Solving PDEs with Multigrid Methods

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Outline

- Modern Scientific Computing
- Multigrid Methods
- Self-Correcting Multigrid Methods
- Current and Future Work

Why Compute?

- Interested in modeling physical processes
  - Diffusion (Heat, Energy, Chemical)
  - Fluid Flow
  - Particle Transport
  - Elastic Materials
- Can describe these processes through differential equations (both ODEs and PDEs)
- Cannot write down closed form solutions
- Need to find (approximate) solutions in other ways

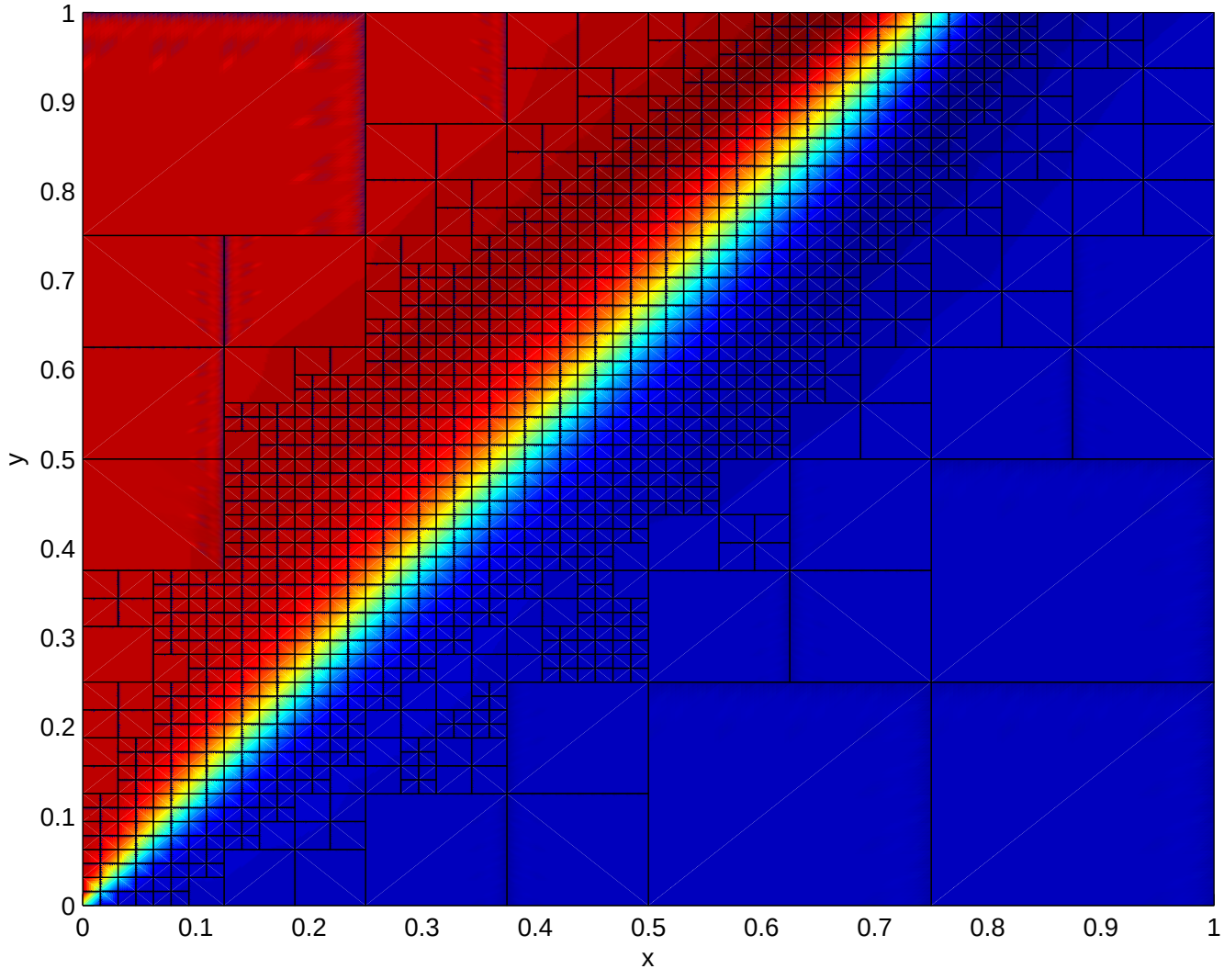
Scientific Computation

- Interested in simulating complex physical systems with parameters, and hence solutions, which vary on multiple scales
- Accuracy constraints lead to discretizations with tens of millions, or even billions, of degrees of freedom (DOFs)
- Need scalability, both algorithmic and parallel

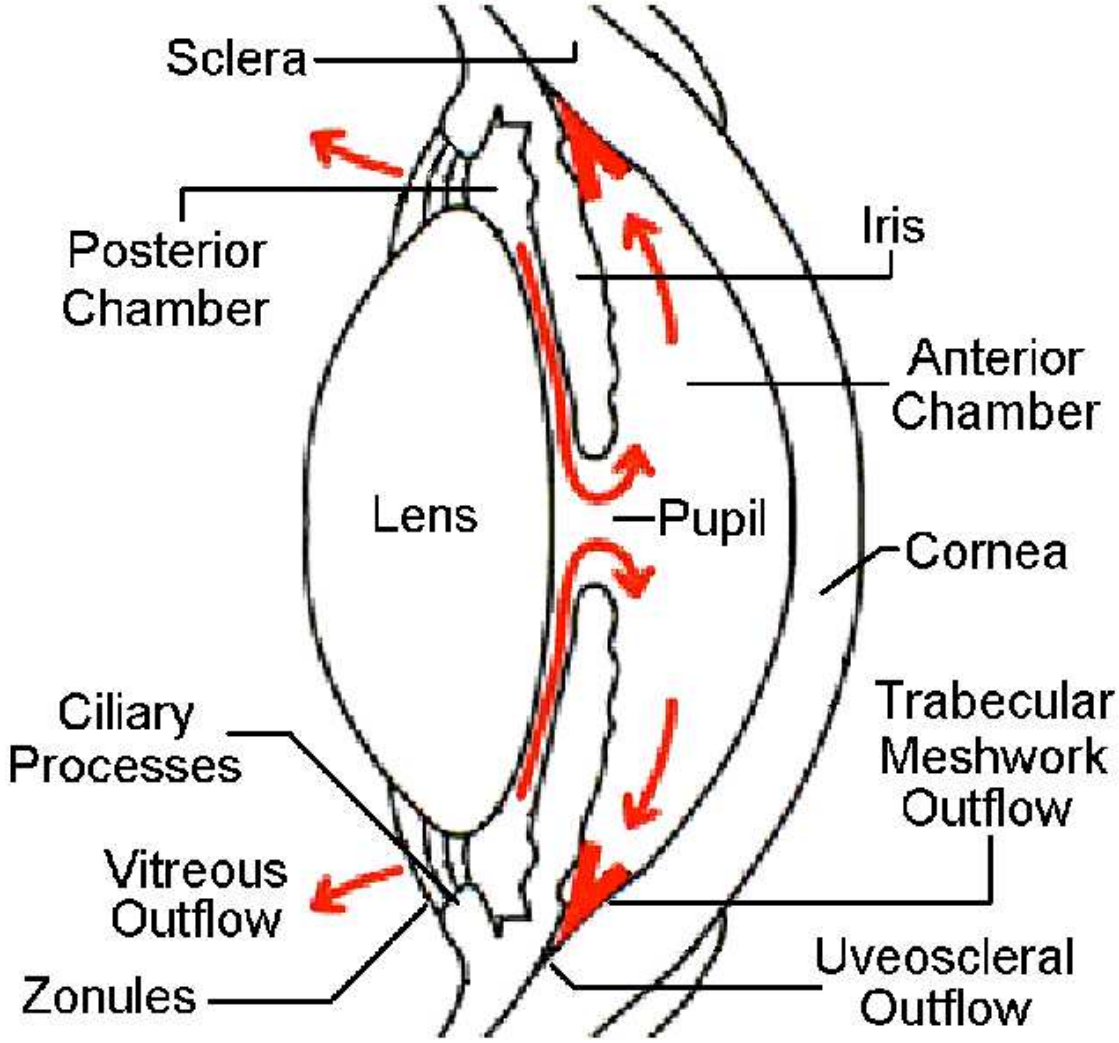
Challenges - Problem Size

- 3D Tsunami Model: 200 million cells, 3 weeks on 1200 processors
- Protein Folding: 18,000 atoms, 10 microsecond simulation, 6 months on 84 processors
- Transport: 500 million - 1 billion degrees of freedom
- Even with optimal methods, three-dimensional problems can be very expensive to solve

