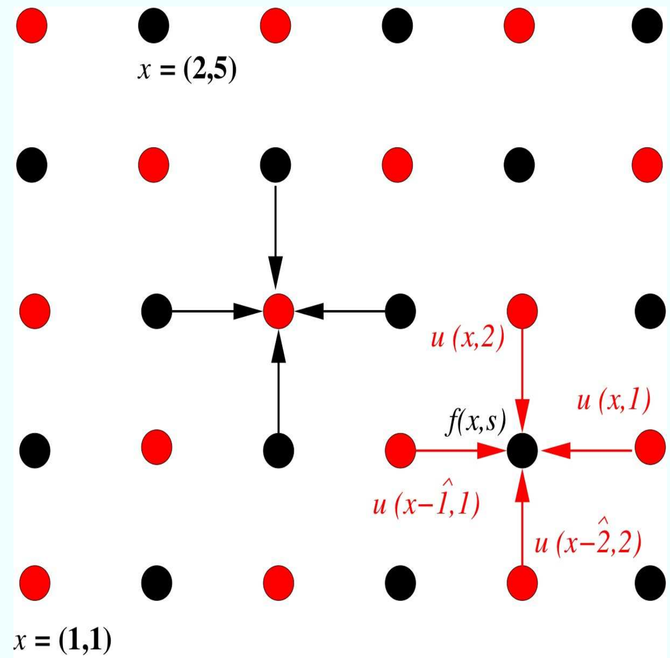
Adaptive Algebraic Multigrid

αAMG and αSA surprisingly effective on a wide range of problems

- Highly irregular meshes
- Strongly anisotropic
- Adaptively refined meshes
- Discontinuous coefficients (heterogeneous material)
- Singularities
- Hyperbolic problems
- QCD

Adaptive AMG for Lattice QCD

- Quantum Chromodynamics (QCD) calculations involve huge linear systems and large-scale (petascale) computing
- Requires solving the complex and non-hermitian discretized Dirac operator
- Each equation may be solved 1000s times

