SAND2019-14998C

Algebraic Multigrid for Highly Convective Flow Simulations

Ray Tuminaro
Center for Computing Research
Sandia National Laboratories

L. Berger-Vergiat, C. Siefert @ Sandia,
M. Brazell@NREL,
D. Mavriplis @ U. of Wyoming

Dec 2019

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Outline

- Multigrid background for solving

$$A\,u = f$$

ideal setting → *more complex situations*

(stability of coarse operators)

- Non-symmetric smoothed aggregation (NSA) & polynomials
  - Error expressions & stability
  - Model problem results
- Piecewise constant grid transfers & mass stabilization
  - Algorithmically simpler
  - Hypersonic problems in Sandia's SPARC code

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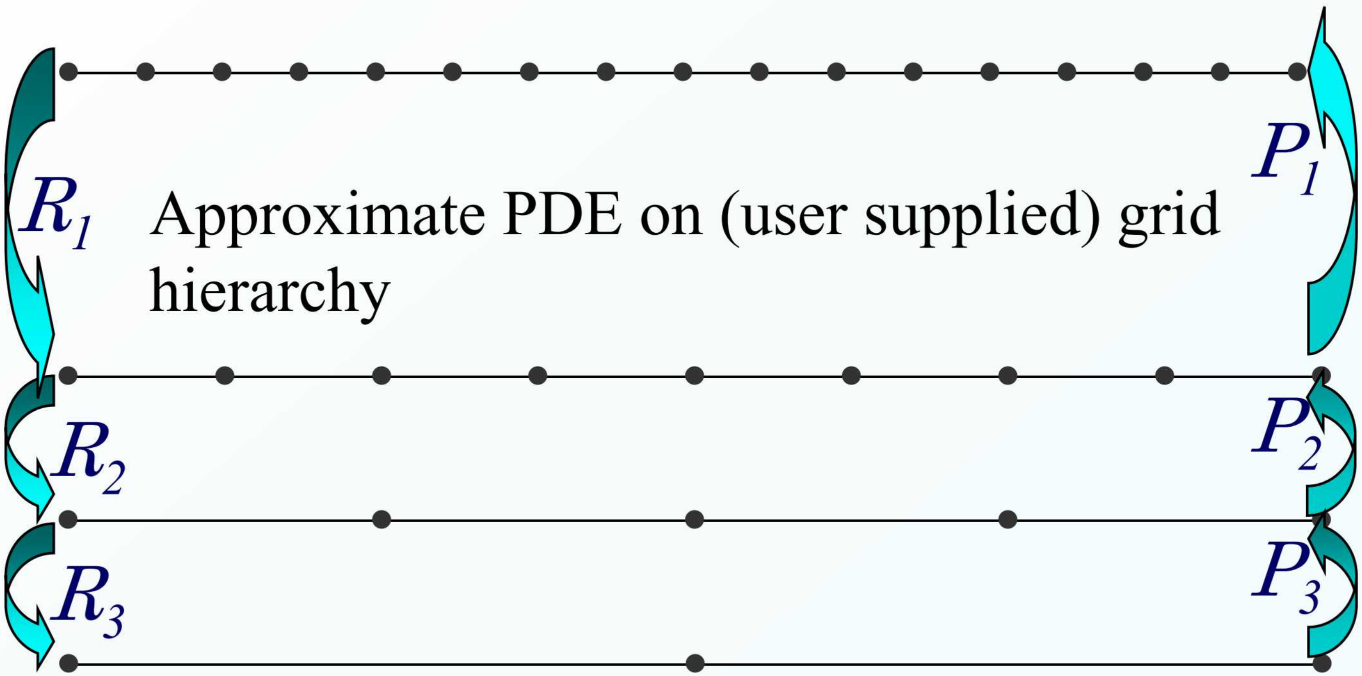
Geometric Multigrid



Approximate PDE on (user supplied) grid hierarchy

Solve

$A_0 \, u_0 = f_0 \quad S_0$

$A_1 \, u_1 = f_1 \quad S_1$

$A_2 \, u_2 = f_2 \quad S_2$

$A_3 \, u_3 = f_3 \quad S_3$

Develop <u>smoothers</u> (approximate solve on a level)

Jacobi, Gauss-Seidel, CG, etc.

Develop grid transfers (e.g. linear interpolation)

Use coarse A_k's to accelerate convergence for A_0

Algebraic Multigrid (AMG) for $A = A^T$

- Given A_0, automatically build remaining MG operators:

$$A_k\,, P_k\,, R_k\,, S_k\text{'s}$$

- Once P_k's are defined, the rest follows "easily":
  - $R_k = P_k^{\,T}$
  - $A_{k+1} = R_{k+1} A_k P_{k+1}$ (Galerkin coarsening)

•No need to supply mesh hierarchy!

•Divorces application a bit from MG development!

•Greater code reuse!

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Algebraic MG behavior

- High & low frequencies not available algebraically.
- These notions are replaced with $\| \, . \, \|_{A_k}$ or $\| \, . \, \|_{A_k^2}$

  - $\| e_k \|_{A_k}$ or $\| e_k \|_{A_k^2}$ small $\Rightarrow$ low frequency
  - $\| e_k \|_{A_k}$ or $\| e_k \|_{A_k^2}$ large $\Rightarrow$ high frequency

- <u>Properties of AMG methods</u>

  – S_k smooths errors with high energy ($\| e_k \|_{A_k}$ large).
  – P_k must accurately interpolate low energy errors (small $\| e_k \|_{A_k}$).
  – P_k must interpolate errors not damped by smoothing.