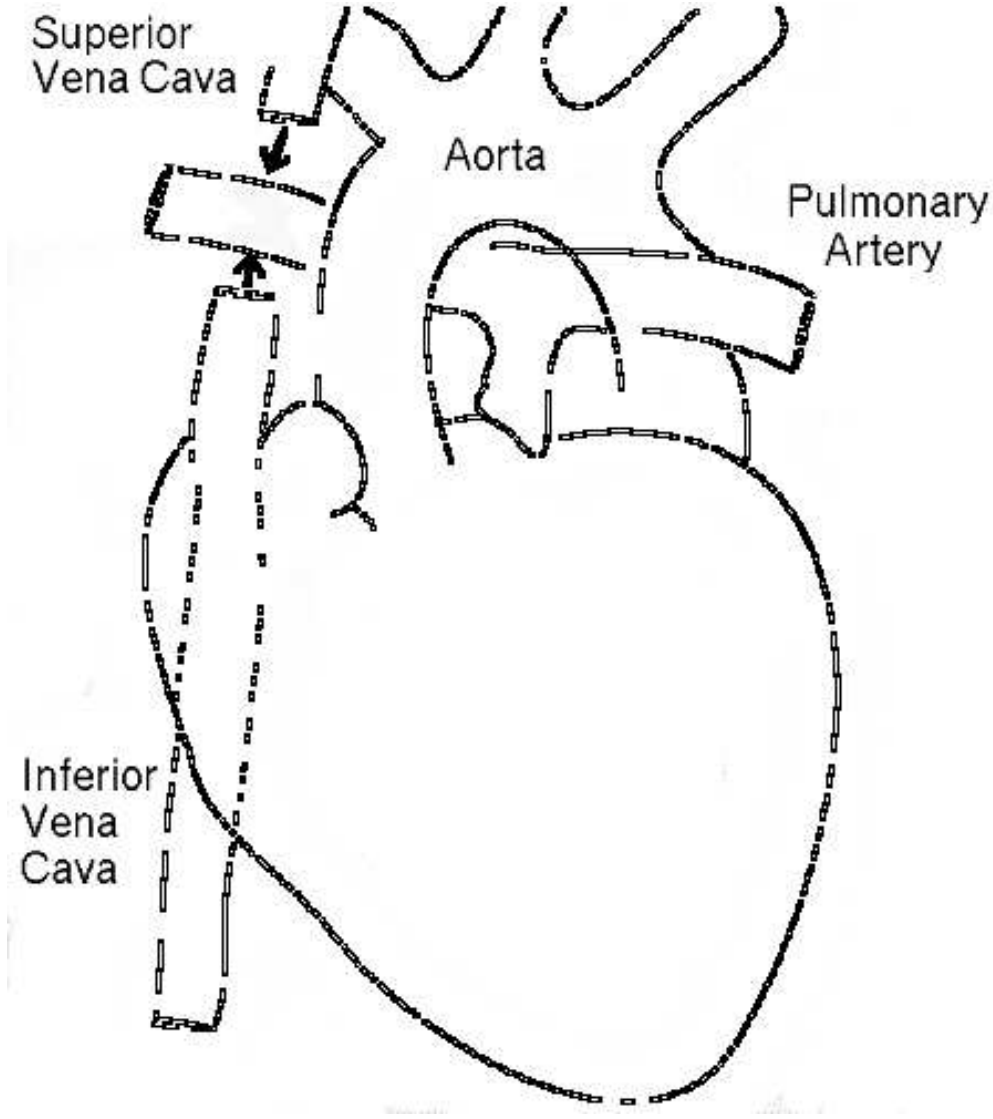
Challenges - Local Refinement



Challenges - Complex Geometry



Challenges - Coupled Systems



Properties of Discretizations

- We consider (primarily) discretizations of the underlying differential equations via finite elements or finite differences
- The matrices from these discretizations tend to be
  - Sparse (number of nonzeros per row doesn't change with n)
  - Ill-conditioned
  - Symmetric (if DE is)
  - Positive-Definite (if DE is)

Direct Methods

- Interested in solving $Ax = b$
- Gauss Elimination involves factoring linear system into an upper- and a lower-triangular part
- Naive cost is $O(N^3) = O(n^9)$ for a 3-dimensional problem
- Utilizing bandedness of our discretization matrix can reduce cost to $O(n^7)$

Stationary Iterative Methods

- Stationary iterative methods choose approximations $B = A^{-1}$ and iterate using the error equation
- If $Ae = A(x - x^k) = b - Ax^k$, then $x^{k+1} = x^k + B(b - Ax^k)$
- The Jacobi iteration chooses B to be the diagonal of A
- The Gauss-Seidel iteration chooses B to be the lower-triangular part of A
- SOR chooses B to try and minimize $\rho(I - BA)$

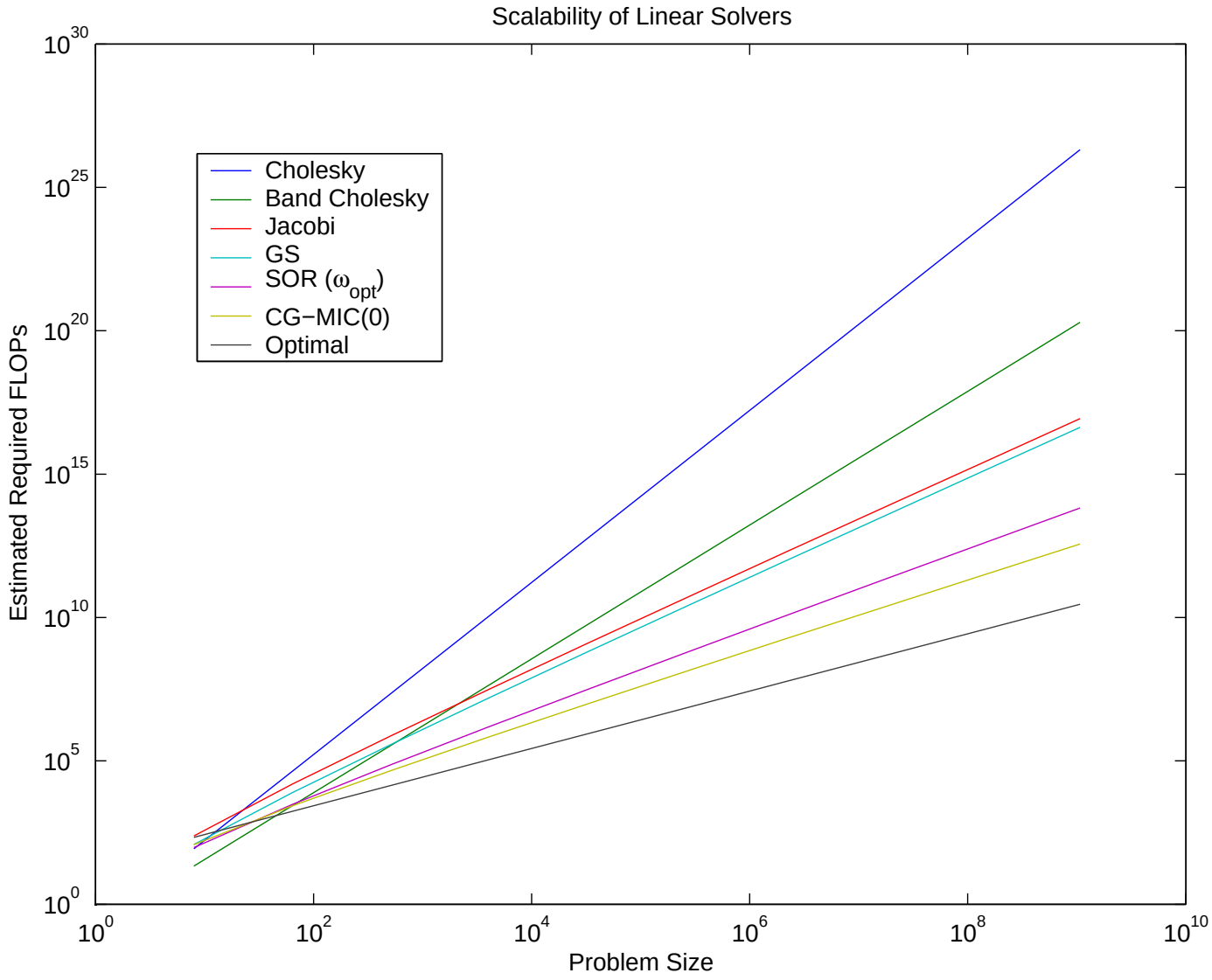
Stationary Iterative Methods . . .

