

Parallel Algebraic Multigrid Methods for Fusion and Higher Order PDEs

Sophie Boileau, Atmik Das, **Kellen Kanarios**, Lucia Krajčoviechová



Mentor: Dr. Jean-Michel Maldague

Sponsors: Dr. Robert Falgout, Dr. Wayne Mitchell, Dr. Daniel Osei-Kuffuor

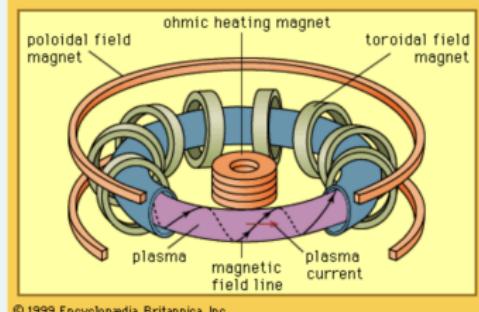
This material is based upon work jointly supported by Lawrence Livermore National Laboratory and the National Science Foundation under Grant No. 2015553.

Motivation

COGENT Proxy Problem

$$-au_{xx} - bu_{yy} + acu_{yyxx} = g, \quad b, c \gg a$$

- Thermonuclear fusion by magnetic confinement.



Preliminaries

- Transferring a PDE into a linear system

$$Au = f.$$

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- Example: 2D Poisson equation

$$-u_{xx} - u_{yy} = f.$$

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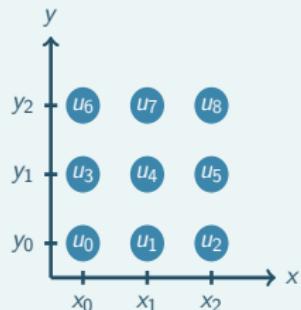
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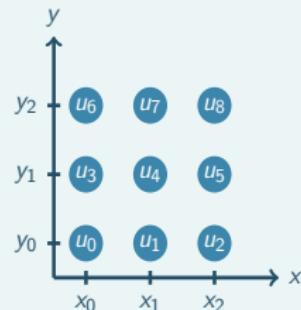
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Its discretization (finite differences) on a 3×3 grid has

$$A = \begin{pmatrix} 4 & -1 & -1 & & \\ -1 & 4 & -1 & & \\ & -1 & 4 & \ddots & \\ & & \ddots & \ddots & \ddots \end{pmatrix} \quad \text{or} \quad A \sim \begin{bmatrix} -1 & -1 & \\ -1 & 4 & -1 \\ -1 & & \end{bmatrix}.$$

stencil
matrix

Taxonomy of Multigrid

1 Iterative Methods

2 Multigrid

3 Algebraic Multigrid

4 Our Approach

Iterative Methods

- Consider the linear system

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$$e^{(k+1)} = (I - M^{-1}A)e^{(k)} = \sum_{i=1}^N (I - M^{-1}\lambda_i)c_i^{(k)}v_i.$$

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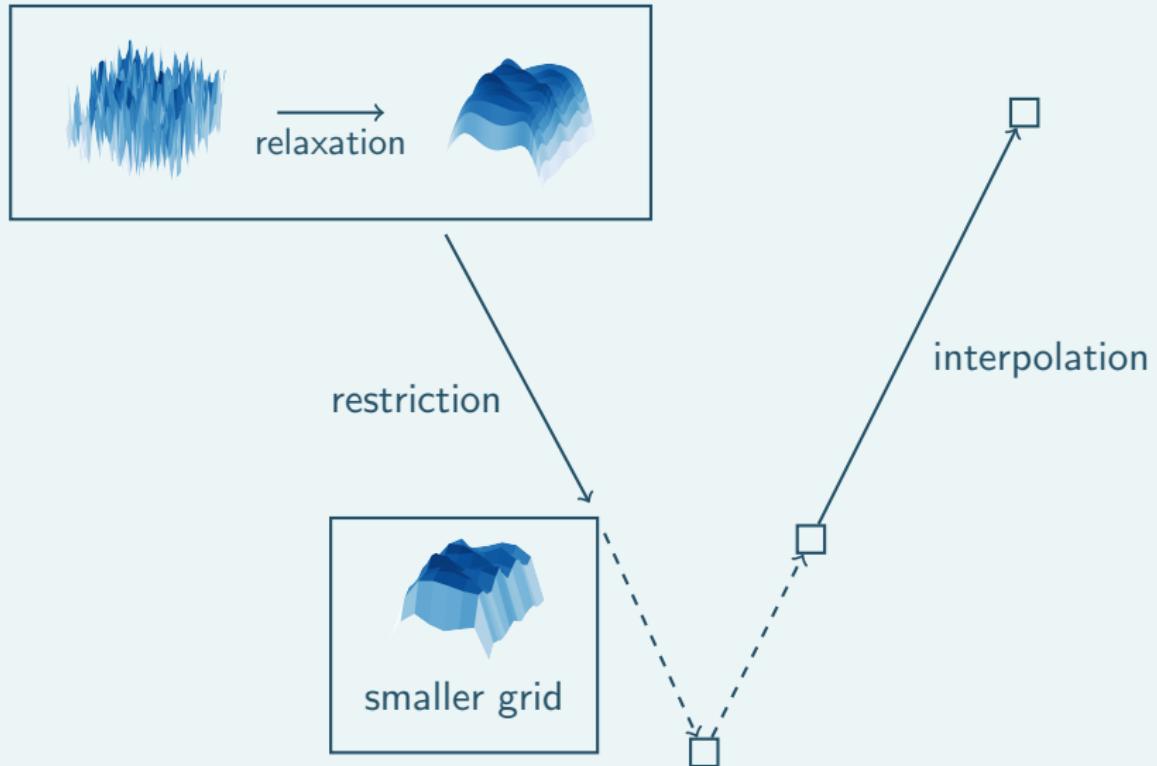
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$$e^{(k+1)} = (I - M^{-1}A)e^{(k)} = \sum_{i=1}^N (I - M^{-1}\lambda_i)c_i^{(k)}v_i.$$

- Small eigenvalues → **slow** convergence.