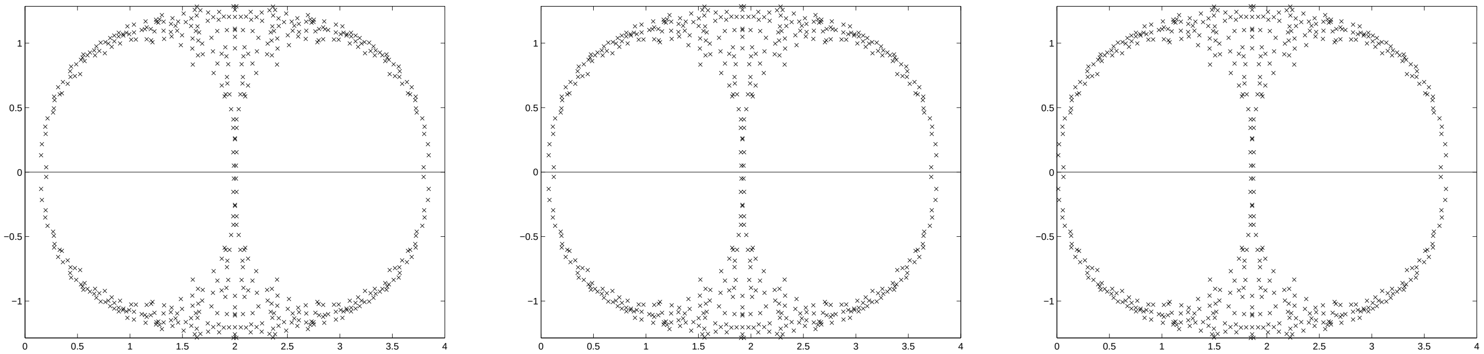


$$M(\mathcal{U}) = D(\mathcal{U}) - m_0 I$$

$$= \begin{bmatrix} A - m_0 I & B \\ -B* & A - m_0 I \end{bmatrix}$$

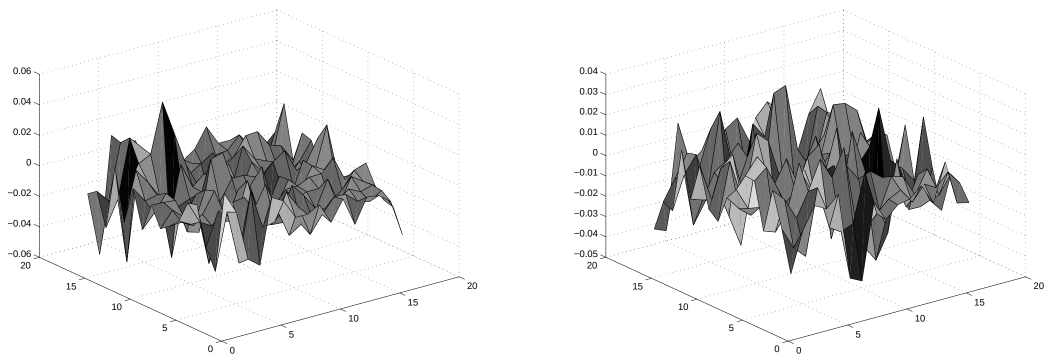
QCD: 2D Schwinger Model

- The system becomes extremely ill-conditioned for typical choices of m_0



$m_0 = 0$ $\longrightarrow$ $m_0 \approx m_{cr}$

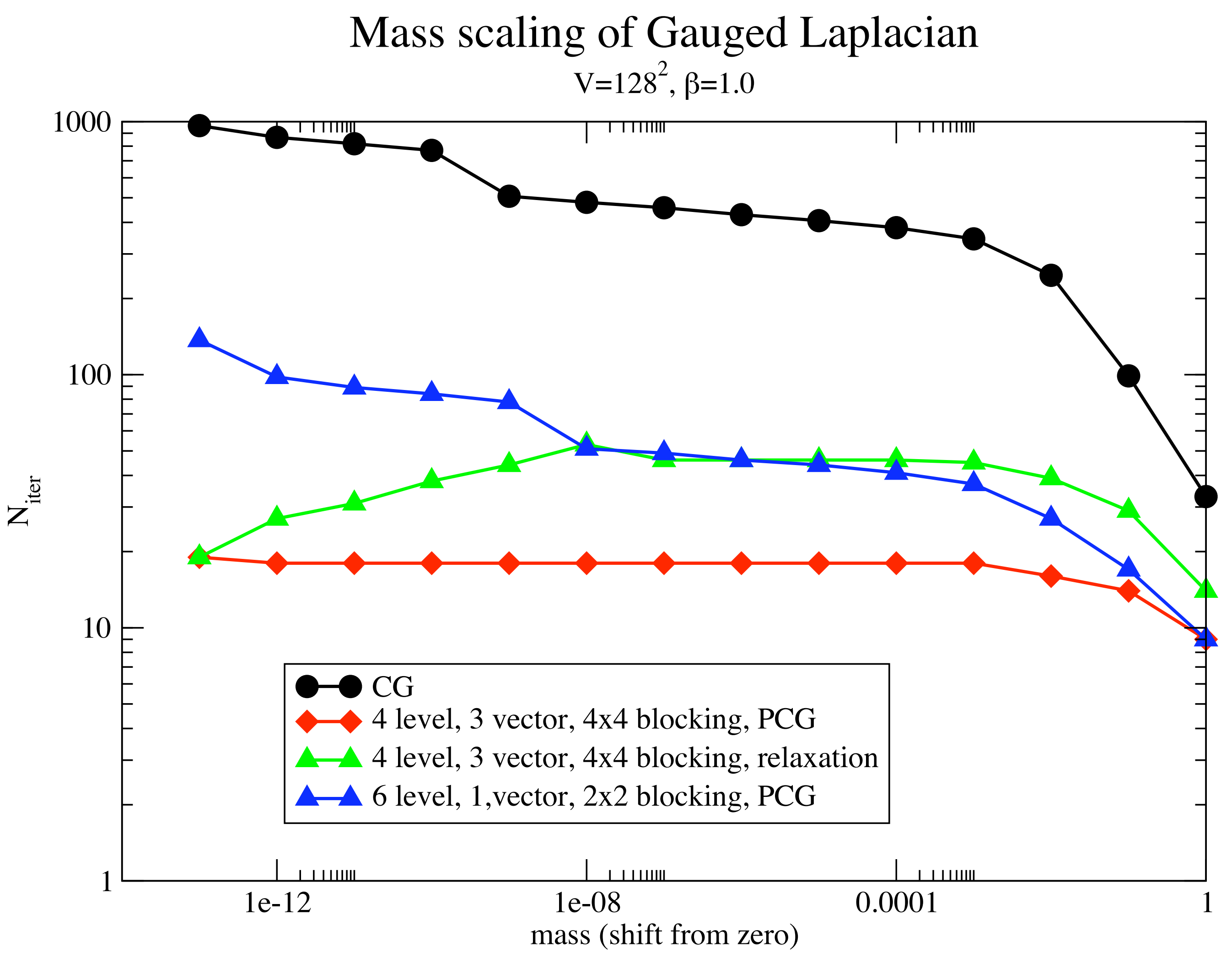
- Near null space is unknown and oscillatory



2D Schwinger Model

- Form the normal equations and apply αSA
- Set-up requires 100s of Work Units
  - (WU = matrix vector multiply)
- Interpolation requires 8 – 10 columns on each aggregate
- For small mass shift, faster than the current method (Diagonally scaled PCG) on even one right-hand side

QCD


Mass scaling of Gauged Laplacian
V=128^2, β=1.0
1000
100
10
1
N_iter
1e-12
1e-08
0.0001
1
mass (shift from zero)
CG
4 level, 3 vector, 4x4 blocking, PCG
4 level, 3 vector, 4x4 blocking, relaxation
6 level, 1,vector, 2x2 blocking, PCG

Real Problem

- Real Problem: 4D model – preliminary results promising

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αSA allows the QCD community to do problems that they could not do before

Conclusions

- Linear systems from PDEs require multilevel algorithms
- GMG optimal for structured grids
- AMG/SA effective for unstructured grids, known (near) null-space
- αAMG/SA greatly expand the domain of applicability

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- Adaptive AMG/SA a group effort

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