Advancing parabolic operators in thermodynamic MHD models: Explicit super time-stepping versus implicit schemes with Krylov solvers

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Slides available at: www.predsci.com/~caplanr/astro16





The problem

- Implicit schemes with Krylov solvers
- Explicit Super Time-stepping schemes
- The MAS thermodynamic MHD model
- Real-world test case and HPC setup
- Performance and scaling results
 Outlook



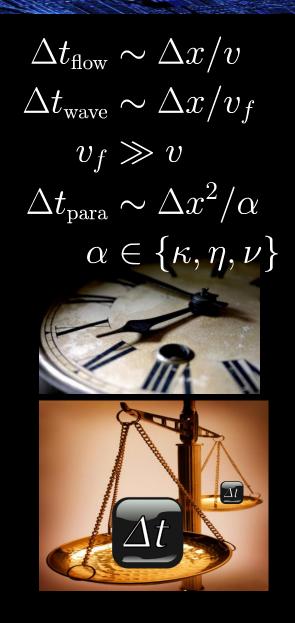
The Problem

- Thermodynamic MHD models have multiple time scales Ψ leading to vastly different explicit time-step stability requirements
- In order to make coronal simulations *tractable*, we need to Ψ exceed such explicit limits
- Focus on parabolic terms Ψ
 - Implicit methods (need iterative solvers) Ψ
 - Explicit methods with unconditional/extended stablility Ψ
 - Reformulation of the model (e.g. thermal waves) Ψ
- Here, we compare a super time-stepping method to an Ψ implicit method



Exceeding time scales!

NOTE! When exceeding explicit time-step limits, one must be very careful about accuracy. Using too large of a time step can result in large errors!



Method Comparison

Implicit Scheme with Krylov Solver



2nd-order Runge-Kutta Legendre scheme (RKL2) [Meyer et al, 2014]

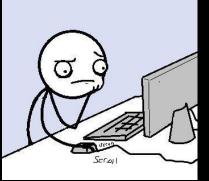
Backward-Euler solved with Proconditioned Conjugate Grad

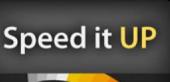
Preconditioned Conjugate Gradient (BE+PCG)

Comparison Criteria

- Basic validation of accuracy and stability
- Ease/difficulty of formulation and implementation
- Features and limitations
- Overall performance
 - Number of iterations needed for each large time-step
 - Computational cost per iteration
- Parallel performance
 - Parallel communication needed per iteration
 - How well does the method scale?

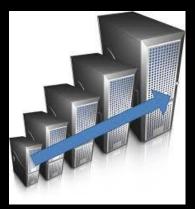












Implicit scheme with Krylov solvers: Backward Euler (BE)

Backward Euler (BE): simplest L-stable method Ψ

$$\frac{\partial u}{\partial t} = F(u, \mathbf{r}) \quad \Longrightarrow \quad \frac{u^{n+1} - u^n}{\Delta t} = \mathbf{M} \, u^{n-1} + \mathbf{M} \, u^{n-1} = \mathbf{M} \, u^{n-1} + \mathbf{M} \, u^{n-1} +$$

Applying BE to PDE yields a system of equations to solve Ψ

$$(1 - \Delta t \mathbf{M}) u^{n+1} = u^n$$
 $\mathbf{M} = y$

To avoid the need for nonlinear solvers, we linearize any nonlinear terms Ψ with lagged diffusivity, e.g.

$$\nabla \cdot \left[\kappa(T^{n+1}) \nabla T^{n+1}\right] \quad \blacksquare \quad \nabla \cdot \left[\kappa(T^n) \nabla T^n\right]$$







Implicit scheme with Krylov solvers: PCG

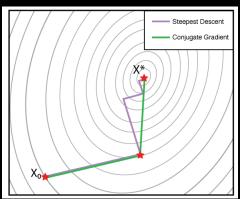
- For operators yielding large sparse matrices, Krylov subspace methods are popular
- For linear symmetric (and nearly-symmetric) matrices: Conjugate Gradient
- Preconditioned Conjugate Gradient: Apply an approximate inverse of the matrix to "precondition" the problem so it will converge more quickly
- Need to balance cost of preconditioner with its reduction in iterations







Aleksey Krylov





Implicit scheme with Krylov solvers: Preconditioners

- We use two preconditioning options: Ψ
 - PC1: Point-Jacobi / Diagonal scaling (DIAG) Cheap, but not very effective... Communication free

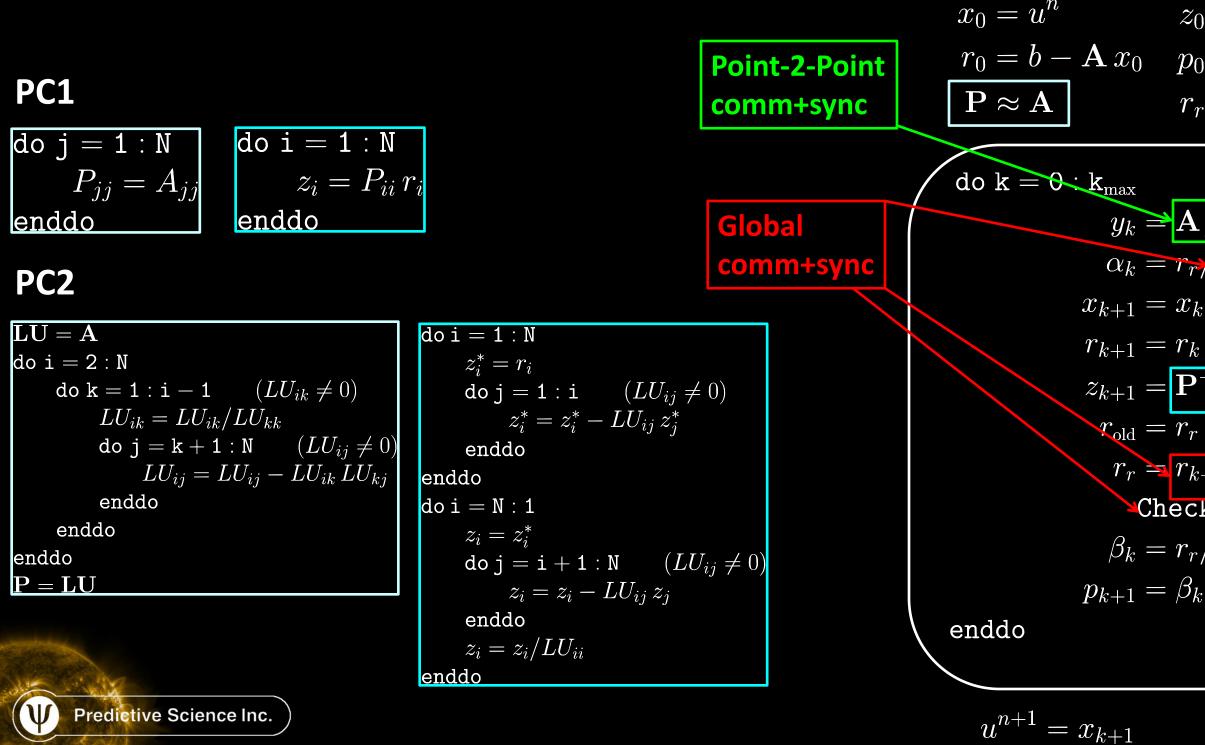
with zero-fill incomplete LU factorization (NDD+ILU0) Expensive, but much more effective! Communication free