- Jacobi and Gauss-Seidel converge to the level of discretization error in $O(n^5)$ operations for the 3-dimensional Poisson problem
- SOR with an optimal parameter choice converges in $O(n^4)$ operations

Krylov Methods

- Krylov methods find the optimal approximation to the solution in a given subspace
- Iteratively increase the size of the subspace to improve accuracy
- For 3D Poisson, the Conjugate Gradient algorithm converges in $O(n^4)$ operations (without any parameter choice)

Scalability



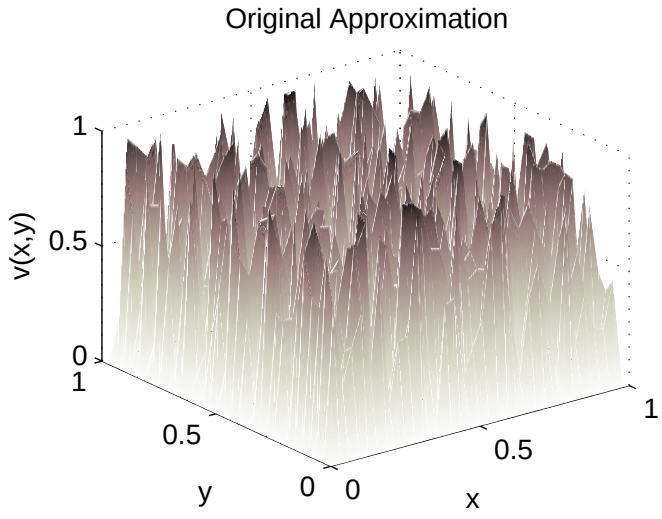
Scalability

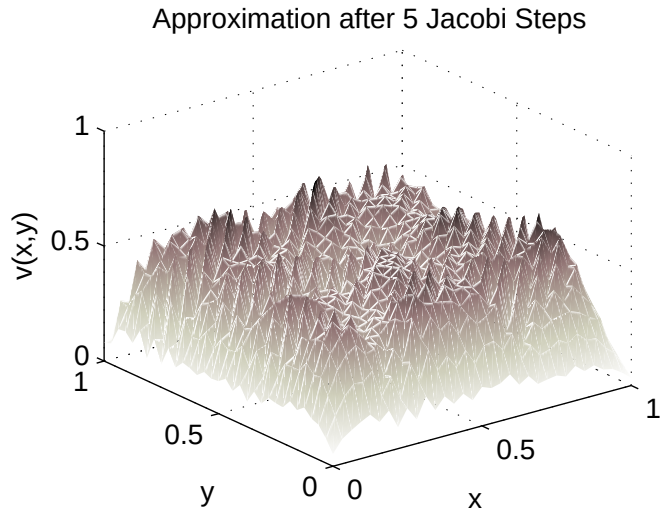
- Because the problems we look to solve are so large, even the cost of $O(N^{\frac{4}{3}})$ is too much
- If $n = 1000$, then $N^{\frac{4}{3}} = 10^{12}$
- An algorithm is said to be scalable (or fast) if it requires only $O(N)$ or $O(N \log N)$ operations
- We must have scalable algorithms in order to solve problems of interest at resolutions of interest

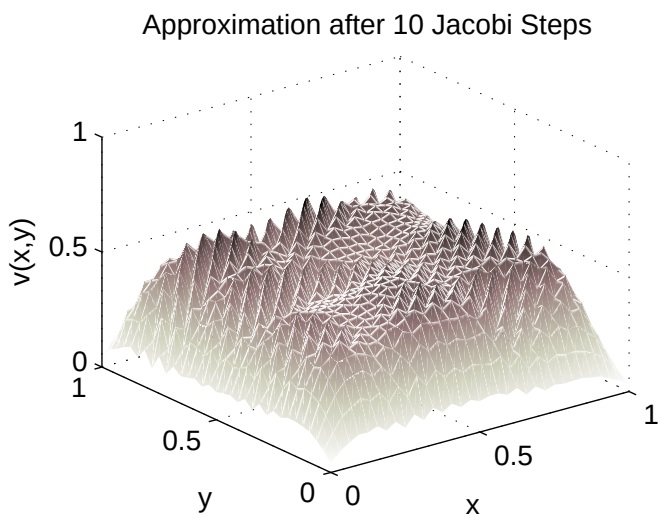
Stationary Iterative Methods . . .

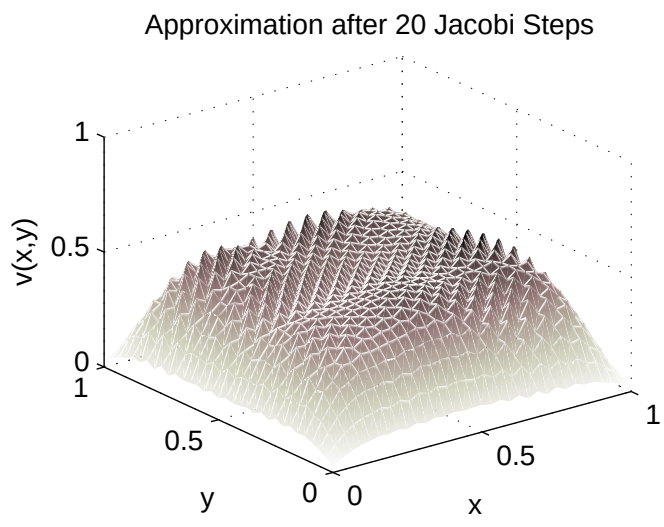
- Jacobi and Gauss-Seidel converge to the level of discretization error in $O(n^5)$ operations for the 3-dimensional Poisson problem
- SOR with an optimal parameter choice converges in $O(n^4)$ operations
- But, Jacobi and Gauss-Seidel resolve some components much faster than others
- In particular, for Poisson the geometrically smoothest components of u are the slowest to be resolved
- For this reason, Jacobi and Gauss-Seidel are often called smoothers - they smooth the error in the approximation