- Note: $||v||_A = \sqrt{v^T A v}$

A 2-level convergence result

Assume

$$\|S_0\, e_0\|_{A_0}^2 \;\leq \|\, e_0\|_{A_0}^2 \; - \alpha\|\, e_0\|_{A_0^2}^2$$

(Jacobi & Gauss Seidel satisfy this for certain SPD matrices)

and

$$\min_{e_1}\|\; e_0 - P_1 e_1\;\|_2^2 \leq \beta\|e_0\|_{A_0}^2$$

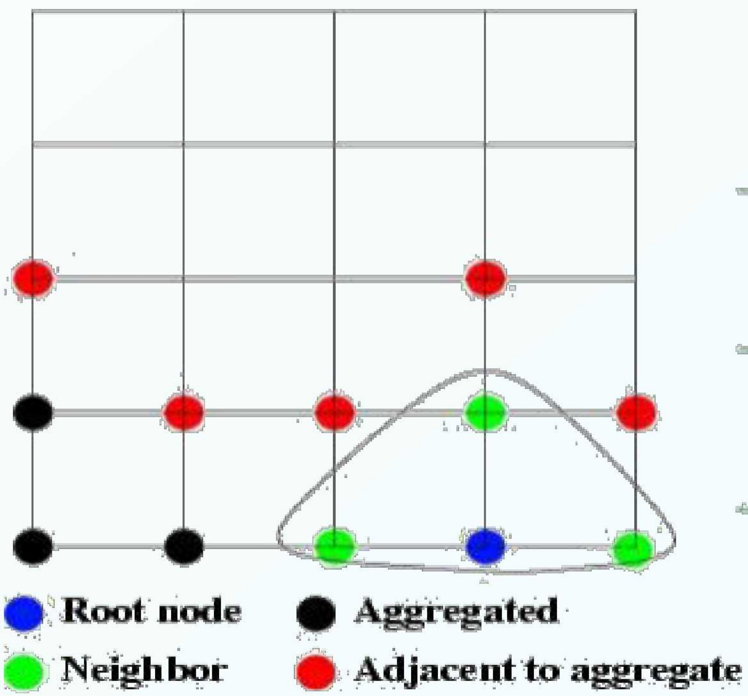
Then, 2-level MG (ST) satisfies the following independent of mesh

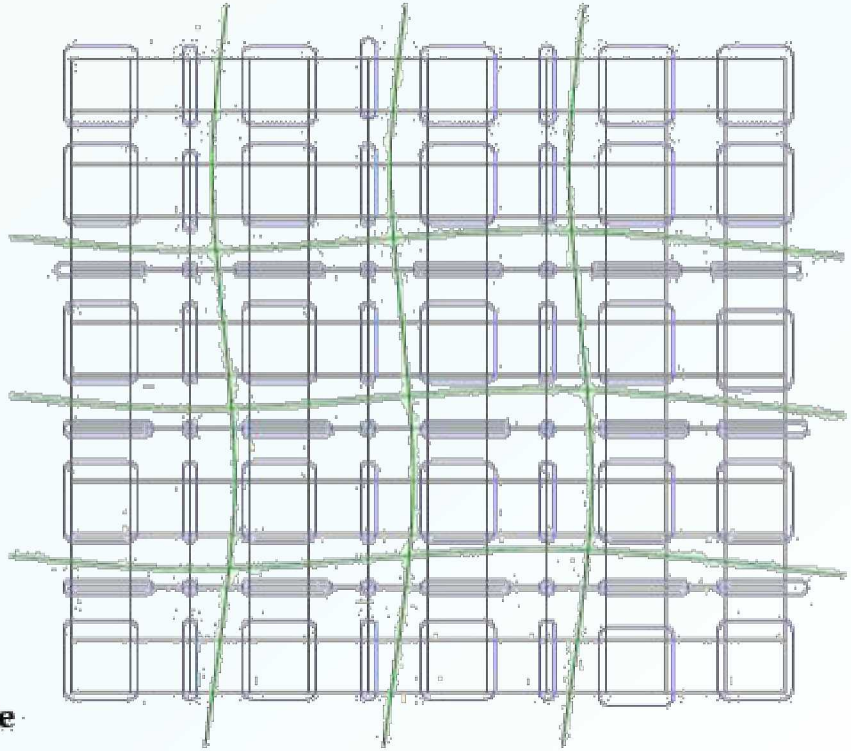
$$\|S_0\, T\|_{A_0} \leq \sqrt{1 - \frac{\alpha}{\beta}}$$

e_0 is fine grid error, e_1 is coarse grid error, S_0 is smoother , T is coarse grid correction operator.

Smoothed Aggregation AMG: P_k

- Coarsen graph of A_k
  - Graph based algorithms
  - Aggregation lumps nodes together
- Compute P_k's coefficients
  - Capture constant
  - Minimize some A-norm type quantity.





