SAND2019-7361D

Algebraic Multigrid for Hypersonic Simulations

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July 2019

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Outline

2 Tracks

- Nonsymmetric smoothed aggregation (NSA) & polynomials
  - Algorithmically interesting, but somewhat more academic
  - Model problem results

- Piecewise constant grid transfers & mass stabilization
  - Algorithmically simpler
  - Hypersonic problems in a realistic setting, Sandia's SPARC code on NGP platforms

NSA not completely ready for hard SPARC problems

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 $\left[-\frac{1.1}{h} \quad \frac{1}{h} \quad \frac{.1}{h}\right] \rho(x)$ 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

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

$\Rightarrow$ unstable ☹

Smoothed Aggregation Multigrid: a polynomial view

MGcycle(A,u,b)
  if not coarsest,
    r = b – A u
    $u_H = 0$
    MGcycle($\hat{R}A\hat{P}$, u_H, $\hat{R}$ r)
    u = u + $\hat{P}$ u_H
  end
  Smooth(A, u, b)

$$\hat{P}_0 = (I - \omega_0 D_0^{-1} A_0) P_0$$

$$\hat{R}_0 = \hat{P}_0^T$$

D : diag(A) or
BlkDiag(A) for PDE systems

ω_0 : damping parameter

P : piecewise constant interpolation

For this talk, smoother will be Jacobi or block Jacobi

For nonsymmetric version,

$$\hat{R}_0 = P_0^T (I - \omega_0 A_0 D_0^{-1}) \quad \Rightarrow \quad \hat{R}A\hat{P} = P_0^T (I - \omega_0 A_0 D_0^{-1}) A_0 (I - \omega_0 D_0^{-1} A_0) P_0$$

Smoothed Aggregation Details

$$\hat{P}_k = (I - \omega_k D_k^{-1} A_k) P_k$$

$$\hat{R}_k = D_{k+1} P_k^T D_k^{-1} (I - \omega_k A_k D_k^{-1})$$

Main *sleight of hand*

Define

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

$$q_{k+1}(.) = q_k() \; (I - \omega_k S_{k-1} \; q_k() \;)^2 \quad k > 0$$

D_{k+1} not *diag*(A_k) for $k > 0$

but we are free to choose it

with

$$S_{-1} = I, \quad S_k = P_{0:k} \; P_{k:0}^T \quad k > 0,$$

$$P_{0:k} = P_0 P_1 \ldots P_k, \quad P_{k:0}^T = P_k^T P_{k-1}^T \ldots P_0^T.$$

Then,

$$D_{k+1}^{-1} A_{k+1} = P_{k:0}^T \; q_{k+1}() \; P_{0:k}$$

⇒ A multigrid iteration can be fully expressed as $D_0^{-1} A_0$ operators on the FINE grid and S_k averaging … IF one does Jacobi smoothing on all levels

Non-sym Smoothed Agg (NSA) summary

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

For a m-level NSA Vcycle with 1 Jacobi 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 Jacobi 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 similar but different than Sala & T, SISC'2008

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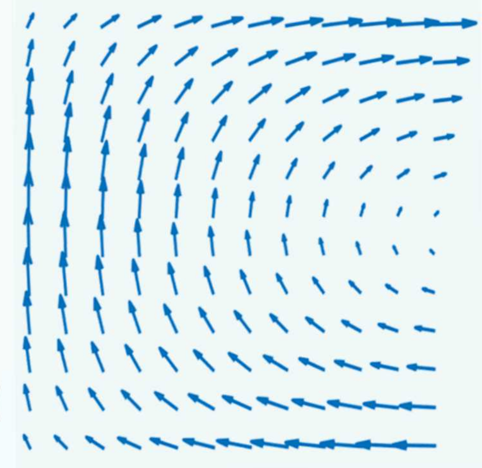
Results: Bent Pipe



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

$u = 0$ 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)

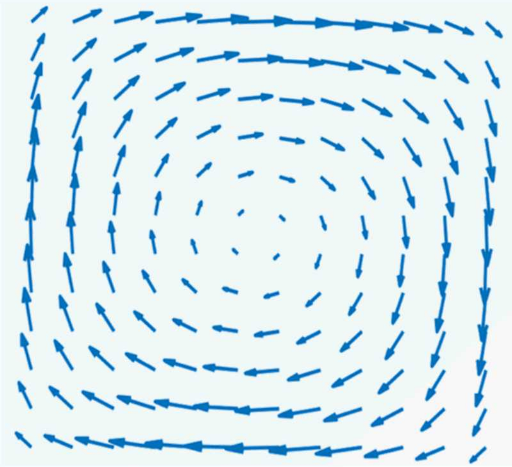
recirculating

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

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)