Smoother Performance









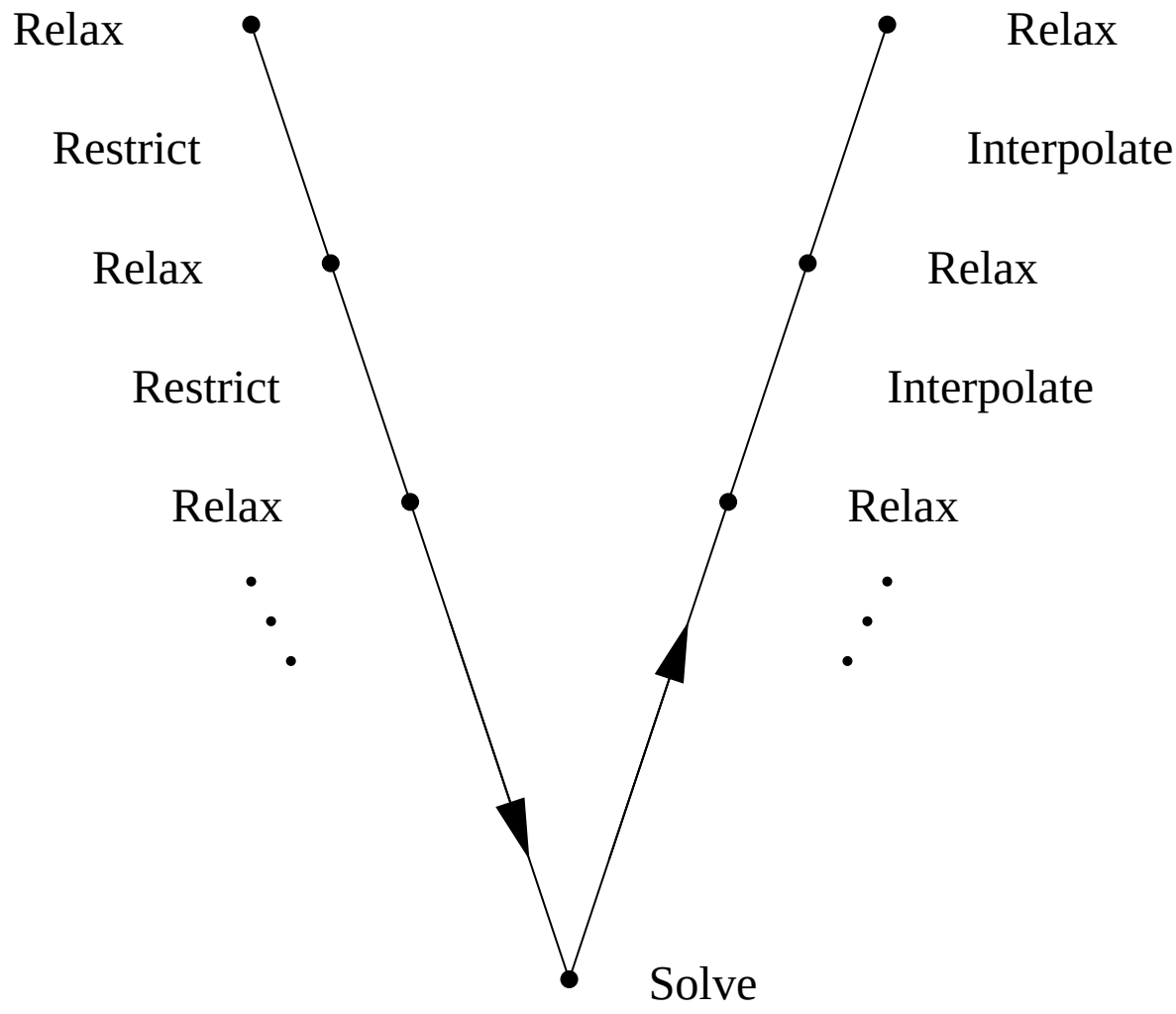
Complementing Relaxation

- If the error left after relaxing is smooth, it can be accurately represented using fewer degrees of freedom
- Problems with fewer degrees of freedom can be solved with less effort
- Error which appears smooth across many degrees of freedom is oscillatory when represented on fewer degrees of freedom

Multigrid Basics

- Multigrid methods obtain optimal efficiency through complementarity
- Use a smoothing process (such as Gauss-Seidel) to eliminate oscillatory errors
- Use coarse grid correction to eliminate smooth errors
- Obtain optimal efficiency through recursion

The V-Cycle

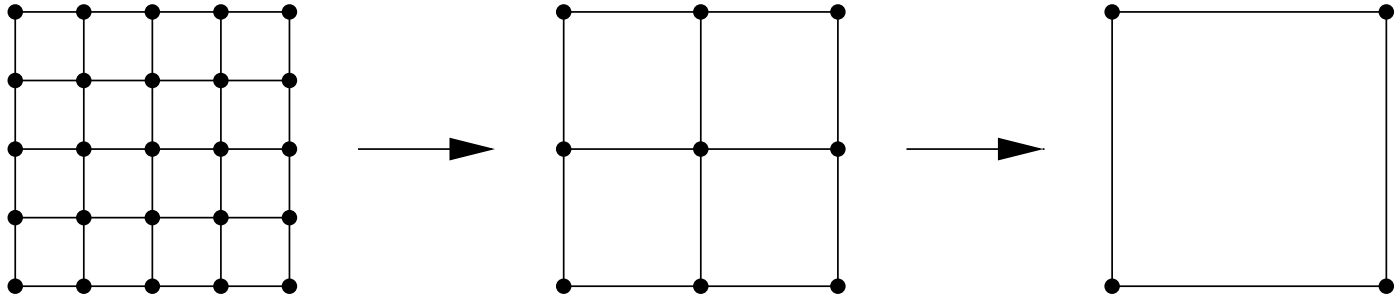

Relax
Restrict
Relax
Restrict
Relax
Solve
Relax
Interpolate
Relax
Interpolate
Relax

Multigrid Operators

- Multigrid V-Cycle requires transfers of residuals and corrections from one grid to the next
- Accomplished through Interpolation (Prolongation) and Restriction operators
- Often pick a form of interpolation (P) and take restriction $R = P^T$ (theoretical benefits)
- Smoothing on coarse grids requires operators on those grids
- These operators must well-approximate the fine grid operator

Geometric Multigrid

- Multigrid algorithms can be broadly classified by how they pick their coarse grids
- If we start with a geometrically regular grid, coarse grids can easily be chosen



Geometric Multigrid

- Interpolation that is accurate for geometrically smooth functions is easy to choose
- Can use linear/bilinear/trilinear averaging to get values at fine-grid points that are not also coarse-grid points
- Restriction can be chosen either by simply taking the fine-grid values at coarse-grid points (injection), or as the transpose of interpolation
- Coarse grid equations can be chosen by rediscretizing the PDE on the coarser grid or . . .

Variational Multigrid

- Multigrid with $R = P^T$ and $A_c = RAP$ is called a *variational formulation*
- Terminology comes from minimization form of $Ax = b$:

$$F(v) = \frac{1}{2}\langle Av, v\rangle - \langle b, v\rangle$$

$$x = \arg\min_{v \in \mathcal{H}} F(v)$$

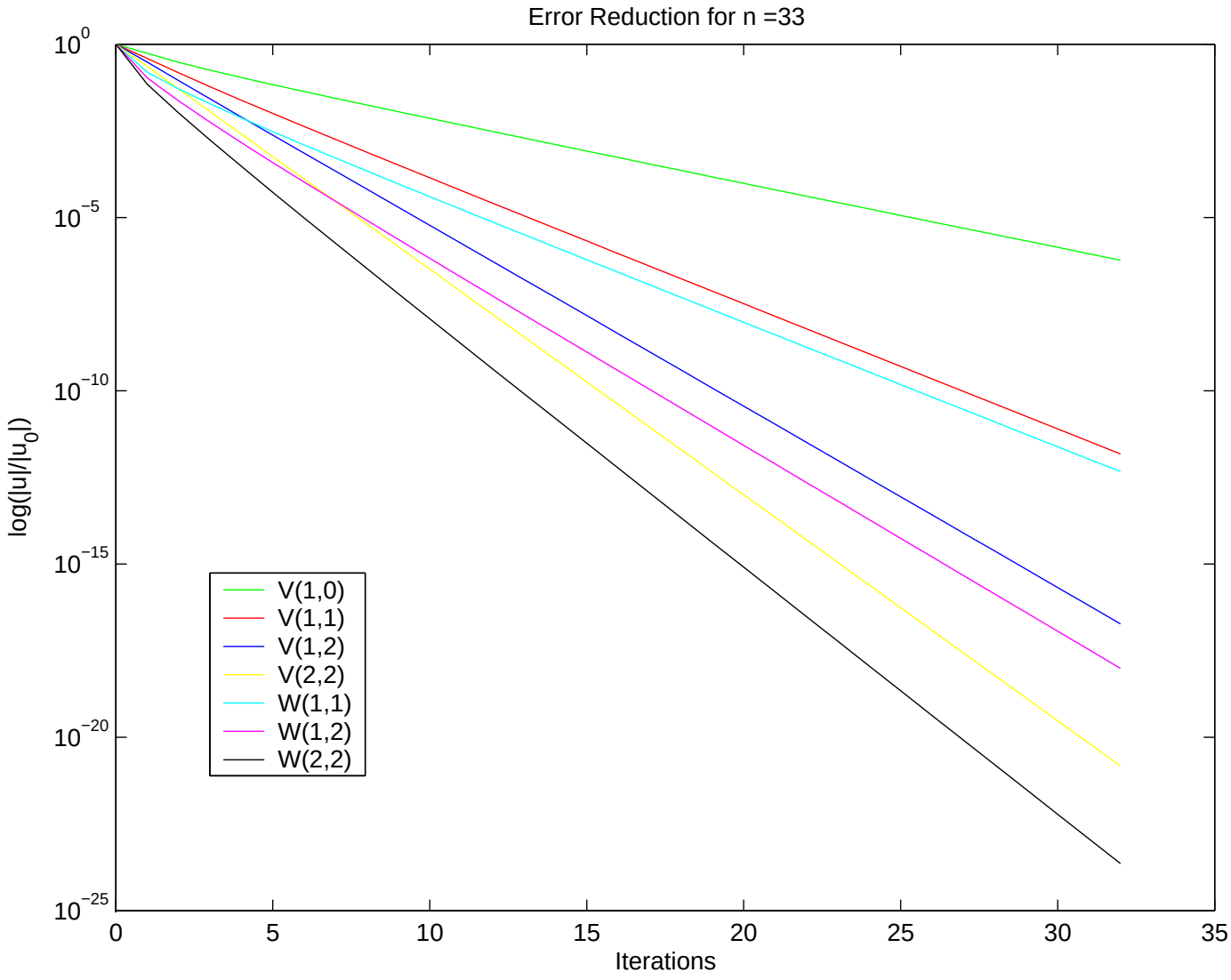
- Given an approximation v to the solution on the fine level, it can be shown that the optimal coarse grid correction Pw solves