Drawback: $N_{\text{processors}} \rightarrow N_{\text{grid}} \longrightarrow \text{PC2} \rightarrow \text{PC1}$

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Implicit scheme with Krylov solvers: PCG



$$egin{aligned} & \mathbf{P}^{-1} \, r_0 \ & \mathbf{p}_0 &= z_0 \ & \mathbf{r}_r &= r_0 \cdot z_0 \end{aligned}$$

$$\begin{array}{c} \mathbf{A} \ p_k \ \mathbf{x} \ \mathbf{y}_k \end{pmatrix} \\ \mathbf{x} \ \mathbf{y}_k + \alpha_k \ p_k \ \mathbf{x} + \alpha_k \ y_k \end{pmatrix} \\ \mathbf{x}_k - \alpha_k \ y_k \ \mathbf{y}_k - \mathbf{x}_k \ \mathbf{y}_k \end{pmatrix}$$

 $r_r = r_{k+1} \cdot z_{k+1}$

Check r_r for convergence

$$r_r/r_{
m old} \ B_k\,p_k+z_k$$

Implicit scheme with Krylov solvers: BE+PCG



- Robust, proven method
- ✓ Can be very efficient
- Pre-made libraries available for many applications
- ✓ L-stability allows the use of very large time-steps



- Requires a quality preconditioner to be efficient, which can be very difficult to formulate, implement, vectorize, and scale. The PCs can also suffer "break down"
- Requires linear operator
- Choosing the convergence tolerance is not trivial
- Global communication for dot products limits scaling (global sync)
- Dot product can suffer from floating point \bigcirc errors requiring quad precision





- Relatively new methods (1996-2015), relatively uncommon Ψ
- Unconditionally stable, but *explicit*! Ψ
- Main idea: Runge-Kutta method with stages added for more stability, rather Ψ than for more accuracy
- Two main flavors are RKC (Chebyshev-based) and RKL (Legendre-based) Ψ and can be recursive or factored [See [O'Sullivan, 2015] (yesterday's talk) for high-order factored RKC (FRKC) methods]
- STS (RKC) is currently being used in several MHD codes with success Ψ (FLASH, PLUTO, Lare3D) and is planned for inclusion in others
- We use the 2nd-order recursive RKL2 from [Meyer et al, 2014] because it Ψ can have better stability properties for non-uniform and non-linear diffusion coefficients



Explicit Super Time-stepping: RKL (Derivation [Meyer et al, 2014])

PDE: $\frac{\partial u}{\partial t} = \mathbf{M} u(t)$ Solution expansion: $u(t) = e^{t \mathbf{M}} u(0) \approx \left(1 + t \mathbf{M} + \frac{1}{2} (t \mathbf{M})^2 + ...\right) u(0)$ $u^{n+1} = e^z u^n \approx \left(1 + z + \frac{z^2}{2} + \dots\right) u^n, \qquad z = \Delta t \mathbf{M}$ Discretized form:

Multi-step explicit scheme: $u^{n+1} = R(\Delta t \mathbf{M}) u^n$ For accuracy, need: $R(z) = 1 + z + z^2/2 + O(z^3)$ For stability, need: $|R(\Delta t \lambda)| \leq 1, \forall \lambda \in \mathbf{M}$

Example: First-order explicit Euler method $(\lambda \in \mathcal{R})$ R(z) = 1 + z $|1 + \Delta t_{\text{Euler}} \lambda| \leq 1$ $u^{n+1} = (1 + \Delta t \,\mathbf{M}) \, u^n$ $\Delta t_{\mathrm{Euler}} \leq \frac{2}{\left|\lambda\right|_{\mathrm{max}}}$ $\frac{u^{n+1} - u^n}{\Delta t} = \mathbf{M} \, u^n$ 1D HEAT EQ: $\Delta t_{
m Euler} \leq rac{\Delta x^2}{2}$

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Legendre polynomial $P_s(x)$ $P_{j}(x) = (1/j) \left[(2j - 1) x P_{j-1}(x) - (j - 1) P_{j-2}(x) \right]$ $|P_s(x)| \le 1, \ x \in [-1,1]$

RKL: $R(z) = a_s + \overline{b_s P_s(1 + w_1 z)}$ Accuracy $O(\Delta t) \qquad \qquad O(\Delta t^2)$ $a_{s} = 1 - b_{s} \qquad a_{s} = 1 - b_{s}$ $b_{s} = 1 \qquad b_{s} = \frac{s^{2} + s - 2}{2s(s+1)}$ $w_{1} = \frac{2}{s^{2} + s} \qquad w_{1} = \frac{4}{2s(s+1)}$ $w_1 = \frac{4}{s^2 + s - 2}$

Recursion relation leads to easy implementation



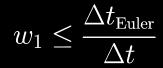
$\Delta t \ll 1$

Stability

- $-1 \le 1 + w_1 \,\Delta t \,\lambda \le 1$
 - Select s, get max dt:

$$\Delta t \le \frac{\Delta t_{\text{Euler}}}{w_1}$$

Select dt, get min s:



Explicit Super Time-stepping: RKL2 [Meyers et al, 2014]

$$y_{0} = u^{n}$$

$$F_{0} = \mathbf{M} y_{0}$$

$$y_{1} = y_{0} + \tilde{\mu}_{1} \Delta t F_{0}$$

$$do \ j = 2 : s$$

$$y_{j} = \mu_{j} y_{j-1} + \nu_{j} y_{j-2} + (1 - \mu_{j} - \nu_{j}) y_{0}$$

$$+ \tilde{\mu}_{j} \Delta t \mathbf{M} y_{j-1} + \gamma_{j} \Delta t F_{0}$$
enddo
$$u^{n+1} = y_{s}$$

$$b_{0} = b_{1} = b_{2} = \frac{1}{3} \qquad b_{j} = \frac{j^{2} + j - 2}{2j(j+1)}$$

$$\tilde{\mu}_{1} = \frac{4}{3(s^{2} + s - 2)} \qquad \tilde{\mu}_{j} = \frac{4(2j-1)}{j(s^{2} + s - 2)} \frac{b_{j}}{b_{j-1}}$$

$$\mu_{j} = \frac{2j - 1}{j} \frac{b_{j}}{b_{j-1}} \qquad \nu_{j} = -\frac{j - 1}{j} \frac{b_{j}}{b_{j-2}}$$

$$\gamma_{j} = (b_{j} - 1) \tilde{\mu}_{j}$$

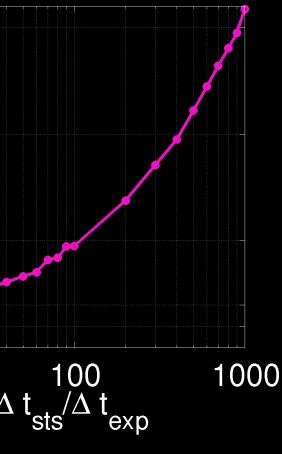
$$s \ge \begin{bmatrix} \frac{1}{2} \left(\sqrt{9 + 16 \frac{\Delta t}{\Delta t_{Euler}} + 16 \frac{\Delta t}{\Delta$$

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ime Stepping



Explicit Super Time-stepping: RKL2



- Very easy to implement (ideal for directive parallelization e.g. **OpenMP/OpenACC**)
- ✓ No global synchronization points
- ✓ Can include nonlinearities and/or flux limiting



- New method low circulation
- Number of sub-cycles can be large depending on the problem and grid
- Amplification factor not monotonically decreasing for increasing wave modes – *may* lead to undesirable results when using large time-steps and/or short simulation times



Thermodynamic MHD model: MAS

- Established MHD Solar coronal/heliospheric model with over 10 years of development
- Written in FORTRAN 90, parallelized with MPI-2



- Has been used extensively in solar physics research described in numerous publications
- Available for use at NASA's Community **Coordinated Modeling Center** http://ccmc.gsfc.nasa.gov







Thermodynamic MHD model: MAS [Governing Equations]

$$\begin{split} &\frac{\partial \mathbf{A}}{\partial t} = \mathbf{v} \times (\nabla \times \mathbf{A}) \\ &\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \, \mathbf{v}) \\ &\frac{\partial T}{\partial t} = -\nabla \cdot (T \mathbf{v}) - (\gamma - 2) \left(T \, \nabla \cdot \mathbf{v}\right) \end{split}$$

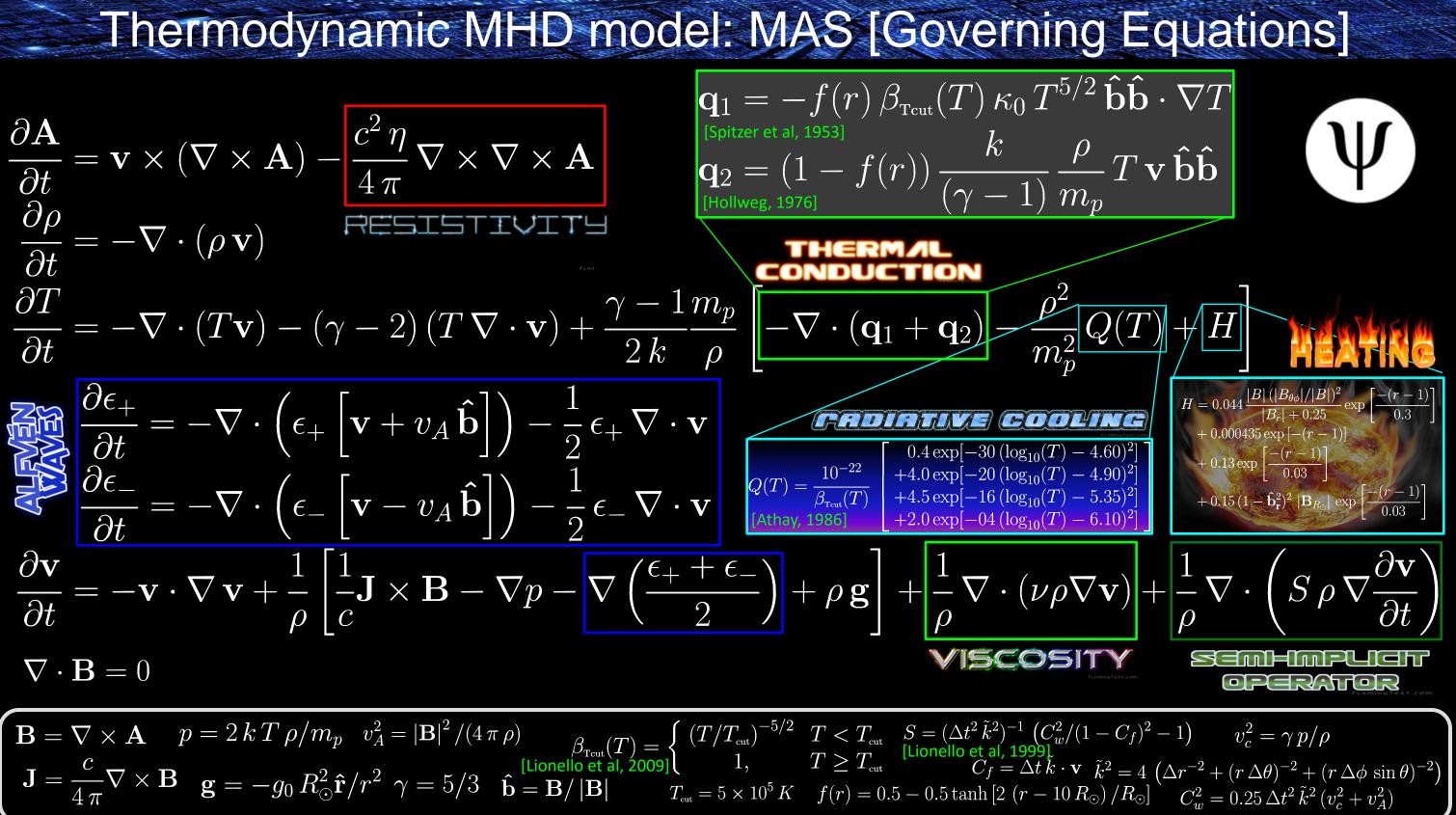
$$\frac{\partial \mathbf{v}}{\partial t} = -\mathbf{v} \cdot \nabla \mathbf{v} + \frac{1}{\rho} \left[\frac{1}{c} \mathbf{J} \times \mathbf{B} - \nabla p + \rho \mathbf{g} \right]$$