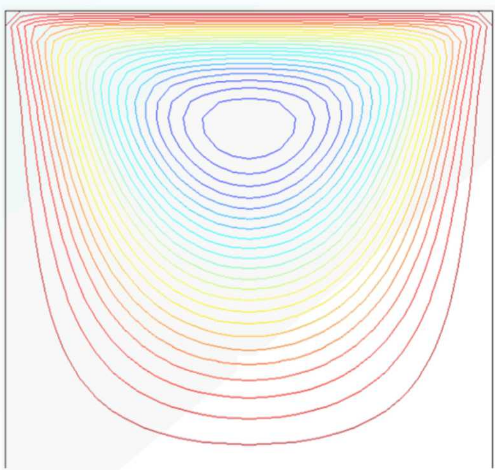


(1,1) block of **lid driven cavity** incomp. NS via IFISS

using W cycle

(last Newton solve)

Mesh	Re 100	500	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	115 /
257 x 257			



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

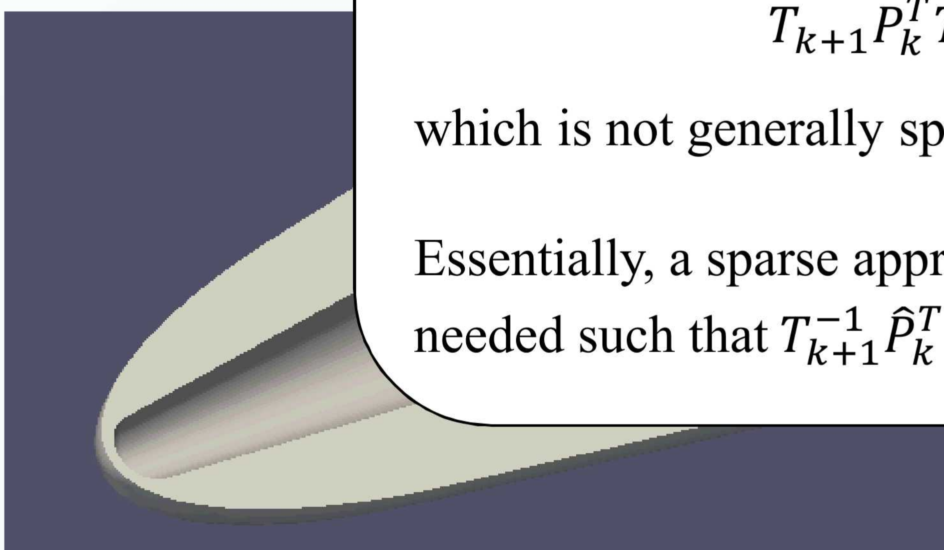
- Basic idea: small pseudo-steps needed initially for nonlinear convergence, try to aggressively advance to large pseudo-steps to accelerate to steady-state

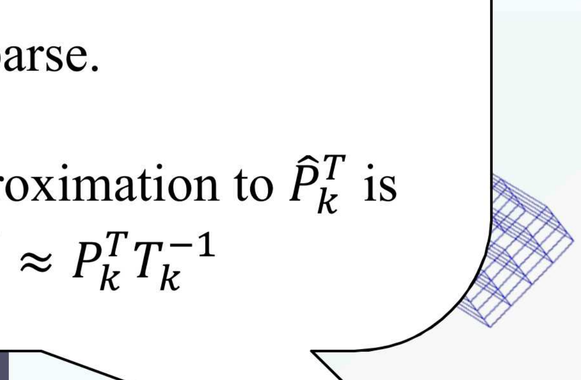
Mesh Structure

Hypersonic objects generate strong shock-waves leading to

- Strongly flow directio
- 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 ☹