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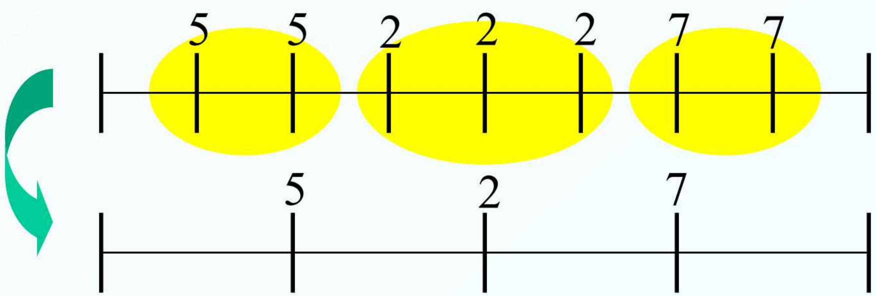
Smoothed Aggregation: P_k coefficients

Finding P_k



- **Build <u>tentative</u> ^tP_k to interpolate constant**

  – **where** $^tP_k(i,j) = \begin{cases} 1 & \text{if } i^{th} \text{ point within } j^{th} \text{ aggregate} \\ 0 & \text{otherwise} \end{cases}$

♦ Smoothed aggregation

+ Improves ^tP_k with Jacobi's method: $P_k = (I - \omega_{k-1}\, diag(A_{k-1})^{-1} A_{k-1})\, {}^tP_k$
+ P_k emphasizes what is not smoothed by Jacobi
+ $R_k = (P_k)^T$

<u>Seek to adapt smoothed aggregation to highly convective systems</u>

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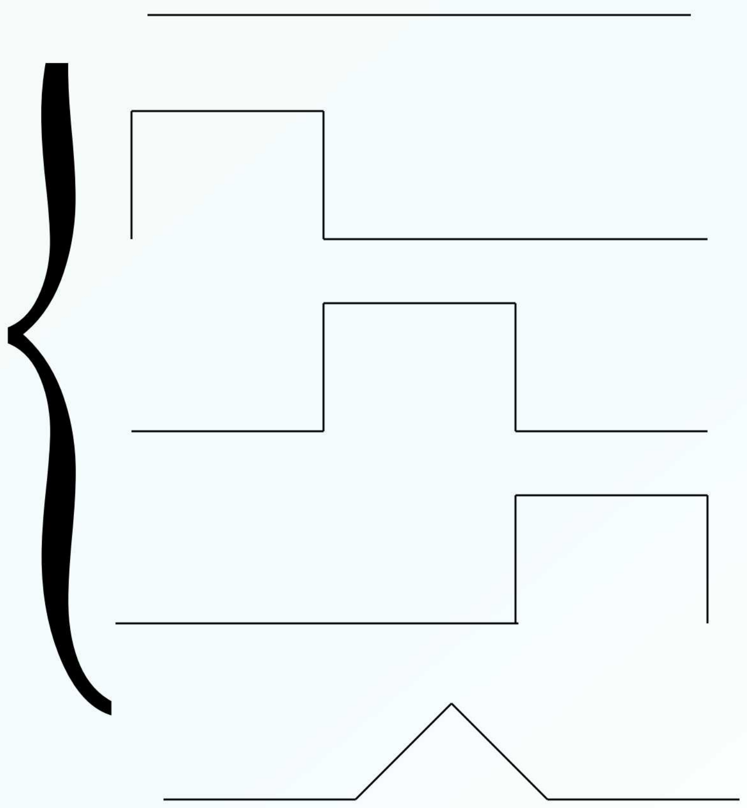
Smoothed Aggregation

• take constant

• split into local basis functions

• smooth basis functions



What can go wrong?

- Lots of things, but we'll focus on

- Simple smoothers (Jacobi & Gauss-Seidel) may not smooth all high frequency errors

- A_k's ($A_k = R_k A_{k-1} P_k$, $k > 0$) are not guaranteed to be stable even if A_0 is stable, especially in non-symmetric case

  e.g., linear interpolation for P_k with $R_k = P_k^T$ often leads to unstable A_k's for highly convective flows

Seek to adapt smoothed aggregation to highly convective systems

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Coarse Grid Stability & Piecewise Constant Transfers (PCT)

PCT considered relatively *safe*

A_0 (fine level discretization) is M-matrix + PCT's $\Rightarrow$

A_k (coarse discretizations) are M-matrices

However, consider $\rho(x)u_x = f$

with stencil $\left[-\frac{1.1}{h} \;\; \frac{1}{h} \;\; \frac{.1}{h}\right]\rho(x)$ and mesh space *h*.

Then

$$11\rho(x_i) = \rho(x_i + 26h) \quad \Rightarrow \quad A_{i,i-1} = -A_{i+26,i+27}$$

where i^{th} row corresponds to x_i. Then, aggregating *i* to *i+26* gives

$$\left[-\frac{1.1}{h} \;\; 0 \;\; \frac{1.1}{h}\right]\rho(x)$$

$\Rightarrow$ unstable ☹

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AMG error expressions

Mg(A_k, u_k, b_k, k)

~~$u_k \leftarrow S_k(A_k, u_k, b_k)$~~

if not coarsest,

$r_k \leftarrow b_k - A_k u_k$

$u_{k+1} \leftarrow 0$

Mg($R_{k+1} A_k P_{k+1}$, u_{k+1}, $R_k r_k$, $k+1$)