$$(P^T AP)w = P^T(b - Av)$$

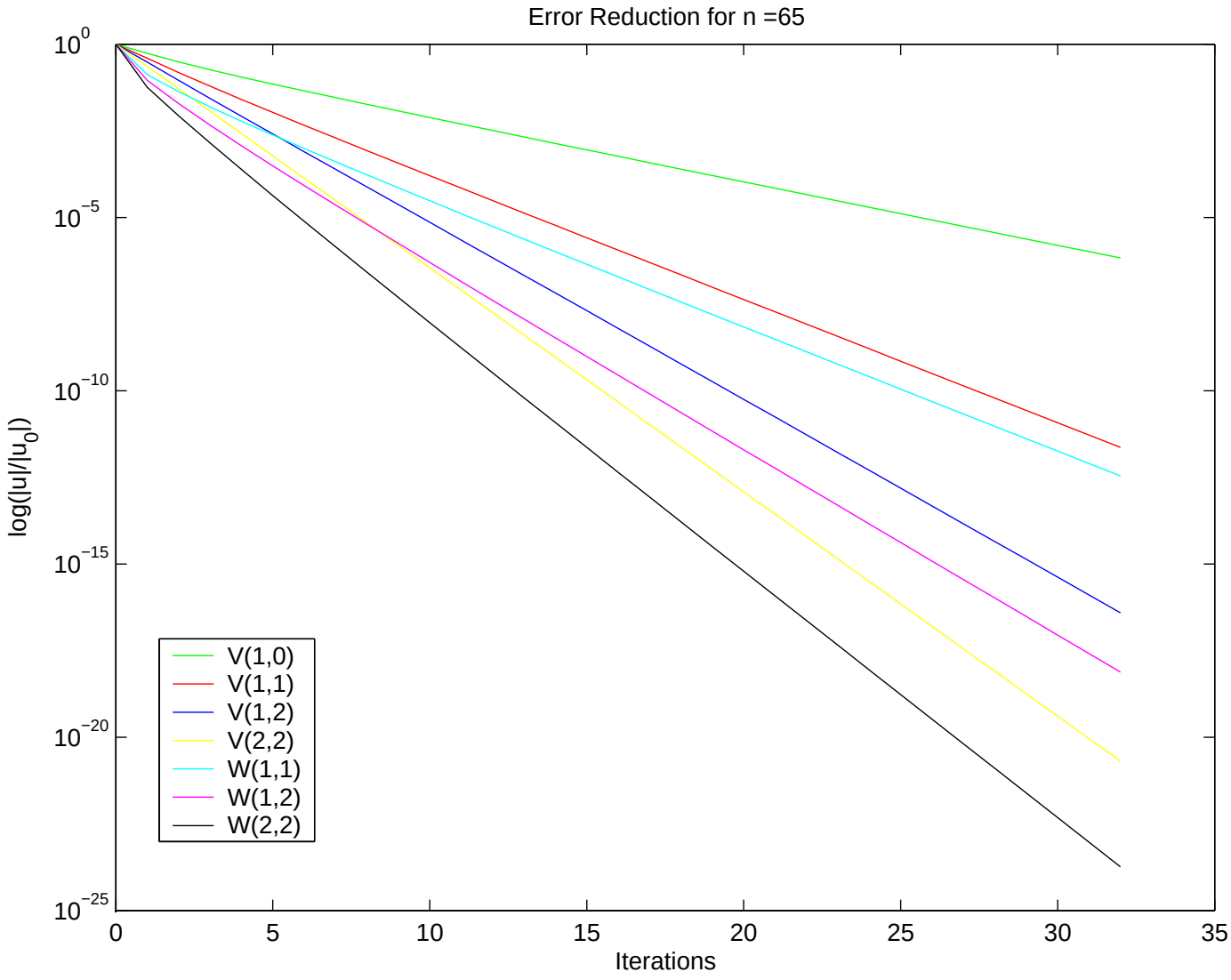
Theoretical Results

- Convergence in a fixed, finite number of V-cycles for finite differences
- Convergence in a fixed, finite number of V-cycles for finite element discretizations for H^1-elliptic operators