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

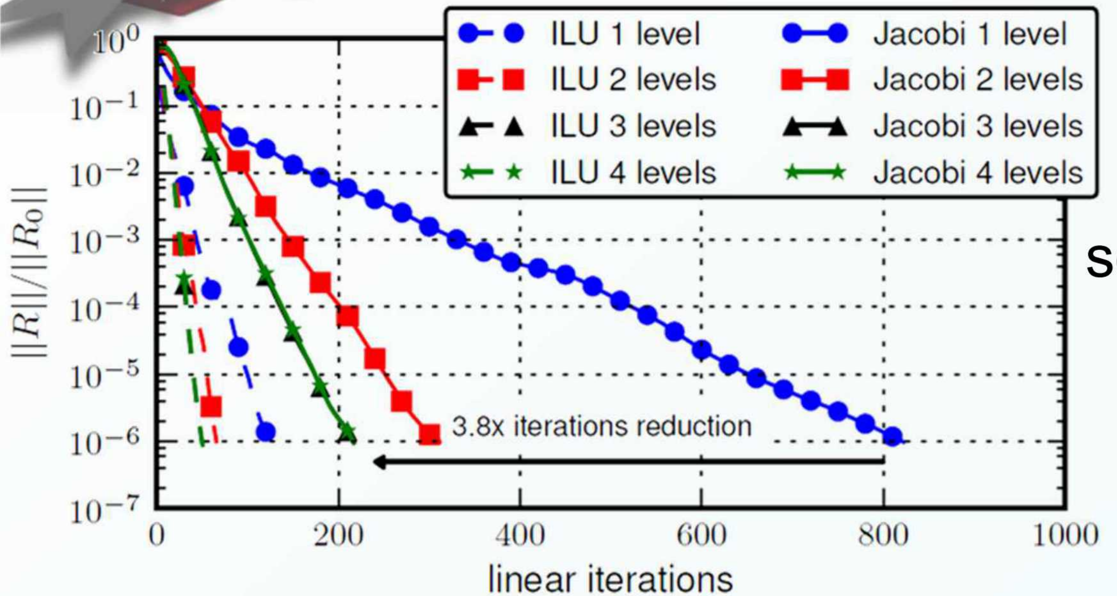
Table: Number of linear iterations (tol=1e-6)

Observations:

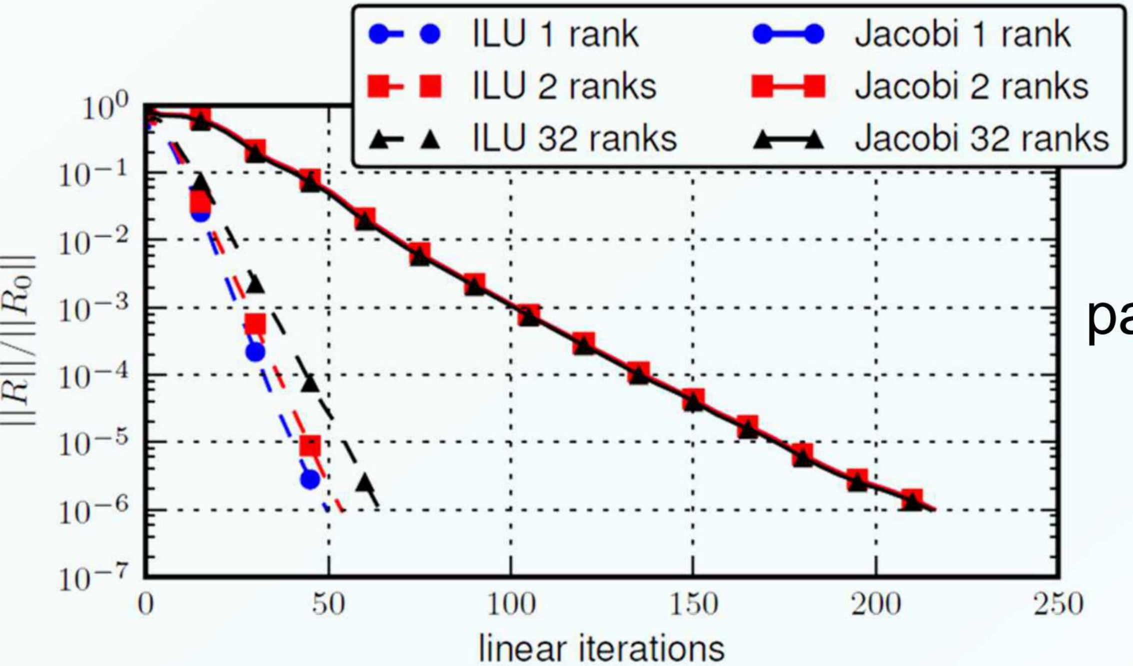
1. linear interpolation with structured aggregation diverges
2. three and four level methods give same convergence
3. no scaling for either structured/unstructured methods