$u_k \leftarrow u_k + P_{k+1} u_{k+1}$

end

$u_k \leftarrow S_k(A_k, u_k, b_k)$

<u>Assumptions</u>

1) $u_0 \leftarrow S_0(A_0, u_0, b_0)$

is $u_0 \leftarrow u_0 + \widehat{\omega}_0 D_0^{-1}(b_0 - A_0 u_0)$

2) $u_k \leftarrow S_k(A_k, u_k, b_k)$, $k > 0$

is $u_k \leftarrow u_k + \widehat{\omega}_k (b_k - A_k u_k)$

3) post smoothing only

Resulting multilevel error propagation

$$e_0^{(j+1)} = \prod_{k=0}^{L-1} (I - \widehat{\omega}_k \, \bar{P}_k \bar{R}_k D_0^{-1} A_0)^{m_k} \;\; e_0^{(j)}$$

- m_k is # of Jacobi/Richardson sweeps on level k
- L is # of MG levels
- $P_0 = R_0 = \mathrm{I}$, $\bar{P}_k = P_0 P_1 \ldots P_k$, $\bar{R}_k = R_k \ldots R_2 \tilde{R}_1 R_0$

Consider

$P_k = {}^t P_k$ (piecewise constant)

$R_1 = \Lambda_1 P_1^T D_0^{-1}$

$R_k = \Lambda_k P_k^T$ *for* $k > 1$

and Λ_k is diag such that $\Lambda_k P_k^T$ rows sums are *1*

Then, $\bar{P}_k \bar{R}_k$ is just an aggregate weighted average. When aggregates are equi-sized, it's just simple averages

piecewise constants $\Longrightarrow$ scaled piecewise constant R_k's

$$e_0^{(j+1)} = \prod_{k=0}^{L-1} \left(I - \widehat{\omega}_k \underbrace{\bar{P}_k \bar{R}_k}_{\text{averages}} D_0^{-1} A_0\right)^{m_k} e_0^{(j)}$$

$$P_k = {}^{t}P_k$$

$$R_1 = \Lambda_1 P_1^T D_0^{-1}$$

Note: $A_1 = \Lambda_1 \left[{}^{t}P_k \right]^T (D_0^{-1} A_0)\ {}^{t}P_k$

$$R_k = \Lambda_k P_k^T \quad \textit{for } k > 1$$

and Λ_k force $\Lambda_k P_k^T$ rows sums to be *1*

For L-level cycle with 1 relax. sweep per level has L $D_0^{-1} A_0$'s. If $\bar{P}_k \bar{R}_k = I$, this would imply a V cycle $\approx L$ Jacobi sweeps

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A new non-symmetric Smoothed Aggregation Algorithm

<u>*k > 1*</u>

$$P_1 = (I - \omega_0 D_0^{-1} A_0)\ {}^tP_1 \qquad P_k = (I - \omega_{k-1} A_{k-1})\ {}^tP_k$$

$$R_1 = \Lambda_1 \left({}^tP_1 \right)^T D_0^{-1} (I - \omega_0\, A_0 D_0^{-1}) \qquad R_k = \Lambda_k \left({}^tP_k \right)^T (I - \omega_k\, A_k)$$

$$= \Lambda_1 \left({}^tP_1 \right)^T (I - \omega_0\, D_0^{-1} A_0) D_0^{-1}$$

so

$$R_k \neq P_k^T$$

and

$$A_1 = \Lambda_1 \left({}^tP_1 \right)^T \underbrace{(I - \omega_0\, D_0^{-1} A_0) D_0^{-1} A_0\, (I - \omega_0 D_0^{-1} A_0)}_{\text{polynomial in } D_0^{-1} A_0}\ {}^tP_1$$

Expressions get messy …

Smoothed Aggregation

Expressions get messy, but …

$$A_{k+1} = \bar{R}_{k+1}\, q_{k+1}()\, \bar{P}_{k+1} \qquad k \geq 0$$

piecewise constants

scaled piecewise constants

with $q_0(D_0^{-1}A_0) = D_0^{-1}A_0$

$$q_{k+1}(\;.\;) = q_k()\big(\, I - \omega_k \underbrace{\bar{P}_{k+1}\bar{R}_{k+1}}_{\text{averages}}\, q_k()\;\big)^2$$

$\Rightarrow$ A multigrid iteration can be fully expressed as $D_0^{-1}A_0$ FINE grid operators & averaging

For a L level Vcycle with 1 relax. sweep per level

\# of $D_0^{-1}A_0$ $= 1 + 3 + \ldots 3^{L-1} = (3^L - 1)/2$

Non-sym Smoothed Agg (NSA) summary

$D_k^{-1} A_k$ expression includes 3^k $D_0^{-1} A_0$ operators

For a (m+1)-level NSA Vcycle with 1 relax. sweep per level

of $D_0^{-1} A_0 = 1 + 3 + \ldots 3^{m-1} = (3^m - 1)/2$

For a m-level PCT Vcycle with 1 relax. sweep per level, # of $D_0^{-1} A_0 = m$

A_k not necessarily even close to diagonally dominate

Choosing ω's is problematic for highly non-symmetric problems

BIG ASSUMPTION: Jacobi with proper ω converges

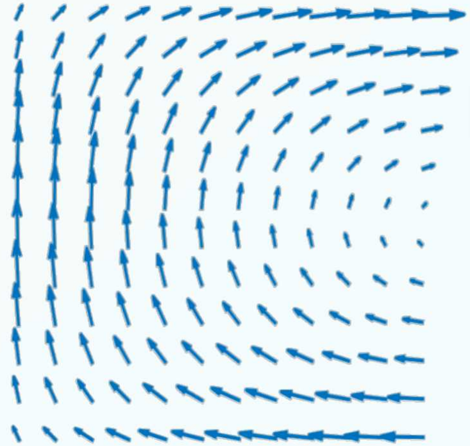
No convergence guarantee, but this is hard for non-symmetric systems.