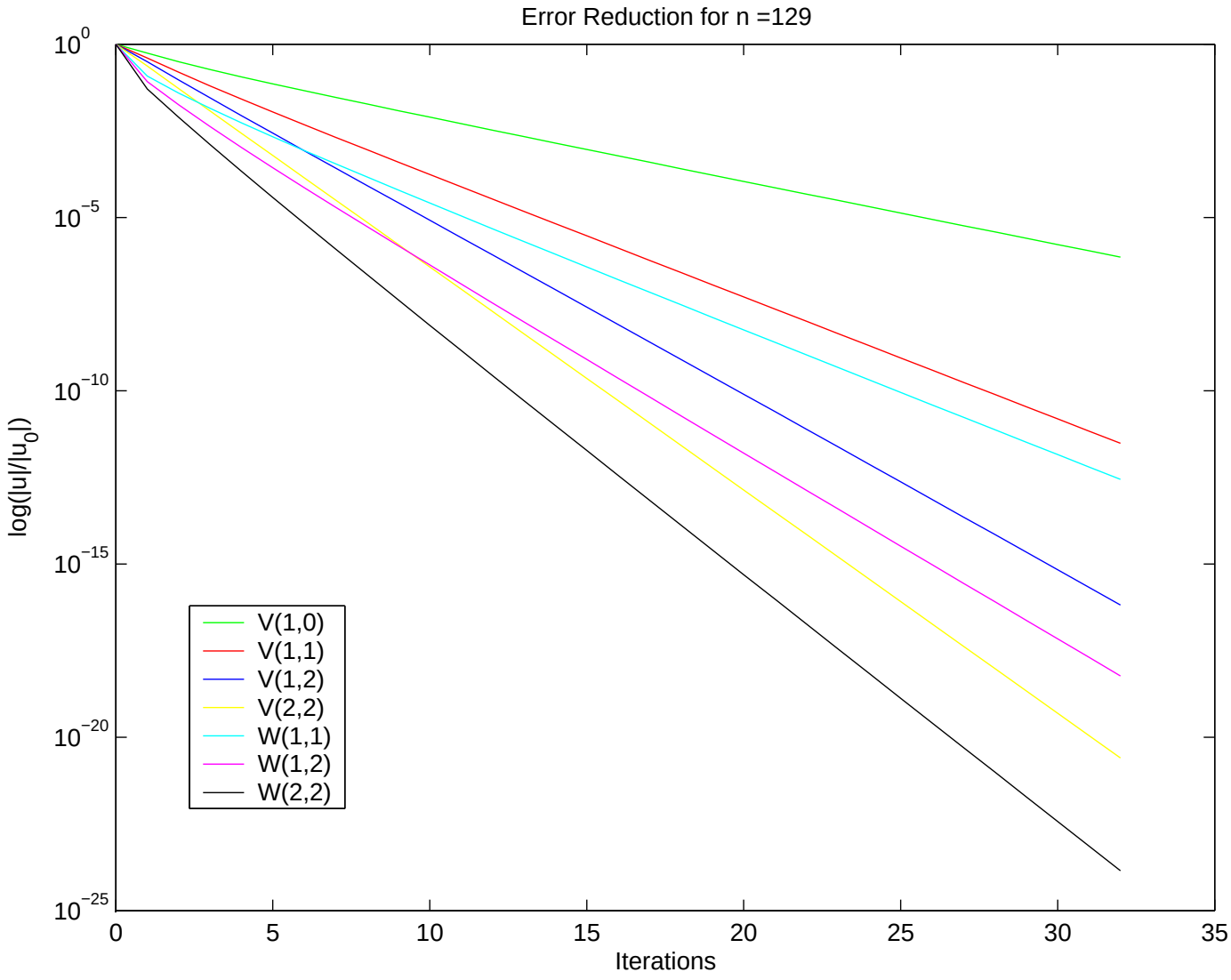
Numerical Results



Numerical Results



Numerical Results



Complications

- Difficult to work out appropriate interpolation for arbitrary geometries
- Some problems don’t have associated geometry (e.g. graph problems)
- Linear interpolation is not appropriate across material boundaries (discontinuities in PDE coefficients)
- Linear interpolation is inefficient in cases of strong anisotropy or convection

Philosophy

- All of the above problems can be solved by tweaking the standard, geometric multigrid algorithm
- Different smoothers and different interpolations can be used
- Each problem requires its own tuning
- Instead, we concentrate on developing an algorithm which is nearly-optimal on a larger number of problems

Algebraic Multigrid

- In the absence of geometric information, choices must be made based on algebraic information
- Interpolation and coarse grids must be chosen based on the ability to interpolate a suitable correction
- Coarse grid operators must be chosen based on the fine-grid operator - Galerkin coarsening may be the most natural choice

Smoothness

- Without geometric information, we can't talk about a vector being "smooth" in the same sense
- We define a vector, e, to be algebraically smooth if it is slow to be reduced by relaxation on $Ae = 0$
- For Jacobi, the condition becomes $\langle D^{-1}Ae, Ae\rangle \ll \langle e, Ae\rangle$
- In general, we think of e as being algebraically smooth if $Ae \ll e$

Influence and Dependence

- Classical (Ruge-Stueben) AMG is all about keeping track of how one gridpoint affects another
- Two gridpoints, i and j are said to be strongly connected if a_{ij} is large
- In particular, we say i strongly influences j if

$$|a_{ij}| > \theta \max_{k \neq j} |a_{kj}|$$

- We say i strongly depends on j if

$$|a_{ij}| > \theta \max_{k \neq i} |a_{ik}|$$

Coarsening Heuristics

- An good choice of a coarse grid is one which can be effectively used to complement relaxation
- That is, we want to choose a coarse grid to allow us to correct the algebraically smooth components on the fine grid
- Ideally, to interpolate to a point i, we would want to have values at all points that it strongly depends on
- In practice, this would yield far too many coarse-grid points
- Instead, we say that for each point j that strongly influences i, either j is a coarse grid point or it is itself strongly dependent on one coarse-grid neighbour of i

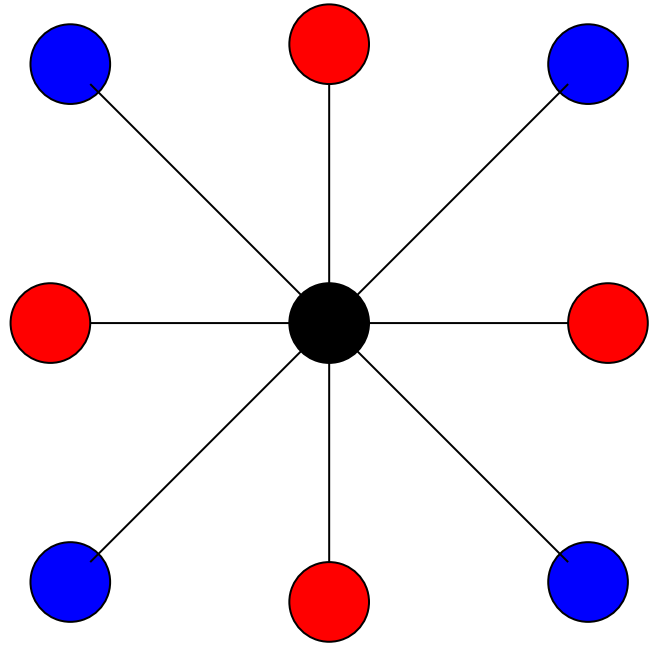
Coarsening Heuristics

- We must also, however, balance the desire for a good interpolation with the need to have a small coarse-grid
- To do this, we insist that the set of coarse points is a maximal subset of the fine-grid such that no coarse-grid point strongly depends on another coarse-grid point
- Implementing these heuristics is accomplished using a colouring algorithm

Defining Interpolation

- For each fine-grid point, i, we want to interpolate its values from neighbouring coarse-grid points

N_i, the Neighbourhood of i



Fine Grid Points

Coarse Grid Points

Defining Interpolation

- For each fine-grid point, i, we want to interpolate its values from neighbouring coarse-grid points
- We consider an interpolation operator that must be accurate for algebraically smooth components, so we start by considering $Ae = 0$, or

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

- Must get rid of connections to points $k \in F_i$

Defining Interpolation

- Points $k \in F_i$ can be either strongly or weakly connected to i
- If k is weakly connected, it isn't important in interpolation, so collapse to the diagonal (i.e. consider $e_k \approx e_i$)
- If k is strongly connected, then we've ensured it is strongly dependent on something in C_i
- So, approximate e_k by a weighted average of $e_j, j \in C_i$

$$e_k \approx \frac{\sum_{j \in C_i} a_{kj} e_j}{\sum_{j \in C_i} a_{kj}}$$

Improvements

- Resulting algorithm can easily handle jumps in coefficients
- No need to know underlying geometry
- Can be adapted to handle anisotropy
- Can be modified to handle more complicated problems, e.g. Elasticity, Stokes Flow, Maxwell's Equations, Hyperbolic PDEs, . . .

Numerical Results

- We start with 2 test problems on $[0,1]^2$, both from bilinear FE discretizations
- Problem 1 is Poisson with pure Dirichlet Boundary Conditions
- Problem 2 is $-\nabla \cdot D(x,y)\nabla p(x,y) = 0$ with Dirichlet BCs on the left and right and Neumann BCs on top and bottom, and

$$D(x,y) = \begin{cases} 10^2 & (x,y) \in [\frac{1}{3}, \frac{2}{3}]^2 \\ 1 & \text{otherwise} \end{cases}$$

Numerical Results

Convergence Factors for AMG

h	Problem 1	Problem 2
$1/32$	0.09	0.14
$1/64$	0.10	0.13
$1/128$	0.14	0.16
$1/256$	0.13	0.15
$1/512$	0.15	0.21

Complications

- Each new type of problem requires a new adaptation
- Coupled Systems become complicated - should tune AMG to each piece of the system
- Very hard to predict what tuning will be necessary
- Many knobs to turn

AMG Assumptions

- Algebraic Multigrid methods attempt to mimic geometric methods in their choices of interpolation operators and coarse grids
- Typically use a fixed, pointwise relaxation scheme
- Classical (Ruge-Stueben) AMG assumes that algebraically smooth error varies slowly along strong connections
- This is equivalent to assuming that algebraically smooth error is essentially (locally) constant

AMG Weaknesses

- AMG assumes the slowest-resolved components are near-constant
- For standard (e.g. finite difference, Galerkin FE) discretizations of scalar differential operators this is usually true
- If discretizations are non-standard or the resulting matrices are scaled, AMG cannot achieve good performance

Importance of Interpolation

- Complementarity is key in multigrid - error components that are not quickly reduced by relaxation must be reduced by coarse-grid correction
- A component can only be corrected from the coarse-grid if it is properly interpolated from that grid
- Interpolation must be most accurate for components that relaxation is slowest to resolve

Choosing Interpolation

- Seek to define interpolation to fit an algebraically smooth vector
- Algebraic smoothness means

$$(Ae)_i \approx 0$$

$$\text{or } a_{ii}e_i \approx -\sum_{j \in N_i} a_{ij}e_j$$

$$= -\sum_{j \in C_i} a_{ij}e_j - \sum_{k \in F_i} a_{ik}e_k$$

- To define interpolation, need to collapse connections from F_i to C_i

Choosing Interpolation . . .