Multigrid



Constructing Smaller System

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- Define restriction and interpolation operators R and P .
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- Let P be interpolation (prolongation) and P^T restriction.
- The coarse-grid operator is defined by the Galerkin procedure,
 $A_c = P^T A P$.
- This gives the “best” coarse-grid correction in the sense that the solution e_c of the coarse system satisfies

$$A_c e_c = P^T r,$$

$$e_c = \arg \min \|e - Pe_c\|_A.$$

Constructing Smaller System

To Do

- Define restriction and interpolation operators R and P .
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$$\begin{array}{ccc} Ae_0 = r_0 & & u_1 = u_0 + Pe_c \\ & \searrow \text{restriction} & \nearrow \text{interpolation} \\ & P^T A P e_c = P^T r_0 & \end{array}$$

Constructing Smaller System

To Do

- Define restriction and interpolation operators R and P .
 - Decide how to pick points for coarser grid.
-
- Error is assumed **smooth**

2D-Poisson



$$-u_{xx} - u_{yy} = f$$

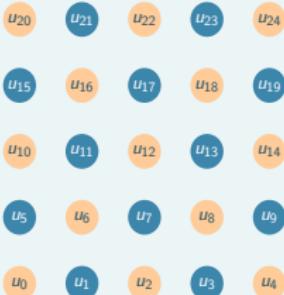
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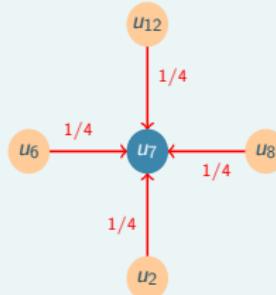
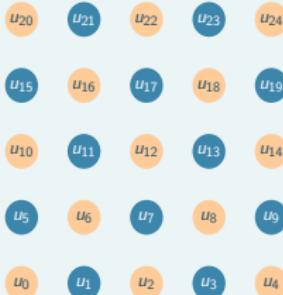
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Constructing Smaller System

To Do

- Define restriction and interpolation operators R and P .
- Decide how to pick points for coarser grid.

- Error is assumed **smooth**, so local linear interpolation often works.



2D-Poisson



$$-u_{xx} - u_{yy} = f$$

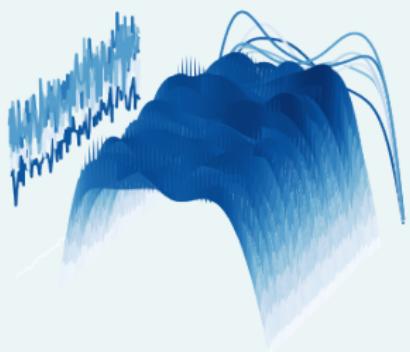
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Anisotropic Example

- Anisotropic, 5×5 grid

$$-u_{xx} - \epsilon u_{yy} = f, \quad 0 < \epsilon \ll 1.$$

- $\sin y$ is an ϵ -eigenfunction.

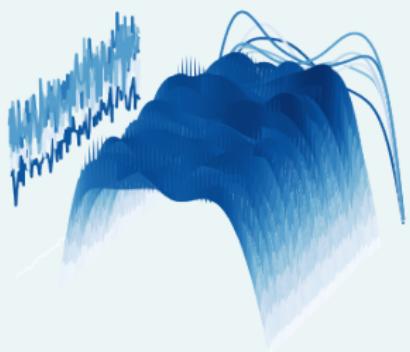


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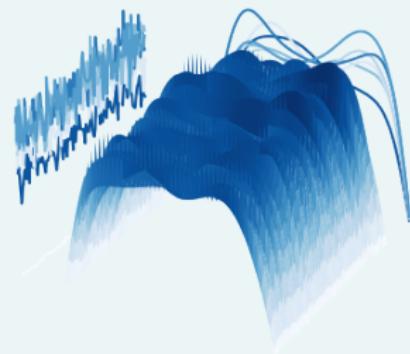
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WHAT DO WE DO?!?