D_0 can be blkDiag(A_0) for PDE systems

Algorithm somewhat similar but different than Sala & T, SISC'2008

Results: Bent Pipe

$$-\epsilon\,\Delta u + \boldsymbol{b}\cdot\nabla u = f \text{ in } (0,1)\times(0,1)$$



$u = 0$ on left, top, bottom BCs

$u = y - .5$ on right BC

$$\boldsymbol{b} = \begin{pmatrix} -2\,x\,(1 - .5\,x) \\ -4\,y\,(y-1)(1-x) \end{pmatrix}$$

$\epsilon = .1 \;\; for \sqrt{(x-.5)^2 + (y-.5)^2}$, otherwise $\epsilon = .001$

iters (levels)

upwind

Mesh	1 Level	PCT	NSA
81 x 81	492	116 (3)	88 (3)
243 x 243	1000+	212 (4)	94 (4)
729 x 729	1000+	391 (5)	113 (5)

nasty

$\frac{1}{8}\left[-\frac{5}{h} \quad \frac{2}{h} \quad \frac{3}{h}\right]$

Mesh	1 Level	PCT	NSA
81 x 81	688	171 (3)	173 (3)
243 x 243	1000+	236 (4)	130 (4)
729 x 729	1000+	416 (5)	130 (5)

GMRES* + MGV(0,1 ω Jacobi)
$\omega \approx 1/\rho(D^{-1}A)$

Stop when residual reduction of 10^{-8}

*no restarts

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Results (with same solver options)

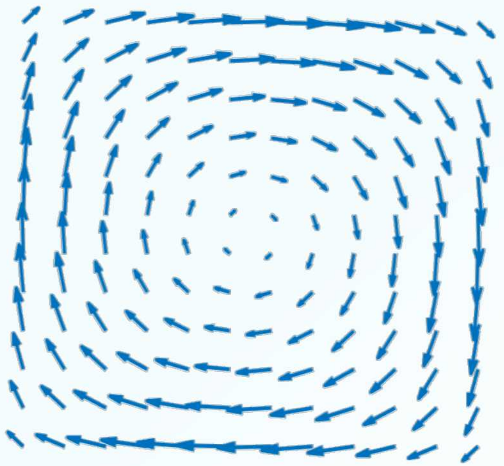
recirculating

$$-\epsilon\, \Delta u + \boldsymbol{b} \cdot \nabla u = f \text{ in } (0,1) \times (0,1) \qquad \boldsymbol{b} = \begin{pmatrix} 4\,x\,(x-1)(1-2y) \\ -4\,y\,(y-1)(1-2x) \end{pmatrix}$$

ϵ & BCs as bent pipe

upwind

Mesh	1 Level	PCT	NSA
81 x 81	1000+	154 (3)	111 (3)
243 x 243	1000+	261 (4)	113 (4)
729 x 729	1000+	440 (5)	121 (5)



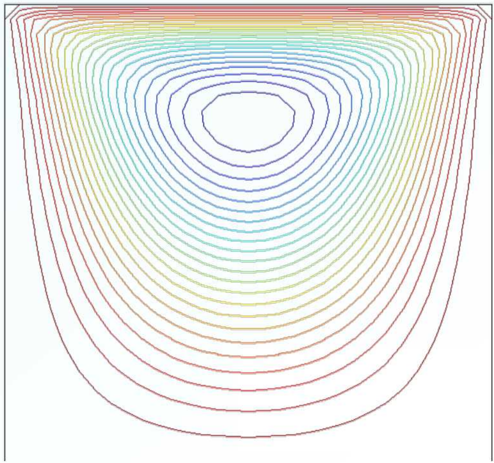
PCT its / NSA its

(1,1) block of **lid driven cavity** incomp. NS via IFISS

using W cycle

(last Picard solve)

Mesh	Re 100	Re 500	Re 1000
33 x 33	37 / 24	64 / 57	92/ 87
65 x 65	54 / 24	91 / 61	117 / 115
129 x 129	70 / 23	117/ 44	146 / 115
257 x 257	119 / 26	198 / 42	249 / 68



Compressible Navier-Stokes

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}_i(\mathbf{U})}{\partial x_i} - \frac{\partial \mathbf{G}_i(\mathbf{U})}{\partial x_i} = \mathbf{0} \qquad (1)$$

with

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho v_j \\ \rho E \end{pmatrix}, \ \mathbf{F}_i(\mathbf{U}) = \begin{pmatrix} \rho v_i \\ \rho v_i v_j + P\delta_{ij} \\ \rho E v_i + P v_i \end{pmatrix} \text{ and } \mathbf{G}_i(\mathbf{U}) = \begin{pmatrix} 0 \\ \tau_{ij} \\ \tau_{ij} v_j - q_i \end{pmatrix} \qquad (2)$$

where ρ is the fluid density, v is the fluid velocity and E the fluid energy per unit of mass which is expressed as $E = \frac{1}{2} v_i v_i + e$ the sum of the kinetic and internal energy e. P is the fluid pressure, τ_{ij} is the viscous stress tensor. $q_i = -\kappa \frac{\partial T}{\partial x_i}$ is the heat flux, T the temperature and κ the thermal conductivity of the gas.