 $\nabla \cdot \mathbf{B} = 0$

$$\mathbf{B} = \nabla \times \mathbf{A} \qquad p = 2 k T \rho / m_p \qquad v_A^2 = |\mathbf{B}|^2 / (4 \pi \rho)$$
$$\mathbf{J} = \frac{c}{4 \pi} \nabla \times \mathbf{B} \qquad \mathbf{g} = -g_0 R_{\odot}^2 \mathbf{\hat{r}} / r^2 \qquad \gamma = 5/3 \quad \mathbf{\hat{b}} = \mathbf{B} / |\mathbf{B}|$$

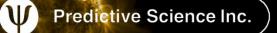


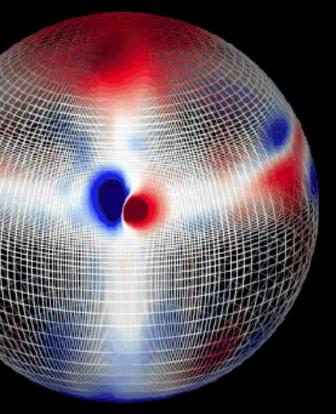




Thermodynamic MHD model: MAS [Numerical Methods]

- Finite difference on logically rectangular non-uniform Ψ spherical grid
- Integrates A on staggered grid to ensure $\nabla \cdot \mathbf{B} = 0$ Ψ
- Advective terms: upwinding Ψ
- Wave terms: Predictor-corrector Ψ
- Semi-implicit term solved using BE+PCG Ψ for both predictor and corrector
- Parabolic terms are operator split and use second-order Ψ central differences
- Matrix operators stored in modified DIA format, Ψ PC2 preconditioner stored in CSR format

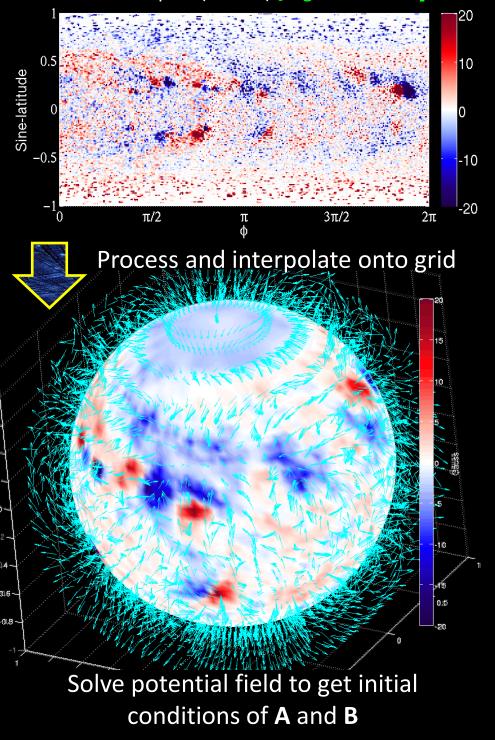


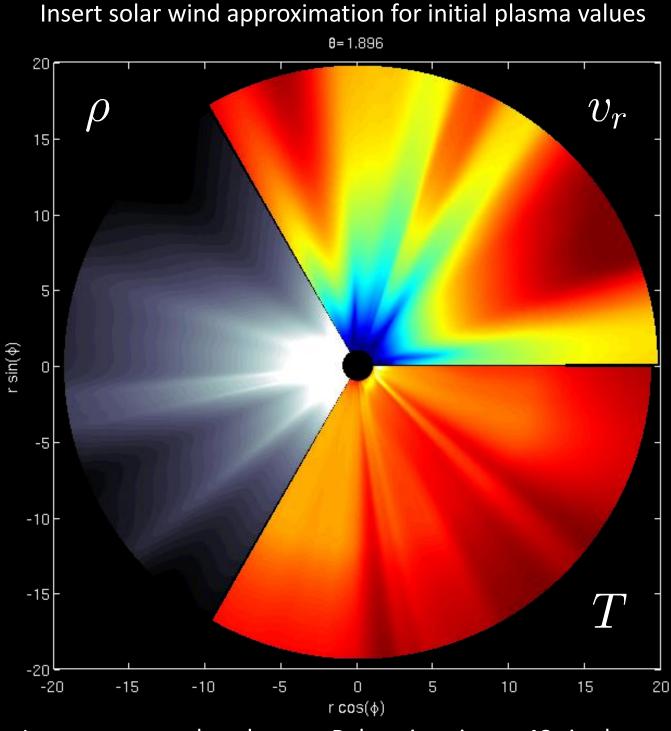


 $(\Delta r, \Delta heta, \Delta \phi)$

Real-world Test Case: Synchronic Coronal Relaxation

Air Force Data Assimilative Photospheric Flux Transport (ADAPT) [Arge et al. 2009]





Integrate to a relaxed state. Relaxation time ~ 48 sim-hours



Validation runs We integrate the relaxation for ~8 sim-hr

Timing runs

We integrate for 6 sim-min starting with the solution after the ~8 sim-hr relaxation

The Grid 181**x**251**x**602 ~27 million points

 $\min[\Delta r] \approx 340 \,\mathrm{km}$ $\max[\Delta r] \approx 590,000 \,\mathrm{km}$ Δr_{i+1} < 6%max