- Seek to define interpolation to fit an algebraically smooth vector
- If $k \in F_i$ is connected to a set of $j \in C_i$, we want to write

$$e_k = \sum_{j \in C_i} w_{kj} e_j$$

- Then, using the definition of algebraic smoothness, we have

$$a_{ii} e_i \approx - \sum_{j \in C_i} a_{ij} e_j - \sum_{k \in F_i} a_{ik} e_k$$

$$a_{ii} e_i \approx - \sum_{j \in C_i} a_{ij} e_j - \sum_{k \in F_i} \sum_{j \in C_i} a_{ik} w_{kj} e_j$$

Choosing w_{kj}

- If we have a vector, $x^{(1)}$, such that $(Ax^{(1)})_k \approx 0$ and so

$$a_{kk}x_k^{(1)} = -\sum_{j \in C_i} a_{kj}x_j^{(1)} - \sum_{j \notin C_i} a_{kj}x_j^{(1)}$$

- Eliminate extra terms by replacing matrix entry a_{kk} with arbitrary d_{kk}

$$d_{kk}x_k^{(1)} = -\sum_{j \in C_i} a_{kj}x_j^{(1)}$$

Choosing w_{kj} ...

- Taking the value of d_{kk} given here, we can write

$$x_k^{(1)} = -\sum_{j \in C_i} \frac{a_{kj}}{d_{kk}} x_j^{(1)} = \sum_{j \in C_i} \frac{a_{kj} x_k^{(1)}}{\sum_{j' \in C_i} a_{kj'} x_{j'}^{(1)}} x_j^{(1)}$$

- Use this formula to collapse all algebraically smooth error

$$e_k = \sum_{j \in C_i} \left(\frac{a_{kj} x_k^{(1)}}{\sum_{j' \in C_i} a_{kj'} x_{j'}^{(1)}} \right) e_j = \sum_{j \in C_i} w_{kj} e_j$$

Adaptive Interpolation

So, we define interpolation to a fine grid point i as

$$e_i = -\sum_{j \in C_i} \frac{a_{ij} + \sum_{k \in F_i} a_{ik} w_{kj}}{a_{ii}} e_j$$

$$= -\sum_{j \in C_i} \frac{a_{ij} + \sum_{k \in F_i} a_{ik} \left(\frac{a_{kj} x_k^{(1)}}{\sum_{j' \in C_i} a_{kj'} x_{j'}^{(1)}} \right)}{a_{ii}} e_j$$

Relation to Ruge-Stueben

- Ruge-Stueben AMG takes $x^{(1)} = 1$
- Substituting this into our interpolation formula gives

$$e_i = -\sum_{j \in C_i} \frac{a_{ij} + \sum_{k \in F_i} a_{ik} \left(\frac{a_{kj}}{\sum_{j' \in C_i} a_{kj'}} \right)}{a_{ii}} e_j$$

- This is the same as the AMG strong-connection-only interpolation formula

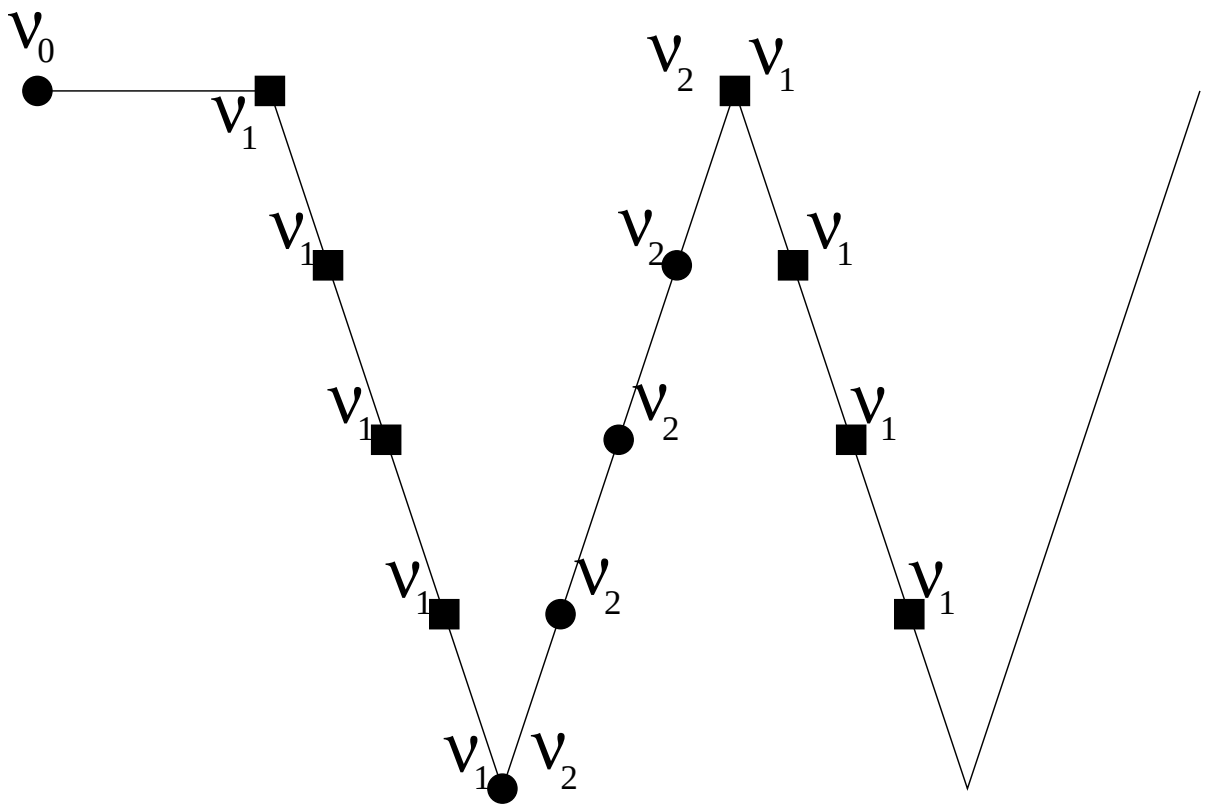
Scaling Invariance

- Combining our interpolation with pointwise relaxation leads to an algorithm that is nearly insensitive to any diagonal scaling
- In particular, if A is scaled to DAD, and $x^{(1)}$ is scaled to $D^{-1}x^{(1)}$, then we achieve the same convergence rates for the scaled problem as for the unscaled problem
- Difficulty lies in generating the scaled vector $D^{-1}x^{(1)}$

Determining $x^{(1)}$

- Choosing a good interpolation operator requires a good approximation, $x^{(1)}$, to the algebraically-smoothest vector of a given matrix A
- Such an approximation could be determined by sufficient relaxation on a random initial guess with a zero right-hand side
- In practice, this requires too much computation to be feasible
- Instead, we use preliminary V-cycles to accelerate the exposure of components for which $Ax \approx 0$

Determining $x^{(1)}$ ...