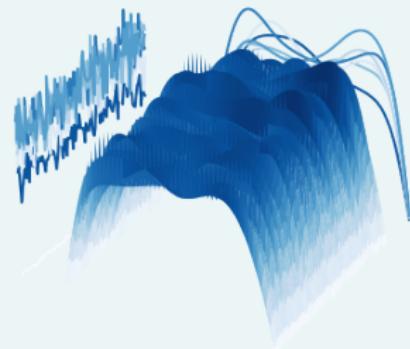
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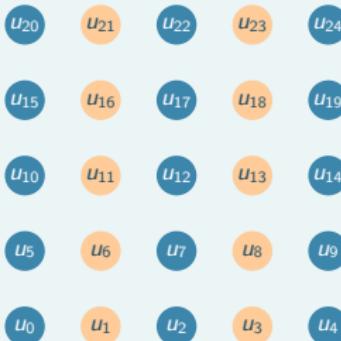
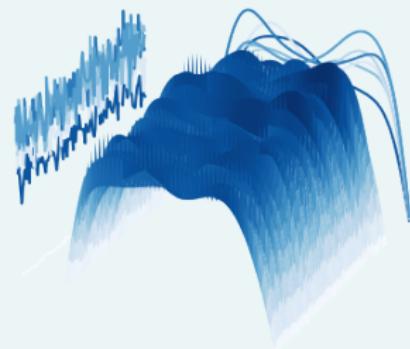
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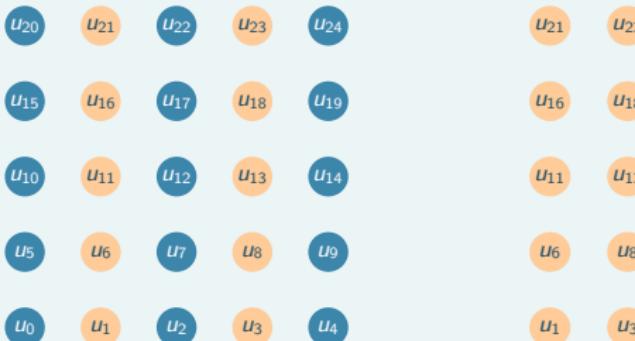
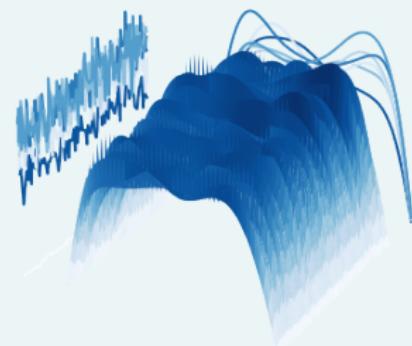
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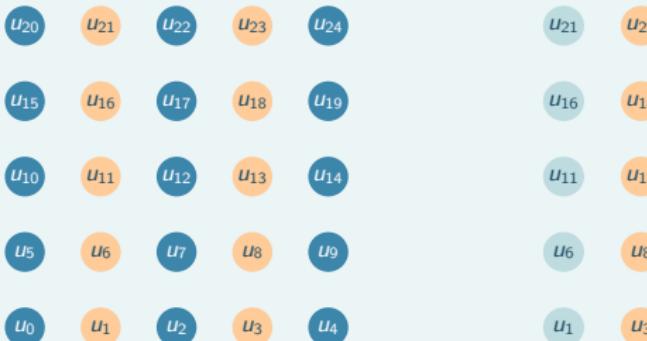
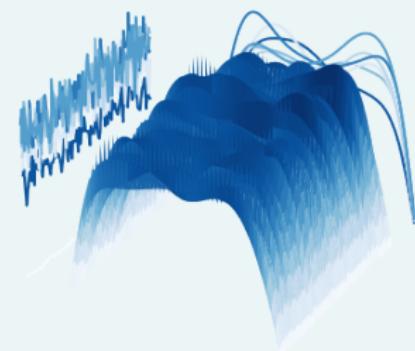
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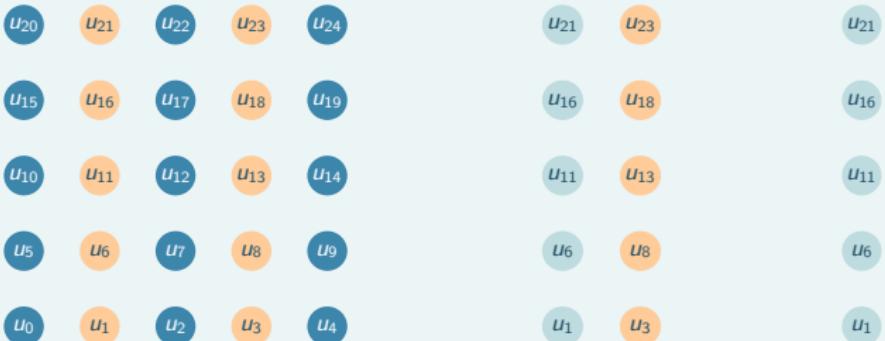
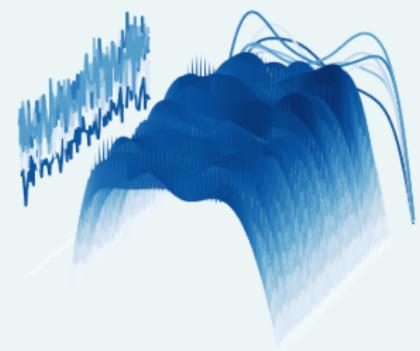
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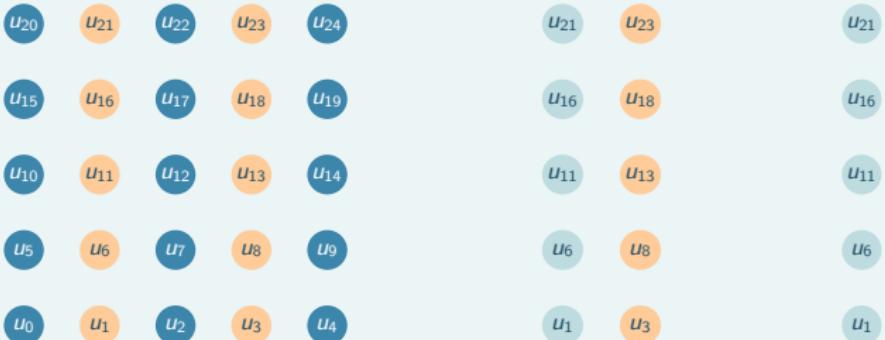
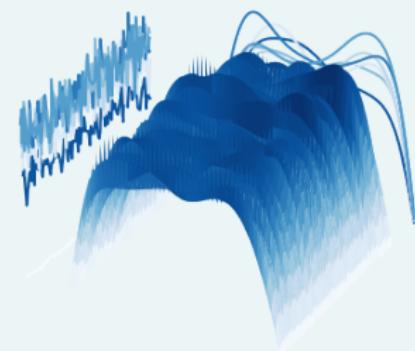
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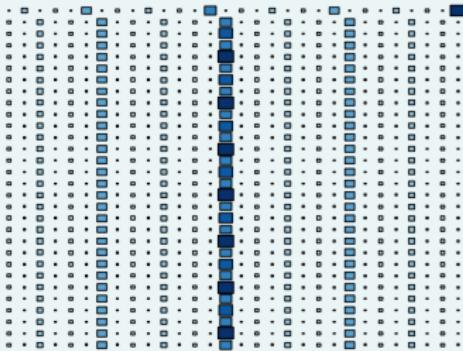
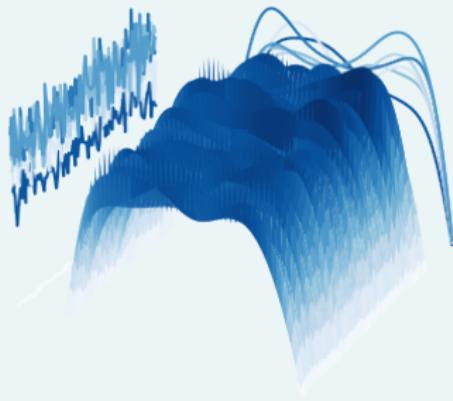


Anisotropic Example

- Use knowledge of underlying PDE and grid.
- Line-relaxation can smooth oscillatory error on coarser grids.



Algebraic Multigrid (AMG)



- Algebraic multigrid follows multigrid principles using only the coefficients of the matrix.
- More robust - can be used in time-dependent simulations.

Strength of Connection

- Smooth error is characterized by small eigenvectors, i.e.

$$\mathbf{e}^T \mathbf{A} \mathbf{e} = \lambda \|\mathbf{e}\|^2 \ll 1.$$

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Definition

A component u_i is θ -strongly connected with a component u_j if

$$-a_{ij} \geq \theta \max_{k \neq j} \{-a_{ik}\}.$$

Example

- Five-point stencil discretization on a 5×5 grid

$$-u_{xx} - \epsilon u_{yy} = f, \quad 0 < \epsilon \ll 1, \quad A \sim \begin{bmatrix} & -\epsilon & \\ -1 & 2 + 2\epsilon & -1 \\ & -\epsilon & \end{bmatrix}.$$

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- Construct strength adjacency matrix:

$$S = \begin{pmatrix} 0 & 1 & & & \\ 1 & 0 & 1 & & \\ & 1 & 0 & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & 0 \end{pmatrix}$$

$S_{ij} = 1$ if u_i and u_j are strongly connected.

Example

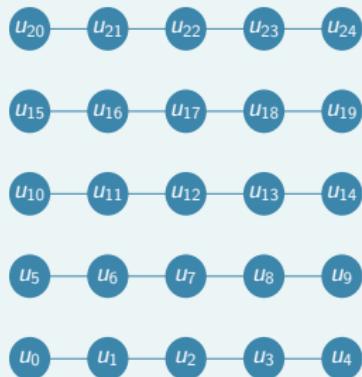
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Graphical representation of S .