Real-world Test Case: HPC Environment



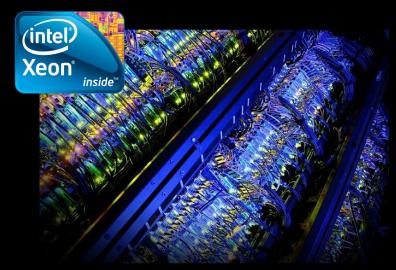
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Allocation provided by:



| Processor Model | Intel Xeon |
|---------------------|------------------------------|
| | E5-2660v3 (Haswell) |
| Clock Speed | $2.5\mathrm{GHz}$ |
| Cores per node | 24 |
| Max Flop/s per node | $\approx 1 \mathrm{TFlop/s}$ |
| DDR4 DRAM per node | 128 GB |
| Total $\#$ of nodes | 1944 |



- Operating 🛞 CentOS system: Intel 2015.2.164 Compiler: **MPI library: MVAPICH** for infiniband v2.1
- timers
- Ψ processors
- Ψ runs



Max # cores per run: 1728

Timings done using MPI

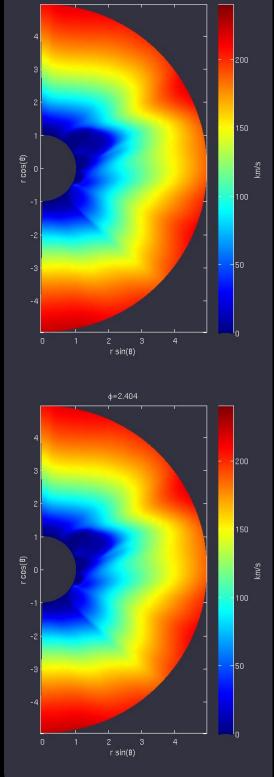
Times for each routine are averaged over all

Time recorded from the best run out of multiple

RKL2



BE+PCG (PC2)

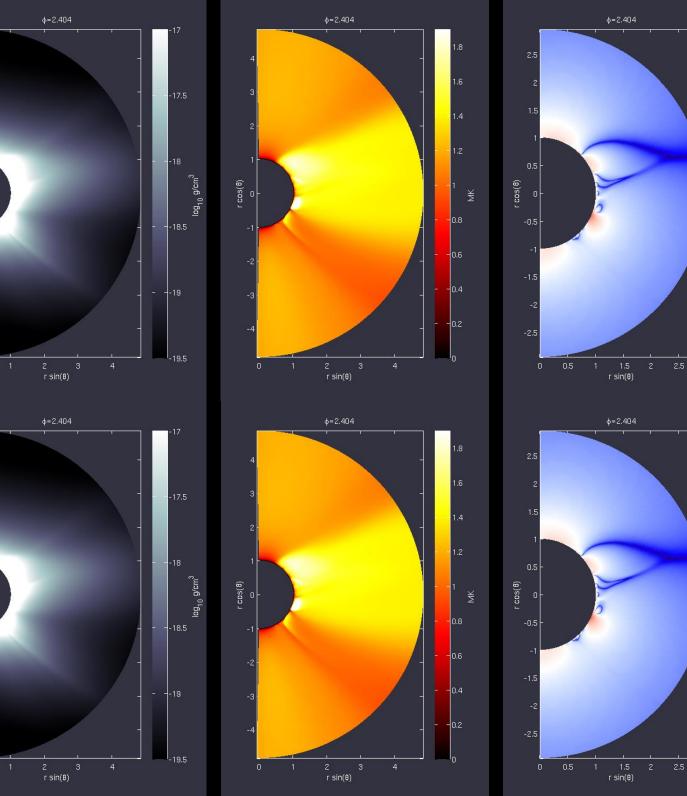


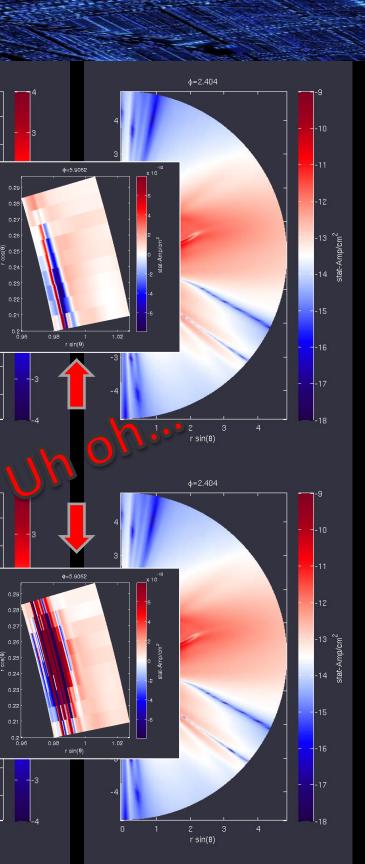
cos(8)

cos(8)