focused on Newtonian fluid & ideal gases, though SPARC also employs non-ideal gas models

Sparc Details

- Only steady-state considered in this talk
- Sparc uses a conservative cell-centered control volume discretization, 7 point stencil (actually 7 block), upwind-ish

for t = 0, …

    Take adaptive pseudo-time step

        1 Step of Newton's method

            Solve 1st order Jacobian approximation system inexactly

- Non-linear residual uses 2nd order Jacobian

- Basic idea: small pseudo-steps needed initially for nonlinear convergence, try to aggressively advance to large pseudo-steps to accelerate to steady-state

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Mesh Structure

Hypersonic objects generate strong shock-waves leading to

- Strongly flow directi
- Low dissipation
- Hard to resolve

To help with thes esh

Recall the sleight of hand …

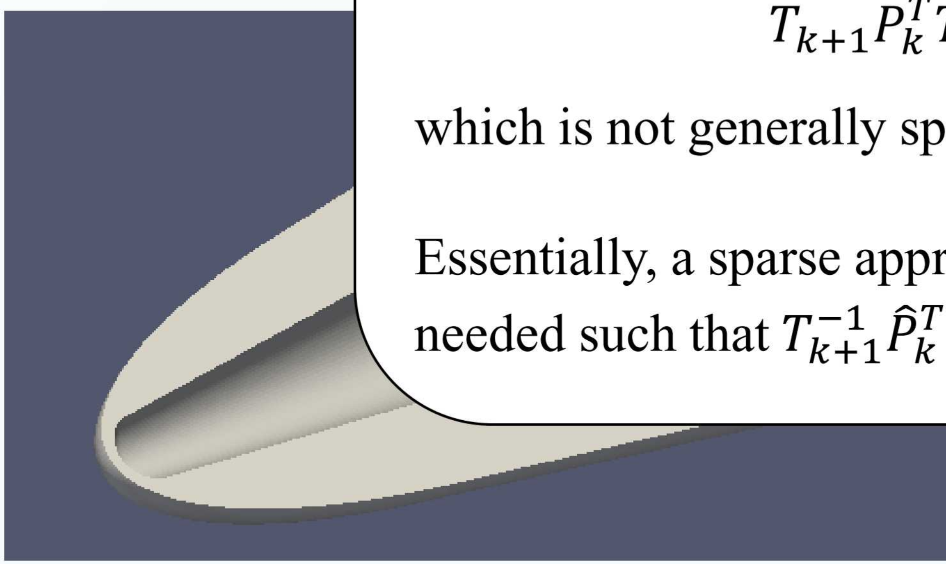
$$D_{k+1} P_k^T D_k^{-1}$$

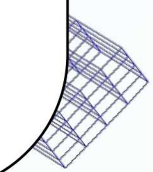
that now becomes

$$T_{k+1} P_k^T T_k^{-1}$$

which is not generally sparse.

Essentially, a sparse approximation to $\hat{P}_k^T$ is needed such that $T_{k+1}^{-1} \hat{P}_k^T \approx P_k^T T_k^{-1}$





Line-Jacobi is the method of choice for linear systems ☹

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Blunt Wedge Problem

Structured mesh: 72^3, 144^3 or 288^3 cells, 5 degrees of freedom per cell, supersonic input flow: Mach 3.
First attempt: use unstructured vs. structured aggregation, 1 sweep ILU(0) as pre-smoother, 4 levels, coarsening rate: 3 per direction.

Mesh size	72^3	144^3	288^3
Unstructured	46	87	N/C
Structured	36	88	256

Table: Number of linear iterations (tol=1e-6)

Observations:

1. linear interpolation with structured aggregation diverges
2. three and four level methods give same convergence
3. no scaling for either structured/unstructured methods

One representative linear system toward the latter part of the simulation with large δt