Algebraic Coarsening

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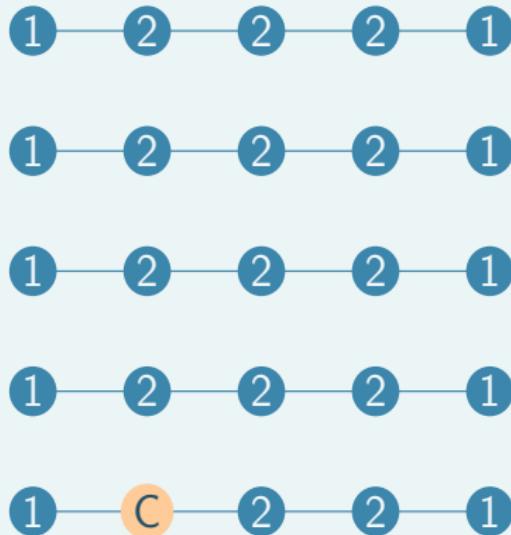
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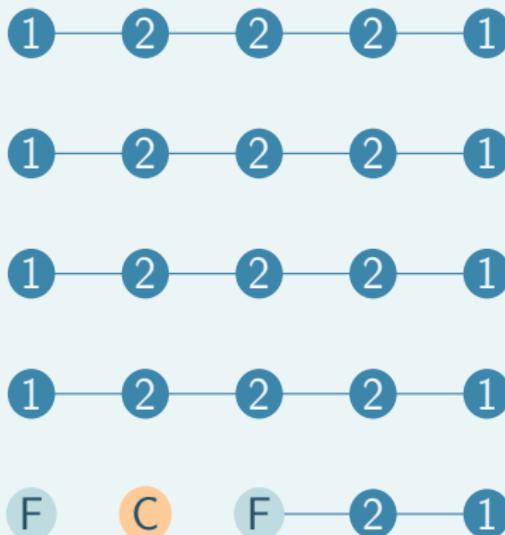
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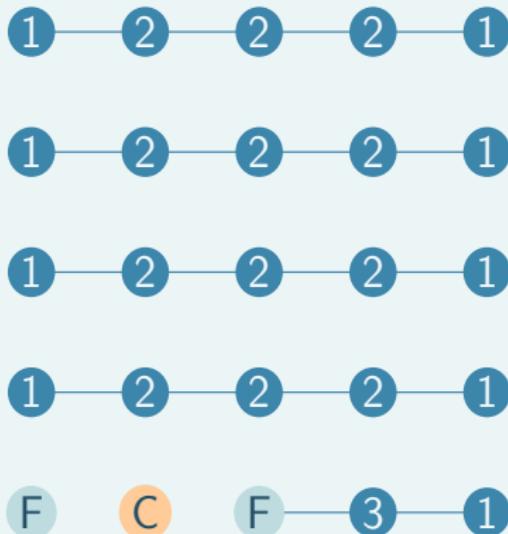
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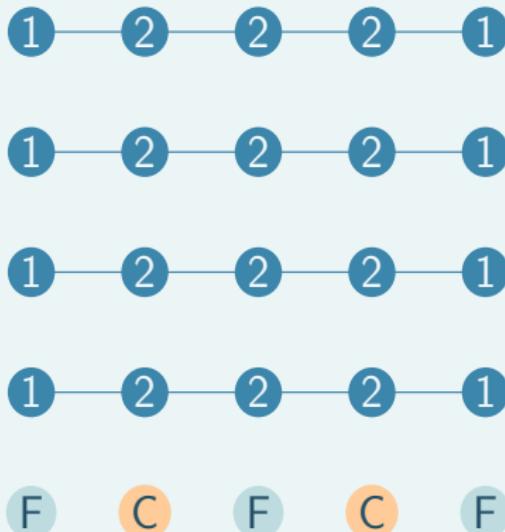
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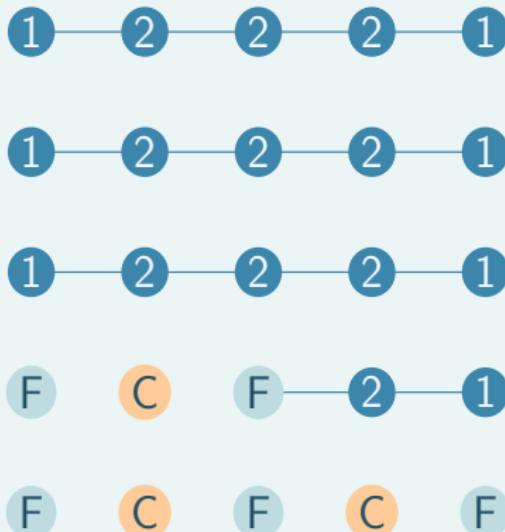
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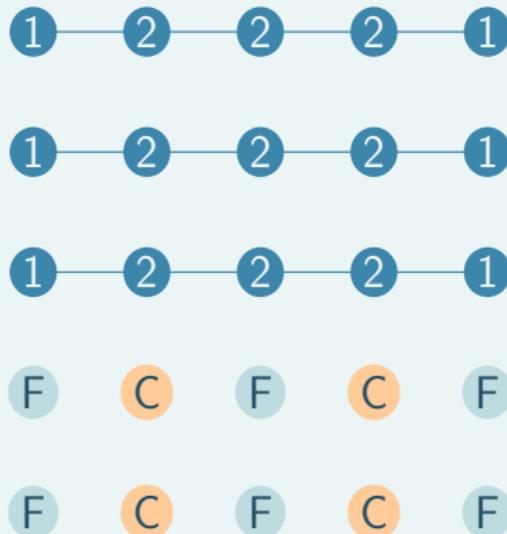
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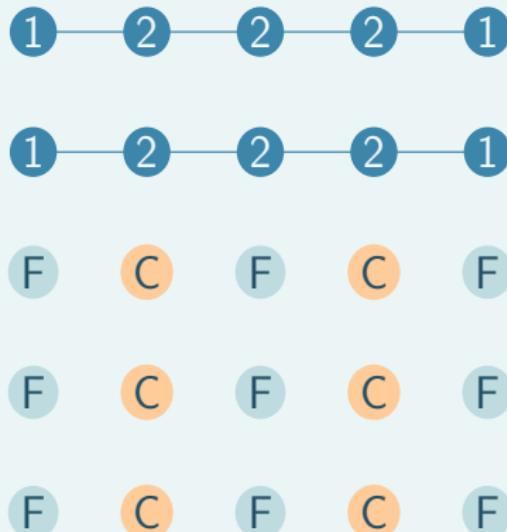
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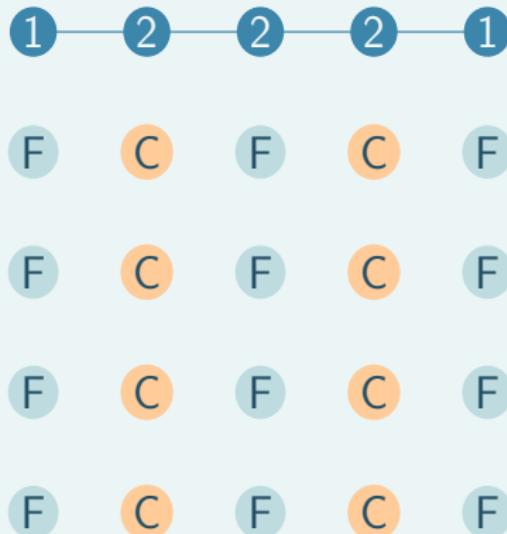
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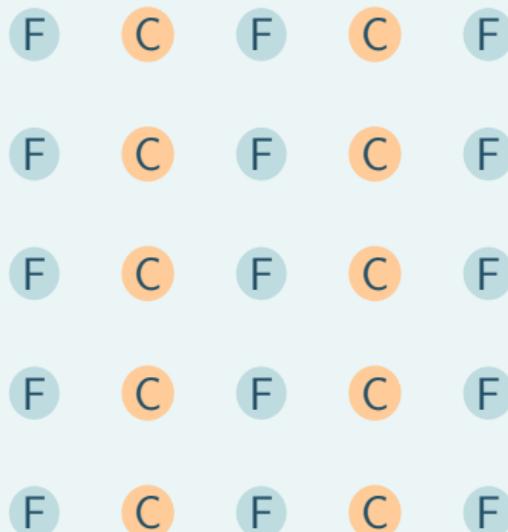
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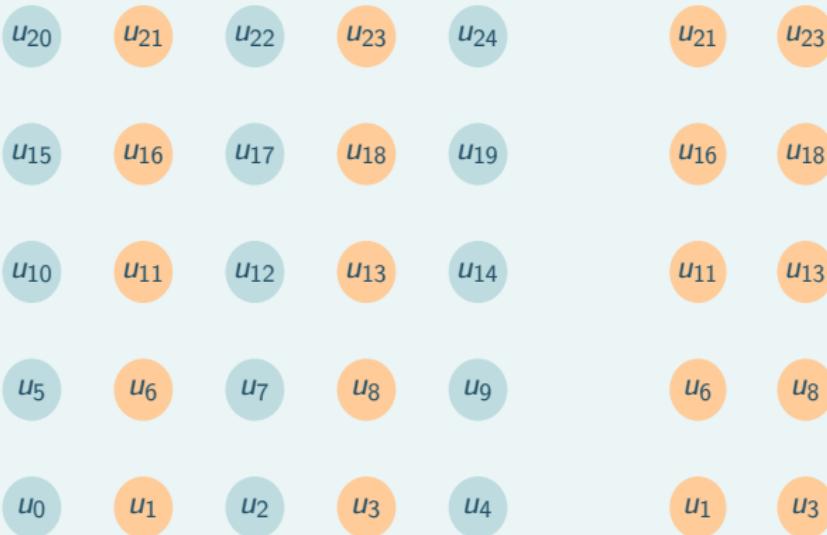
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Algebraic Coarsening