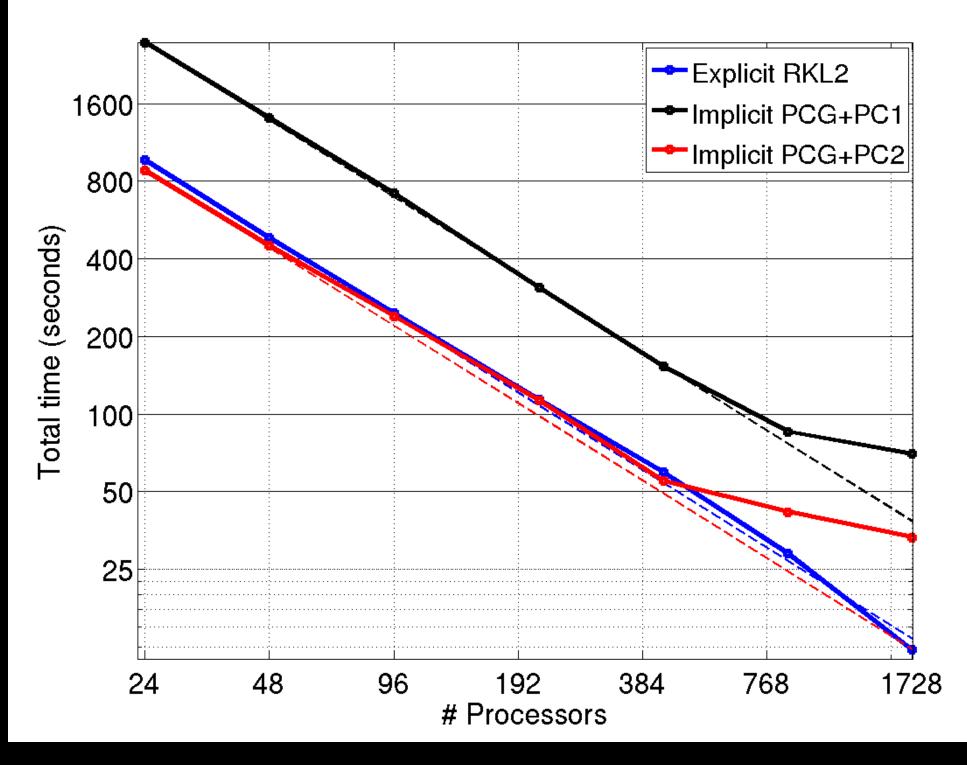
φ=2.404

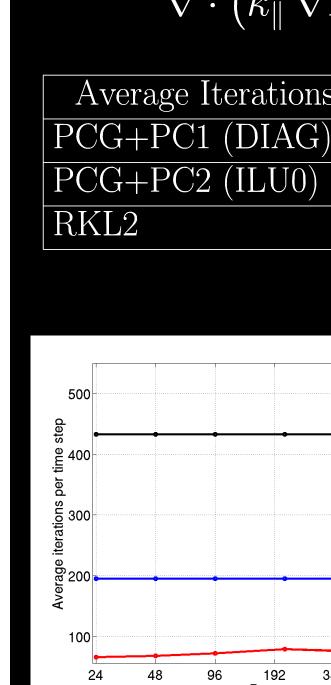






Performance Results: Thermal Conduction

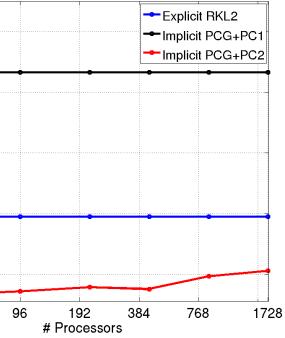




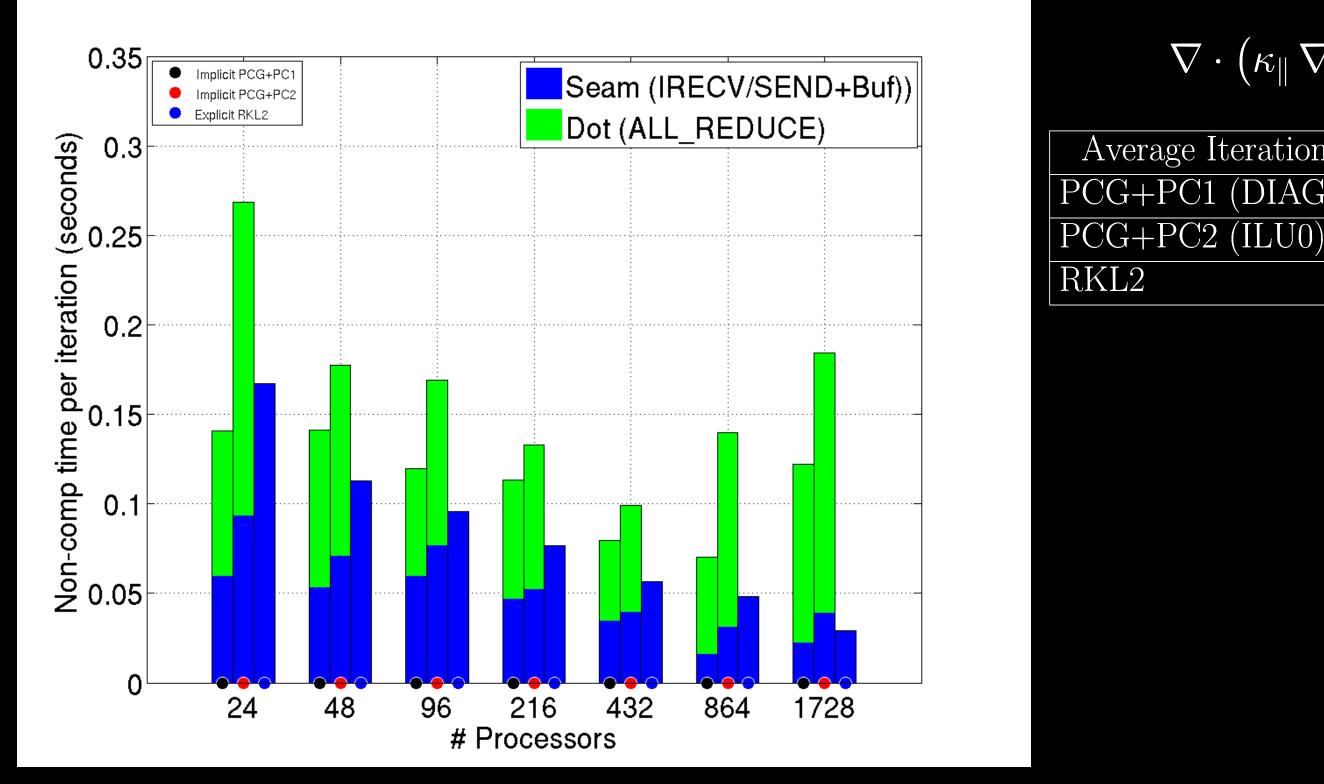


$\nabla \cdot (\kappa_{\parallel} \nabla T)$





Performance Results: Thermal Conduction

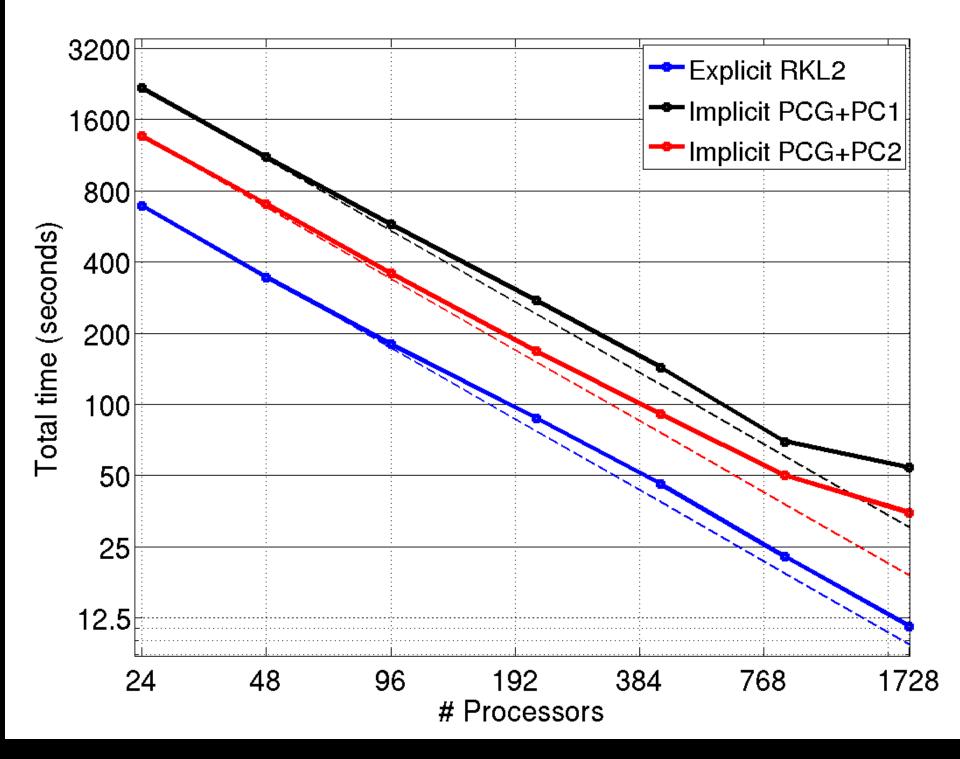




$abla \cdot \left(\kappa_{\parallel} \, abla T ight)$

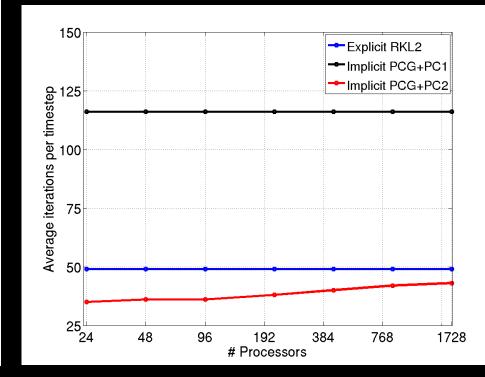
Average Iterations per Step PCG+PC1 (DIAG) 433 $66 \rightarrow 106$ 195