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

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

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

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

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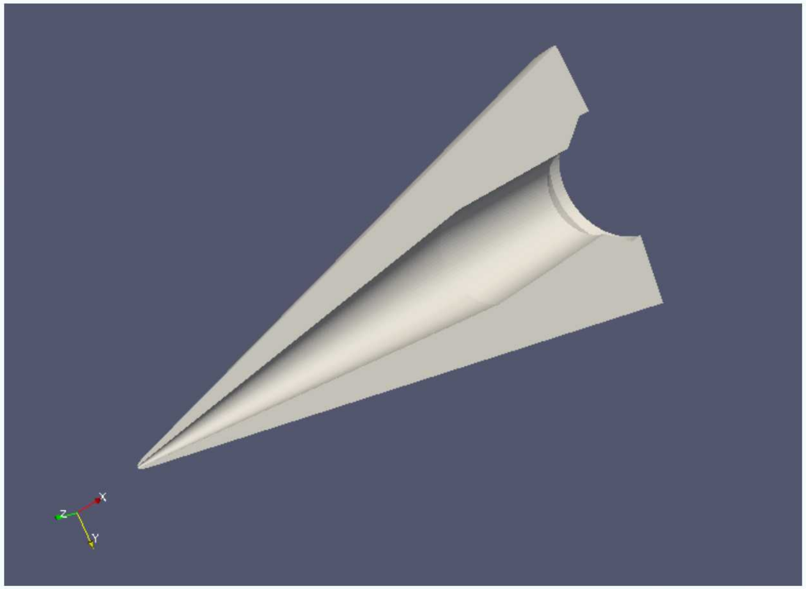
Hifire + SA turbulence model



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

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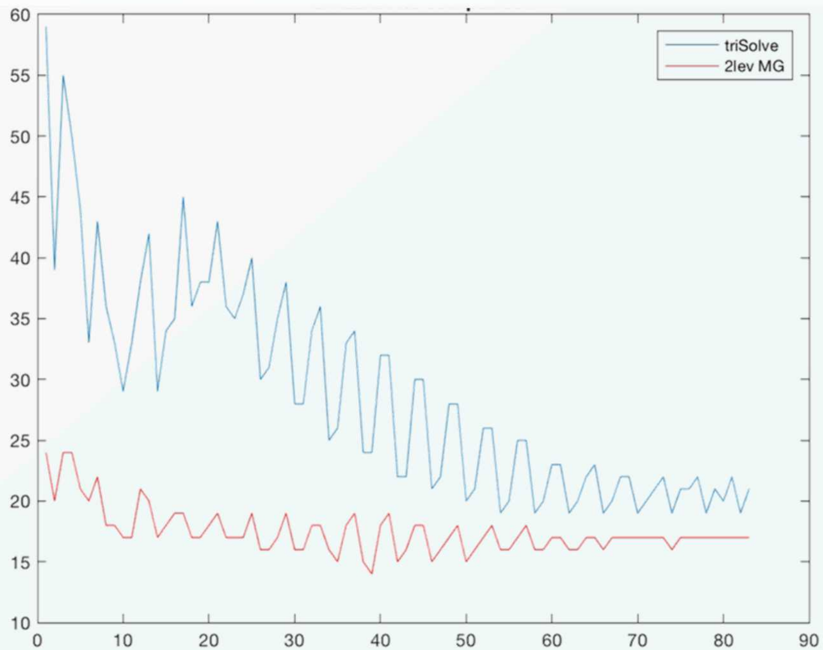
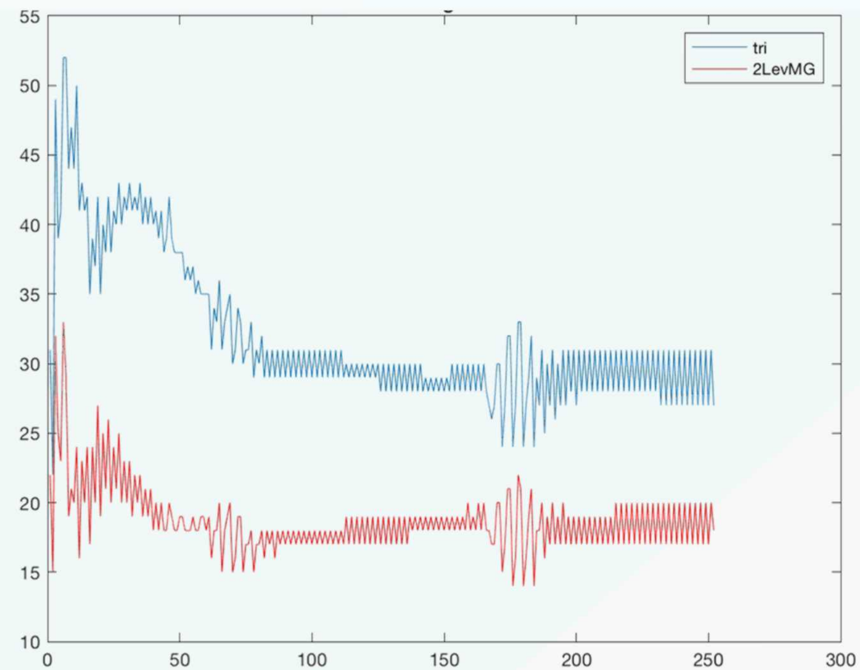
2 level results

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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