Algebraic Interpolation

- Weighted average of neighbouring coarse points.

Algebraic Interpolation

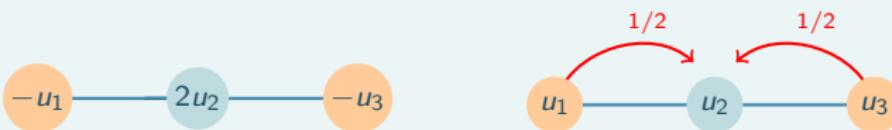
- Weighted average of neighbouring coarse points.
- For the previous problem,

$$u_2 = \left(\frac{a_{21}}{a_{21} + a_{23}} \right) u_1 + \left(\frac{a_{23}}{a_{21} + a_{23}} \right) u_3 = \frac{1}{2} u_1 + \frac{1}{2} u_3.$$

Algebraic Interpolation

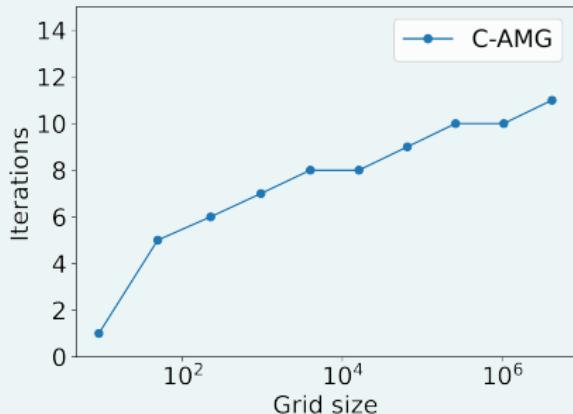
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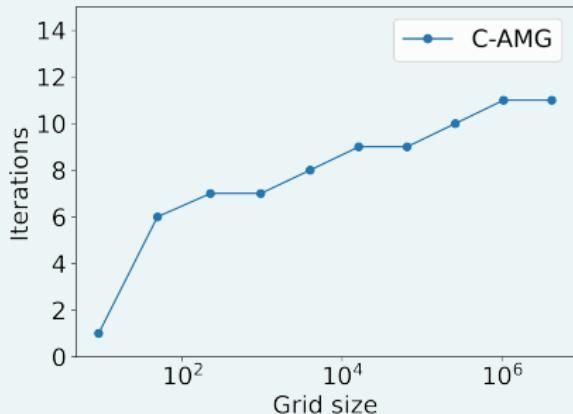


RECOVERED LOCAL LINEAR INTERPOLATION

C-AMG Performance on Diffusion



Isotropic diffusion:
 $A = -u_{xx} - u_{yy}$



Anisotropic in y diffusion:
 $A = -0.00001u_{xx} - u_{yy}$

Problem

- Nine-point stencil
discretization on a 5×5 grid:

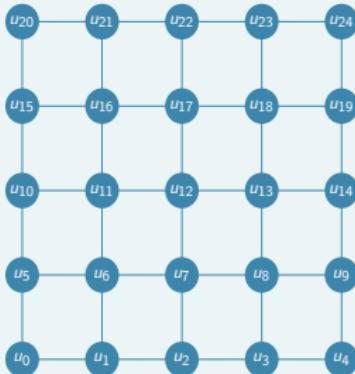
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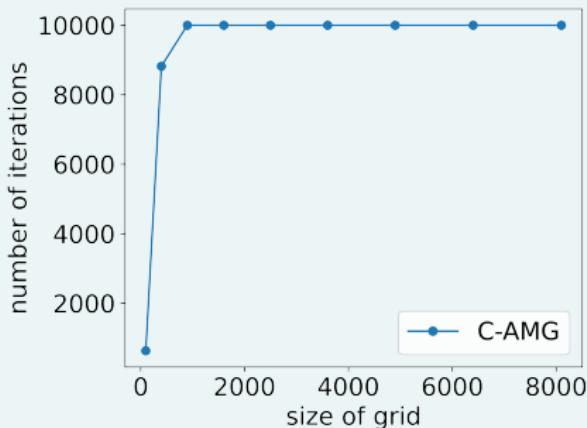


Problem

Standard solving techniques break down for this problem.