Results: Viscosity





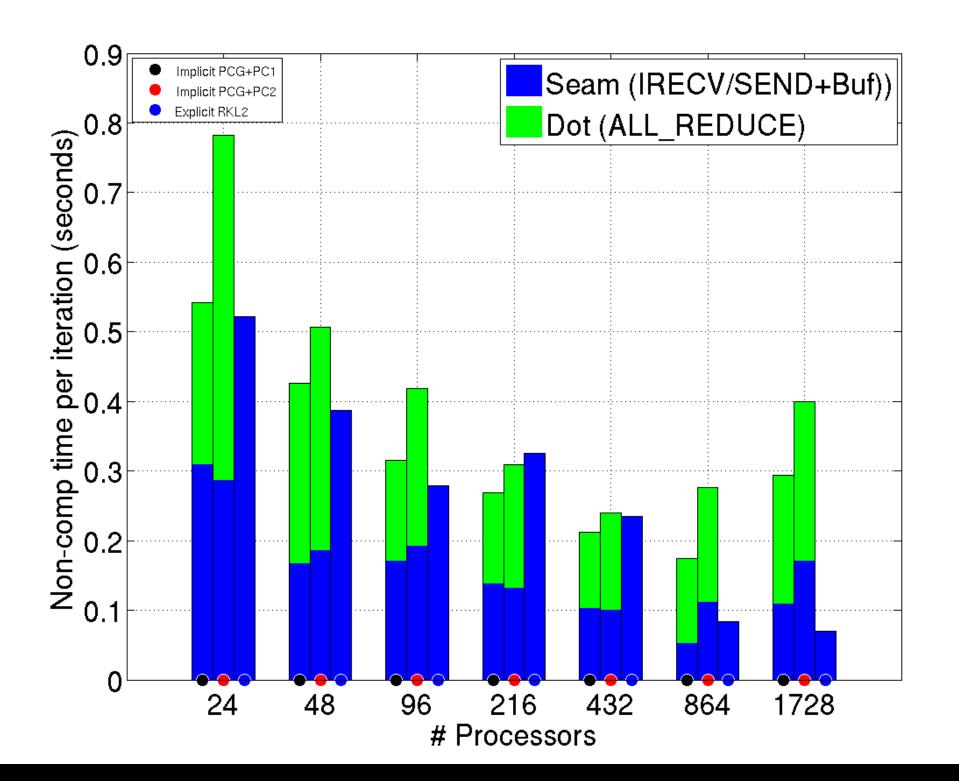




 $\nabla \cdot (\rho \, \nu \, \nabla \mathbf{v})$

Average Iterations per Step PCG+PC1 (DIAG) 116 $35 \rightarrow 43$ 49

Performance Results: Viscosity

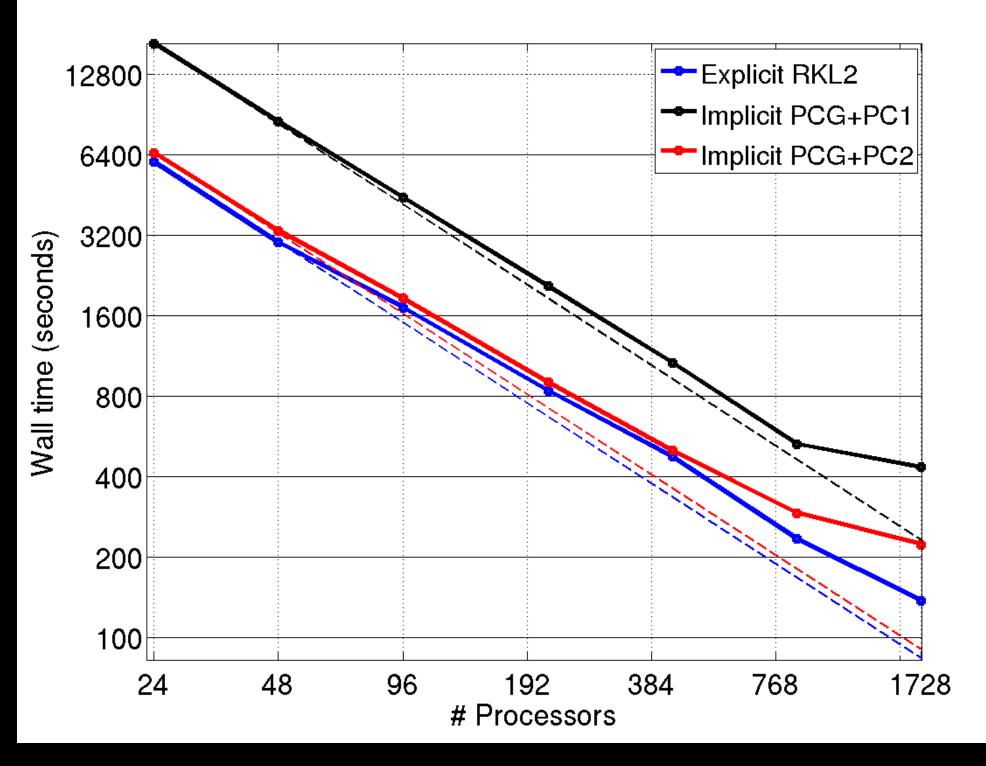


PCG+PC2 (ILU0) RKL2

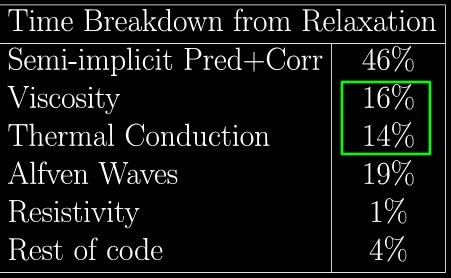
 $\nabla \cdot (\rho \, \nu \, \nabla \mathbf{v})$

Average Iterations per Step PCG+PC1 (DIAG) 116 $35 \rightarrow 43$ 49

Performance Results: Overall Code



Viscosity Thermal Conduction Alfven Waves Resistivity Rest of code



- Super Time-stepping algorithms show potential as an alternative to iterative solvers for parabolic terms in MHD models
- For the problem tested, the STS outperformed the iterative solver, especially in scaling to many CPUs
- For the viscosity term, there are some solution effects to work out
- Can STS methods be used for MHD waves?



Questions?



Slides available at:
www.predsci.com/~caplan/astro16

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Explicit Super Time-stepping: RKL2

- RKL needs the value of the Euler stability time-step to compute the number Ψ of required super-steps (s)