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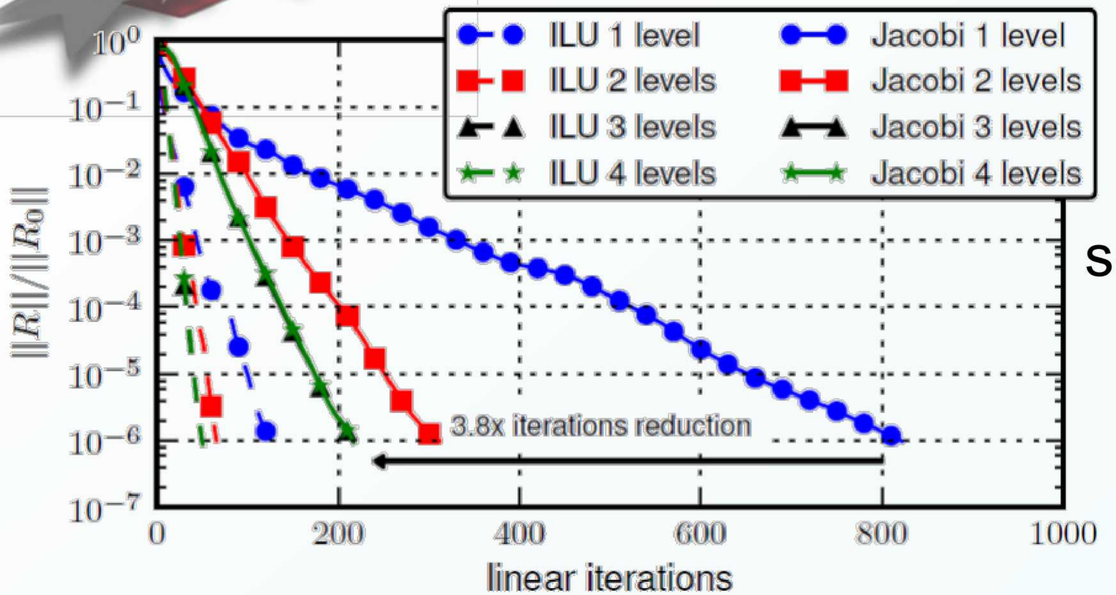
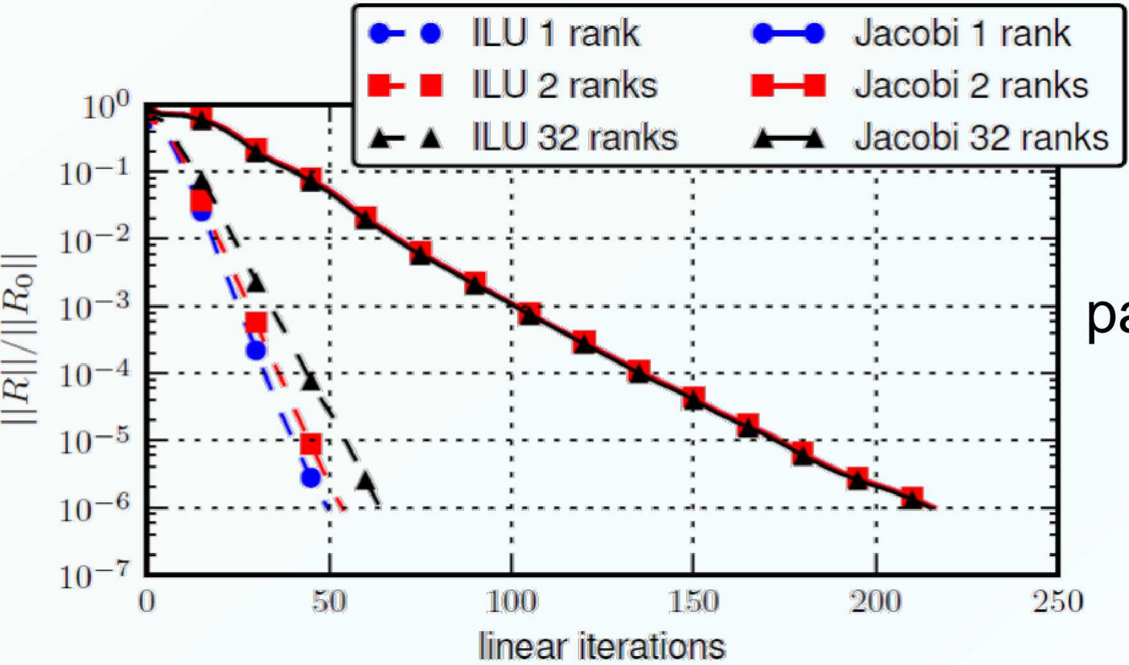
Line-Jacobi vs. ILU smoothing



serial



parallel

Overall good benefit with MG

Domain decomp. ILU takes fewer iterations in serial but scales less well in parallel

Note: Have successfully run NSA on aero-blunt wedge

Mass Stabilization

- Add diagonal term to coarse grid operator

$$A_{k+1} = R_k A_k P_k + (\alpha-1) R_k M_k P_k$$

where M_k's are projected mass matrices

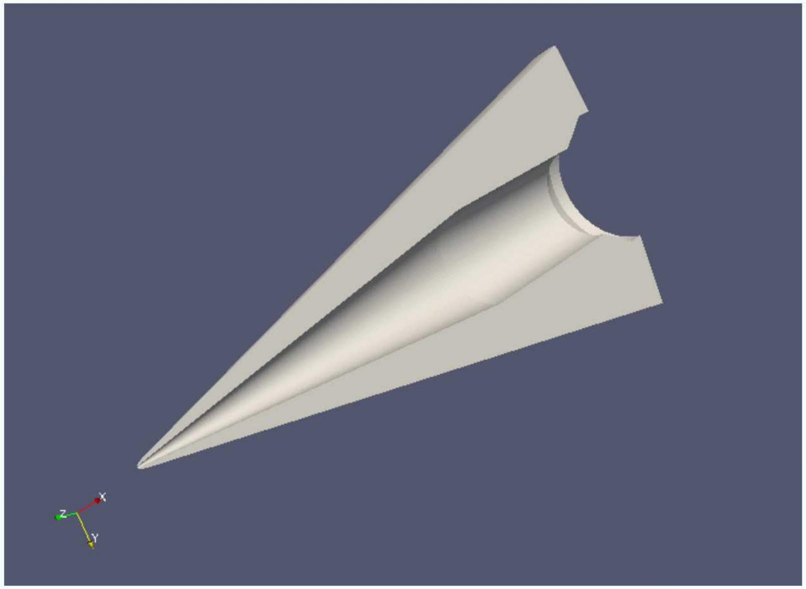
	Unstructured			Structured		
α	72^3	144^3	288^3	72^3	144^3	288^3
1	46	87	N/C	36	88	256
2	45	86	N/C	35	82	205
4	45	87	N/C	34	75	97
6	46	89	N/C	35	74	86
8	46	92	N/C	36	77	83
10	48	95	N/C	37	81	85