COGENT Proxy Problem

$$-au_{xx} - bu_{yy} + acu_{yyxx} = g, \quad b, c \gg a$$



Preliminaries: Total Reduction

- Can write $Au = f$ as equivalent system:

$$\begin{pmatrix} A_{FF} & A_{FC} \\ A_{CF} & A_{CC} \end{pmatrix} \begin{pmatrix} u|_f \\ u|_c \end{pmatrix} = \begin{pmatrix} f|_f \\ f|_c \end{pmatrix}$$

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- For $S = \begin{pmatrix} I_F \\ 0 \end{pmatrix}$,

$$I - A^{-1}A = \underbrace{\left(I - P_* \left(P_*^T A P_* \right)^{-1} P_*^T A \right)}_{\text{coarse-grid correction}} \underbrace{\left(I - S \left(S^T A S \right)^{-1} S^T A \right)}_{F\text{-relaxation}}.$$

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- Want multigrid method with this error propagation.

F-Relaxation

- Use

$$\widetilde{M^{-1}} := S(S^T A S)^{-1} S^T = \begin{pmatrix} A_{FF}^{-1} & 0 \\ 0 & 0 \end{pmatrix}.$$

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- Update is

$$u^{(k+1)} = u^{(k)} + \widetilde{M^{-1}} r^{(k)}$$

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- Update is

$$u^{(k+1)} = u^{(k)} + \widetilde{M^{-1}} r^{(k)}$$

- Error propagation is

$$E_F := I - \widetilde{M^{-1}} A = I - S \left(S^T A S \right)^{-1} S^T A.$$

Coarse Grid Correction

- From multigrid,

$$P_*^T A P_* e_c = P_*^T r \implies e_c = (P_*^T A P_*)^{-1} A e_k.$$

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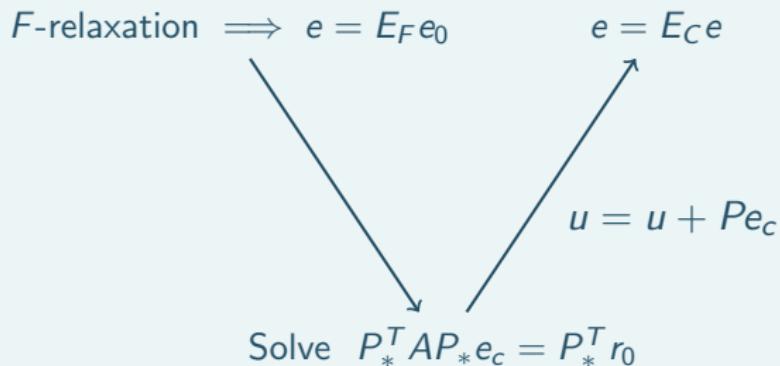
- Then

$$u_{k+1} = u_k + P_* e_c.$$

- Can derive

$$E_C := I - P_* (P_*^T A P_*)^{-1} P_*^T A.$$

Multigrid Reduction



- Exact two-grid method.

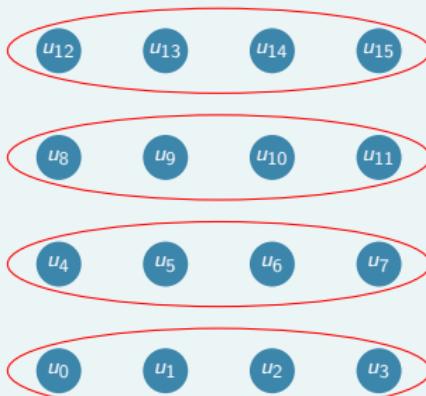
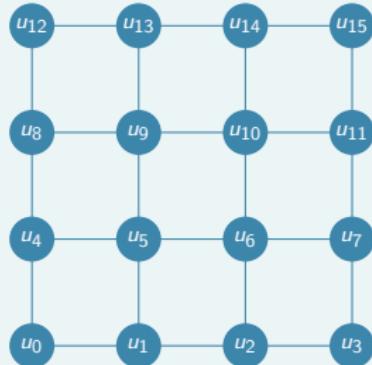
- $e = E_C E_F e_0 = 0$

Solving Fourth Order Term

- First focus on fourth order term.
- We will take multigrid reduction approach.
 - 1 Approximate coarse grid correction
 - 2 Approximate F -relaxation.

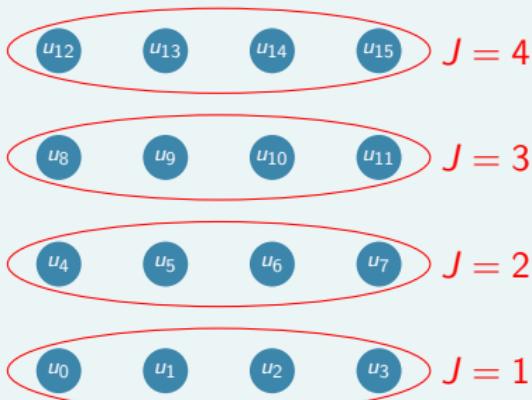
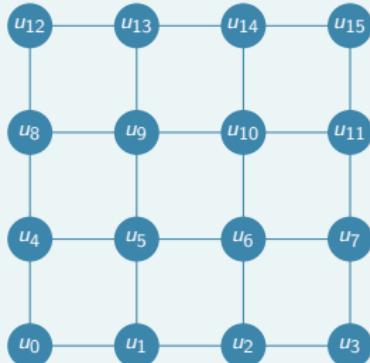
Line Relaxation

- Partition grid into lines.



Line Relaxation

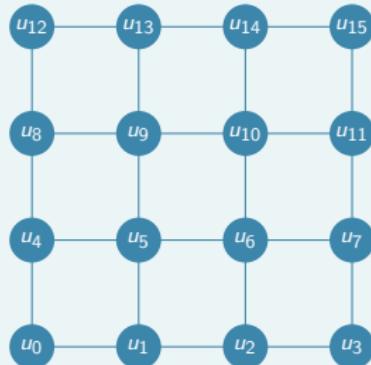
- Partition grid into lines.



- Let J be the J th line.

Line Relaxation

- Partition grid into lines.



- Let J be the J th line.
- Solve each line exactly.

Line Relaxation

- For $J = 1$.

$$A_{J,J} u_J = \begin{bmatrix} 4 & -2 & & \\ -2 & 4 & -2 & \\ & -2 & 4 & -2 \\ & & -2 & 4 \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \end{bmatrix} = f_J - A_{J,J+1} u_{J+1}$$

- Systems are tridiagonal - can be solved in $O(n)$.

Line Relaxation

- Why do we do this?

Line Relaxation

- Why do we do this?
- Can smooth oscillatory near-kernel components.