- In 2D, total cost of relaxation can then be approximated by $\nu_0 + \frac{8}{3}\nu_1 + \frac{4}{3}\nu_2$ work units

Test Problems

- We start with 2 test problems on $[0,1]^2$, both from bilinear FE discretizations
- Problem 1 is Poisson with pure Dirichlet Boundary Conditions
- Problem 2 is $-\nabla \cdot D(x,y)\nabla p(x,y) = 0$ with Dirichlet BCs on the left and right and Neumann BCs on top and bottom, and

$$D(x,y) = \begin{cases} 10^2 & (x,y) \in [\frac{1}{3}, \frac{2}{3}]^2 \\ 1 & \text{otherwise} \end{cases}$$

Test Problems

- The second pair of problems come from diagonally scaling Problems 1 and 2
- To scale, we use the node-wise scaling function

$$1 + \sin(547\pi x_i)\sin(496\pi y_j) + 10^{-7}$$

- This function gives variable scaling on each node, but does not change its character with h

Numerical Results

- Coarse grids are chosen geometrically, based on full-coarsening
- Coarse grid operators are determined by the Galerkin condition.
- Compute asymptotic convergence factor, then use this to estimate number of V(1,1)-cycles needed to reduce error by 10^{-6}
- From number and cost of cycles ($\frac{8}{3}$ work units), can estimate total cost of solution stage

AMG-Equivalent Results

- By fixing $x^{(1)} = 1$, we can generate results indicative of AMG's performance

Work Units for standard AMG

h	Problem 1	Problem 2	Problem 3	Problem 4
$1/32$	12.9	14.5	1297	59.4
$1/64$	13.4	15.6	4075	112.1
$1/128$	13.6	14.9	6122	218.7
$1/256$	13.8	16.4	6122	430.6
$1/512$	13.9	15.2	7350	858.6
$1/1024$	13.9	16.7	7350	1656

Distributing Relaxation

- To choose how to distribute relaxation, we fix the number of work units allotted to the relaxation in the setup phase

$$\nu_0 + \frac{8}{3}\nu_1 + \frac{4}{3}\nu_2 = 12$$

- Best results were achieved for $\nu_0 = 4, \nu_1 = 2, \nu_2 = 2$, with good results also seen for $\nu_0 = 4, \nu_1 = 3, \nu_2 = 0$ and $\nu_0 = 4, \nu_1 = 1, \nu_2 = 4$
- Poor results were achieved with $\nu_0 = 0, \nu_1 = 3, \nu_2 = 3$ and $\nu_0 = 4, \nu_1 = 0, \nu_2 = 6$

Work units for solution

$$\nu_0 = 0, \nu_1 = 3, \nu_2 = 3$$

h	Problem 1	Problem 2	Problem 3	Problem 4
$1/32$	12.9	14.8	12.9	14.7
$1/64$	13.4	15.6	13.5	15.3
$1/128$	13.6	14.7	13.8	15.4
$1/256$	13.8	16.4	13.9	30.3
$1/512$	13.9	24.0	13.9	25.8
$1/1024$	749.0	926.1	103.7	977.2

Work units for solution

$$\nu_0 = 4, \nu_1 = 2, \nu_2 = 2$$

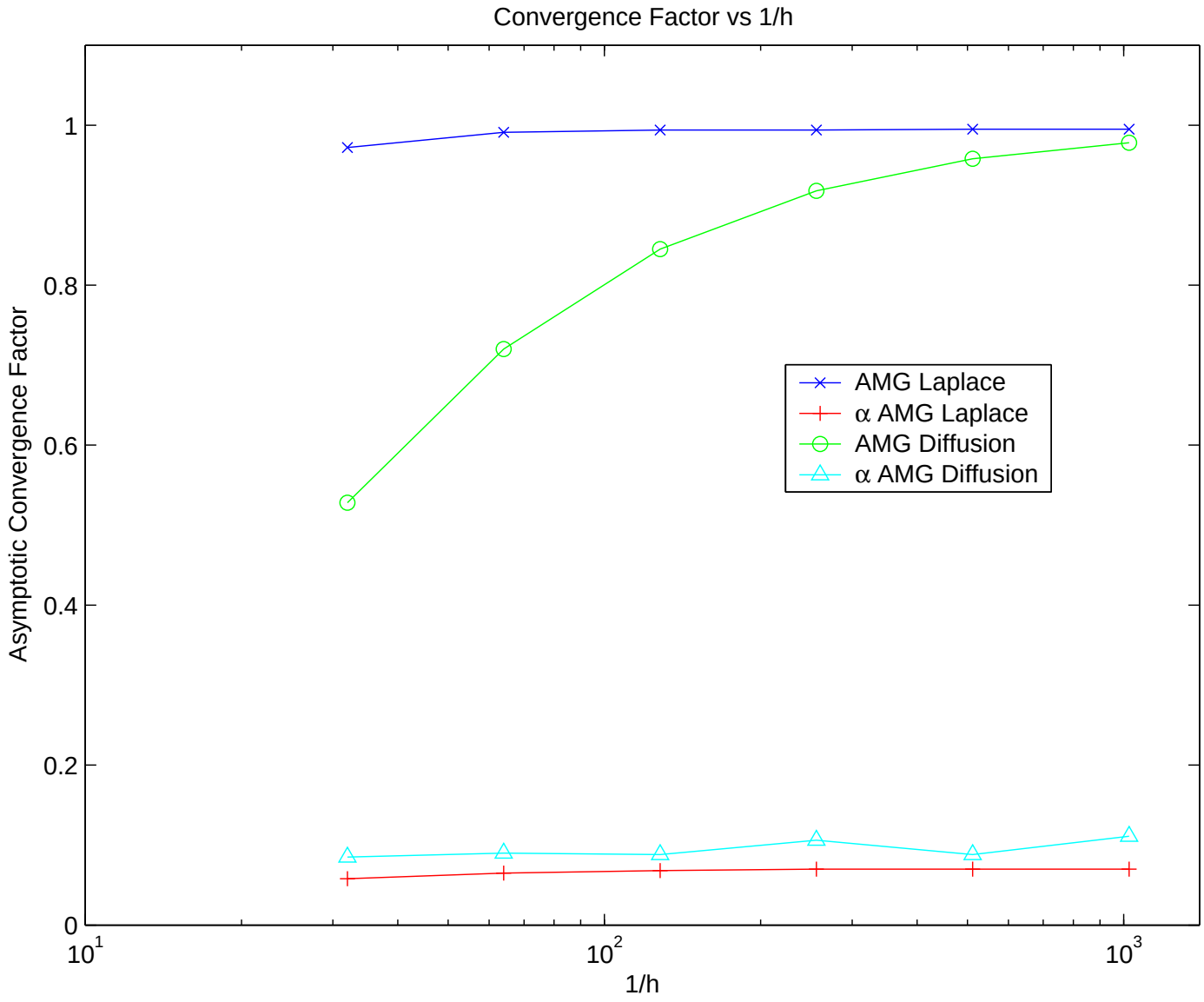
h	Problem 1	Problem 2	Problem 3	Problem 4
$1/32$	12.9	14.7	12.9	14.7
$1/64$	13.4	15.6	13.5	15.4
$1/128$	13.6	14.9	13.7	14.7
$1/256$	13.9	16.4	13.9	25.2
$1/512$	13.9	15.8	13.9	16.4
$1/1024$	13.9	23.2	13.9	25.6

Work units for solution

$$\nu_0 = 6, \nu_1 = 3, \nu_2 = 3$$

h	Problem 1	Problem 2	Problem 3	Problem 4
$1/32$	12.9	14.9	12.9	14.9
$1/64$	13.4	15.6	13.5	15.3
$1/128$	13.6	15.2	13.7	15.3
$1/256$	13.8	16.4	13.8	16.4
$1/512$	13.9	15.2	13.9	15.2
$1/1024$	13.9	16.7	13.9	16.8

Convergence Factors



Current and Future Work

- Developing a theory for self-correcting AMG
- Developing a fully-algebraic version
- Investigating better coarsening procedures (Compatible Relaxation)
- Natural extension to systems
- Alternate smoothers

Summary

- Applications driving need for solvers for large problems
- Classical iterative methods do not scale appropriately for the sizes we are considering
- Multigrid (multiscale) methods do offer optimal efficiency

Summary

- For regular grids, with smooth PDE coefficients, geometric MG works well
- For irregular grids, discontinuous coefficients, algebraic MG works well
- For coupled systems, exotic bases, adaptive algebraic MG offers hope
- All are $O(N)$ algorithms, constants are non-trivial, but not prohibitive