Observations

- helpful with structured coarsening
- optimal α at bottom of U

α is parameterized in terms of a CFL number provided by the user

Hifire + SA turbulence model



6 dofs per node

L3 $\approx$13 M dofs

L2 $\approx$106 M dofs

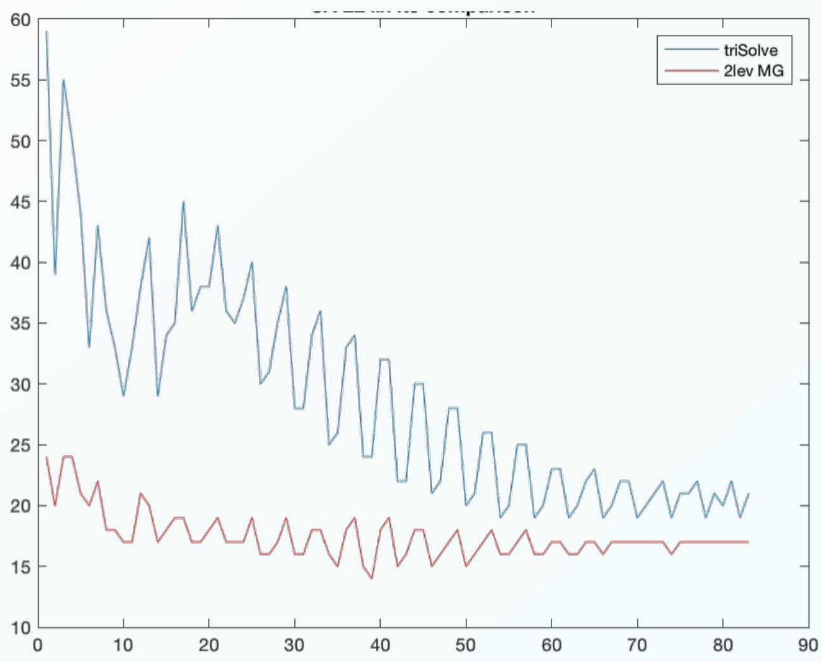
L1 $\approx$856 M dofs

L0 $\approx$6.8 B dofs

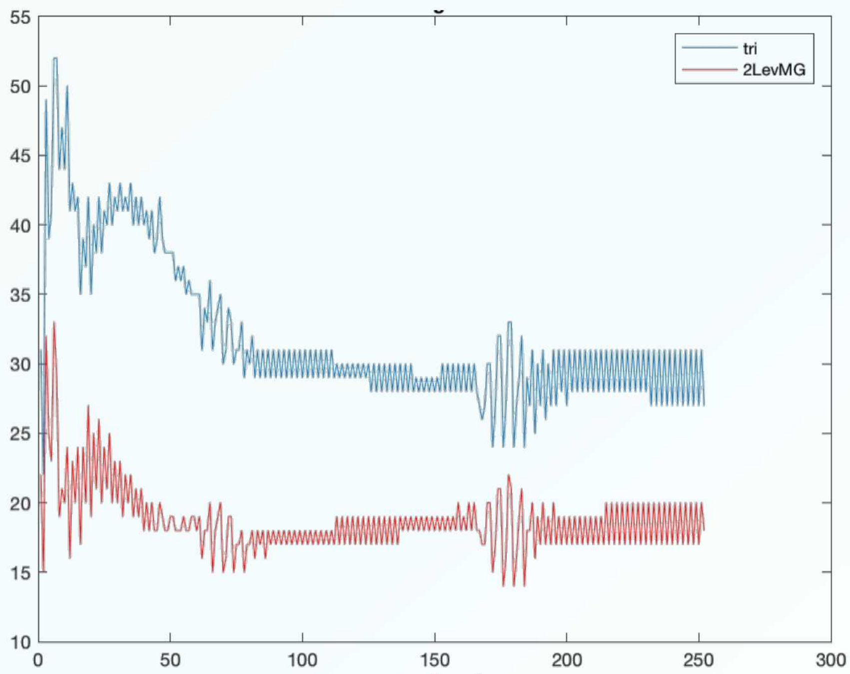
- Lots of nonlinear convergence problems

2 level results

iterations over different linear solves (1 level in blue, 2 level in red)



L2



L1

A sequence of linear solves with moderate time step

Nonlinear solver eventually stalls

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Conclusions

- Hypersonic problems are hard for multigrid

- NSA polynomial connection relevant for strong convection
  - Assumes (block) Jacobi method converges *reasonably*
  - MG iteration can be *equivalent* to fine Jacobi sweeps + averaging
  - NSA generally better than PCT on model problems

- SPARC hypersonic flow application introduces challenges
  - Stability often lost on coarse grid for PCT & NSA
  - An NSA variant can accelerate convergence over PCT for model problem
  - PCT can accelerate convergence on harder SPARC problems for large δt

    … but results are mixed due to stability issues
  - Line solve commuting needs to be worked out for NSA $T_{k+1}^{-1}\hat{P}_k^T \approx P_k^T T_k^{-1}$

Support provided by DOE ASCR program & NNSA ATDM program

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