Line Relaxation

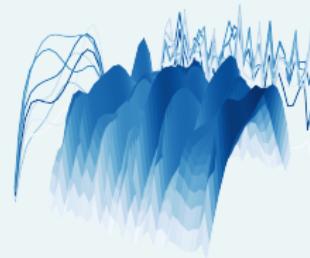
- Why do we do this?
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pointwise



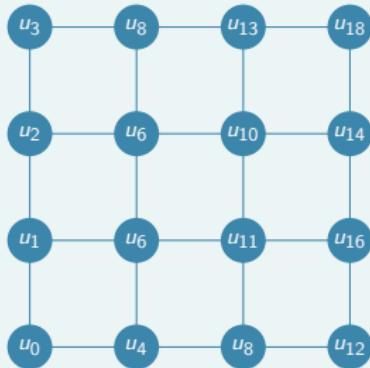
x -line



y -line

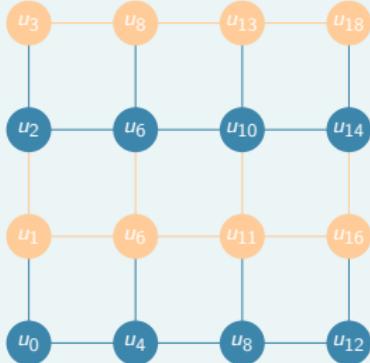
Picking Coarse Points

- Still need to partition points into C/F points



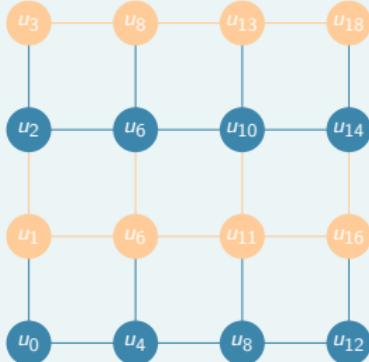
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Picking Coarse Points

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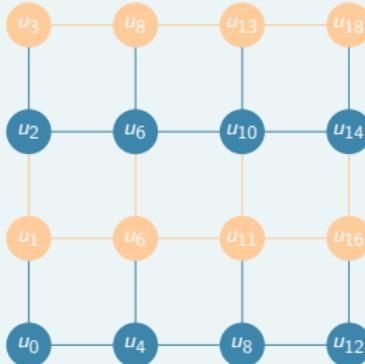


Picking Coarse Points

- Still need to partition points into C/F points
- Choose C -points to be lines in direction opposite relaxation.
- Pick F -lines to be independent
 - F -line relaxation becomes exact.

$$A_{FF}^{-1} = \begin{bmatrix} A_{22}^{-1} & 0 \\ 0 & A_{44}^{-1} \end{bmatrix}$$

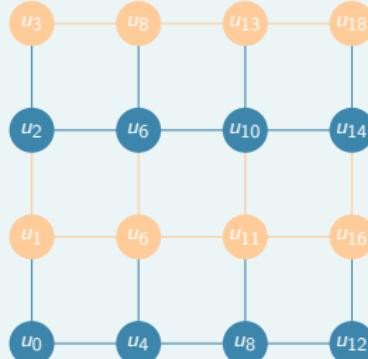
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Picking Coarse Points

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- Can solve in parallel.
- Solve C -lines then F -lines

Important Equation

$$e_J = -A_{J,J}^{-1} A_{J,J-1} e_{J-1} - A_{J,J}^{-1} A_{J,J+1} e_{J+1}$$

Ideal Interpolation

Important Equation

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$$u_{xxyy} \sim \begin{bmatrix} 1 & -2 & 1 \\ -2 & 4 & -2 \\ 1 & -2 & 1 \end{bmatrix}$$

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- Therefore,

$$e_J = \frac{1}{2} e_{J-1} + \frac{1}{2} e_{J+1}.$$

Ideal Interpolation

Important Equation

$$e_J = -A_{J,J}^{-1} A_{J-1,J} e_{J-1} - A_{J,J}^{-1} A_{J+1,J} e_{J+1}$$

- Similarly,

$$u_{xxyy} \sim \begin{bmatrix} 1 & -2 & 1 \\ -2 & 4 & -2 \\ 1 & -2 & 1 \end{bmatrix}$$

- Once again

$$A_{J-1,J} = -\frac{1}{2} A_{J,J} = A_{J+1,J},$$

and

$$e_J = \frac{1}{2} e_{J-1} + \frac{1}{2} e_{J+1}.$$

Ideal Interpolation Cont.

- As a matrix,

$$P = \begin{bmatrix} 1/2 & 1 & 1/2 \end{bmatrix}_c \iff e_J = \frac{1}{2}e_{J-1} + \frac{1}{2}e_{J+1}.$$

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- Note $P^T AP \sim \frac{1}{2}A$.
 - Can use same P on each level.
 - Exact coarse grid correction on every level.
 - Should take 1 iteration for n -level solve.

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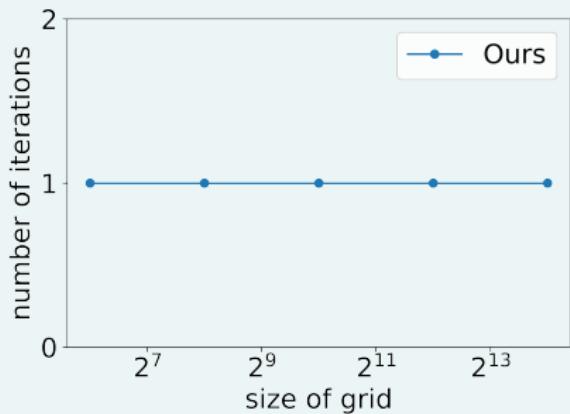
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 - Exact coarse grid correction on every level.
 - Should take 1 iteration for n -level solve.

- Have exact method for fourth order term!



Solving Fourth Order Term

- First focus on fourth order term.
- We will take multigrid reduction approach.
 - 1 Approximate coarse grid correction
 - Semi-coarsen
 - 2pt ideal interpolation
 - 2 Approximate F -relaxation.
 - C/F Line relaxation.

Solving Fourth Order Term

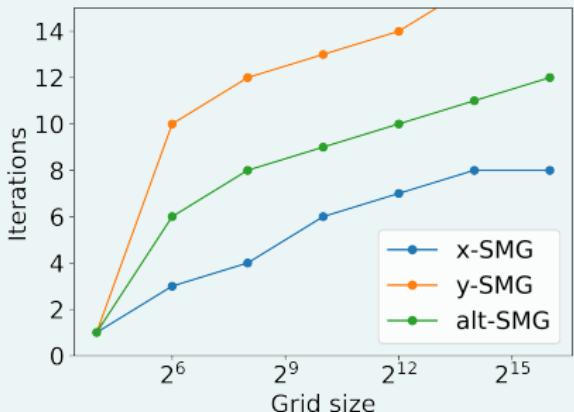
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 - 1 Approximate coarse grid correction
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 - C/F Line relaxation.
- Now we must deal with diffusion term.

Dealing with Diffusion

COGENT Problem

$$-au_{xx} - bu_{yy} + acu_{yyxx} = g, \quad b, c \gg a$$

- Have both diffusion and fourth order term.
 - Showed method is exact for fourth order term.
- Do not have exact coarse-grid correction with diffusion.
- Differences will become more extreme in 3D.



$$-u_{xx} - \epsilon u_{yy} = 0$$

Dealing with Diffusion

- Diffusion term $A = -\epsilon u_{xx} - u_{yy}$ has stencil

$$A \sim \begin{bmatrix} 0 & -1 & 0 \\ -\epsilon & 2 + 2\epsilon & -\epsilon \\ 0 & -1 & 0 \end{bmatrix}.$$

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- In general, if $A = -au_{xx} - bu_{yy}$
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 - Semi coarsen in $x \implies a = (1/2)a$.
 - Semi coarsen in $y \implies b = (1/2)b$.
- Alternate semi-coarsening $\implies A \rightarrow$ isotropic.

Motivation

- Consider $A = -\epsilon u_{xx} - u_{yy}$ for $\epsilon = 1 \times 10^{-3}$.

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- Consider $A = -\epsilon u_{xx} - u_{yy}$ for $\epsilon = 1 \times 10^{-3}$.
- Semi-coarsen in y 20 times then

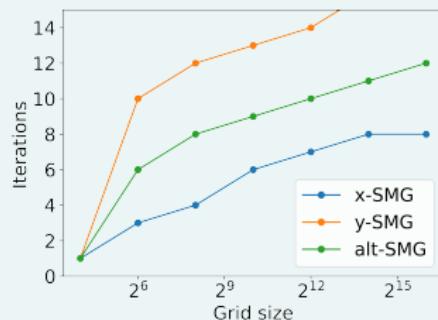
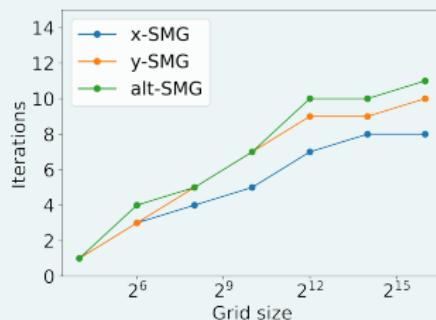
$$A^{(20)} \approx -u_{xx} - \epsilon u_{yy}$$

Motivation

- Consider $A = -\epsilon u_{xx} - u_{yy}$ for $\epsilon = 1 \times 10^{-3}$.
- Semi-coarsen in y 20 times then

$$A^{(20)} \approx -u_{xx} - \epsilon u_{yy}$$

- Do not want to semi-coarsen in y for this system



- Differences is amplified for approximate line solve.

Dealing with Diffusion

What we need

- Need to semi-coarsen in right direction when strongly anisotropic.
- Need to alternate to converge to isotropy.

Dealing with Diffusion

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-
- To do this, we use “smart” coarsening
 - 1 Reconstruct a and b .
 - 2 Coarsen according to the following:

$$\begin{cases} \text{Coarsen in } x, & \text{if } a \geq b \\ \text{Coarsen in } y, & \text{otherwise} \end{cases}$$

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Dealing with Diffusion

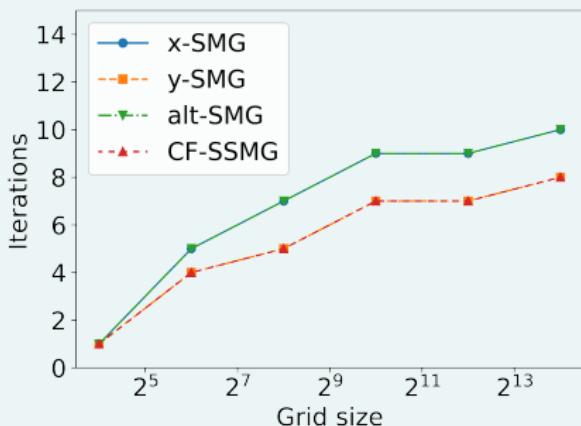
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- Ensures diffusion term is isotropic.
- Correctly coarsens in the case of strong anisotropy.

Semi-Coarsening Comparison

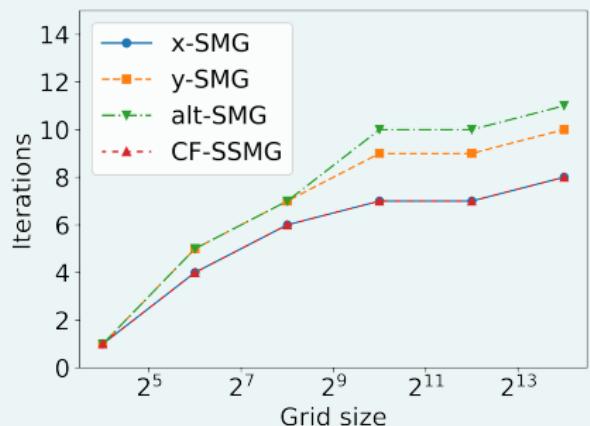
- Anisotropic in y diffusion:

$$A = -\epsilon u_{xx} - u_{yy}$$



- Anisotropic in x diffusion:

$$A = -u_{xx} - \epsilon u_{yy}$$

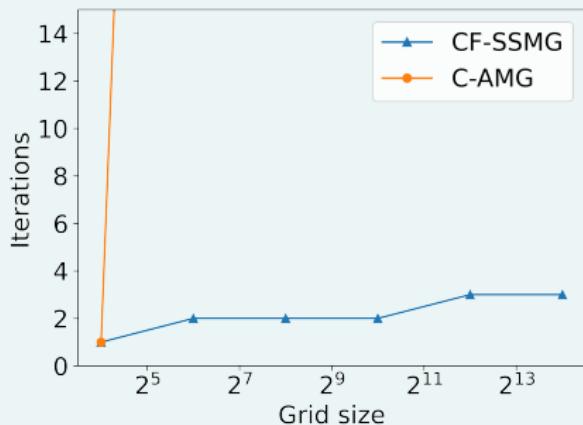


Results

Comparing our algorithm (CF-SSMG) against the prior state of the art algorithm (C-AMG).

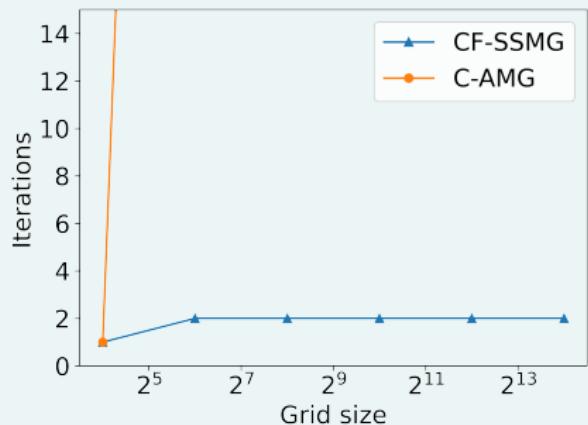
- Fourth Order Term:

$$-\epsilon u_{xx} - \epsilon u_{yy} + u_{yyxx} = 0$$



- COGENT Problem:

$$-0.0003u_{xx} - 2u_{yy} + 2u_{yyxx} = 0$$



QUESTIONS?