- In 3D spherical coordinates, simple upper-bound estimates can be too strict Ψ (especially for anisotropic diffusion)
- Can get much tighter bound using Gershgorin circle theorem: Ψ

Definition 1 Given a square matrix **A**, a Gershqorin disk for every row j is defined as a disk in the complex plane, centered at A_{ij} , with a radius of:

$$R_j = \sum_{i \neq j}^N |A_{i,j}|$$

Theorem 1 Every eigenvalue λ of a square matrix **A** lies in one of its Gershgorin discs:

$$|\lambda - A_{jj}| \le R_j$$

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Since $\lambda \in \mathcal{R}$ and $A_{jj} \in \mathcal{R}$, we get a bound on $|\lambda|$ as:

$$|A_{jj}| - R_j$$

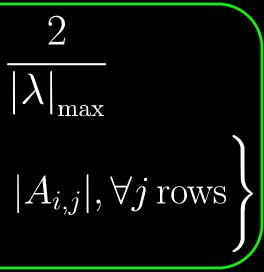
Therefore the maximum value of $|\lambda|$ is bound by:

$$|\lambda|_{\max} \le \max$$

$$\Delta t_{\mathrm{Euler}} \leq |\lambda|_{\mathrm{max}} \leq \max \left\{ \sum_{i=1}^{N} \right\}$$

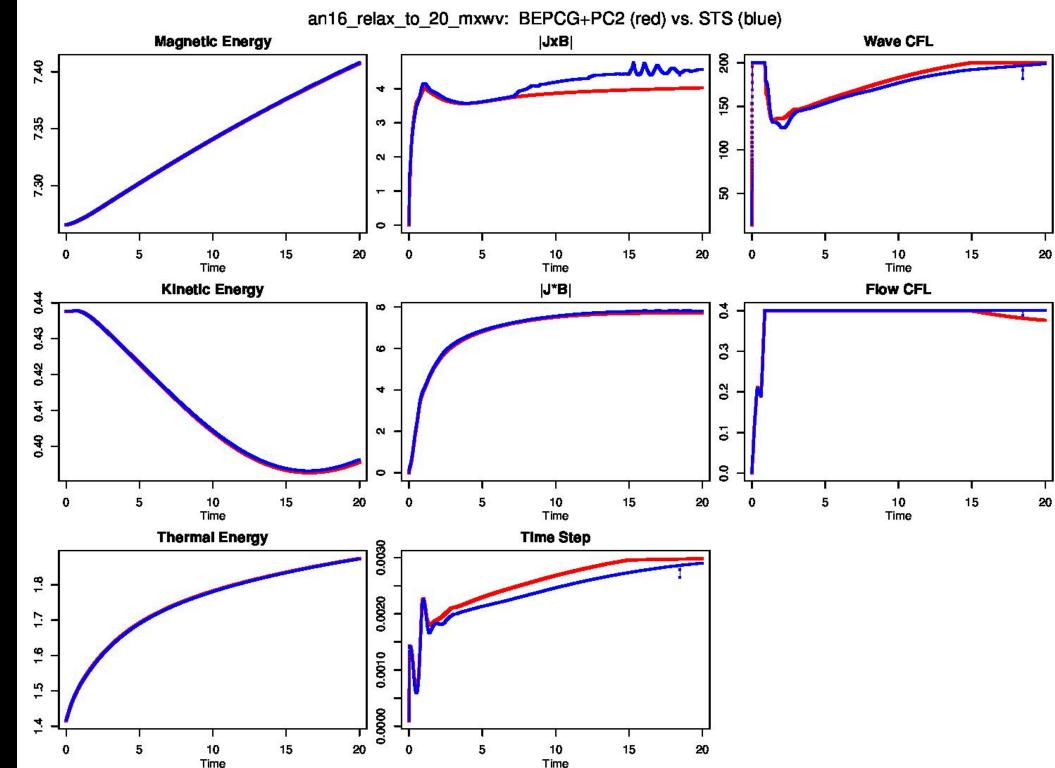
[Scott, 1985]: Max error in bound: $\sqrt{p+1}$

- $\leq |\lambda_j| \leq |A_{jj}| + R_j$
- $\{|A_{jj}| + R_j, \forall j \text{ rows}\}$



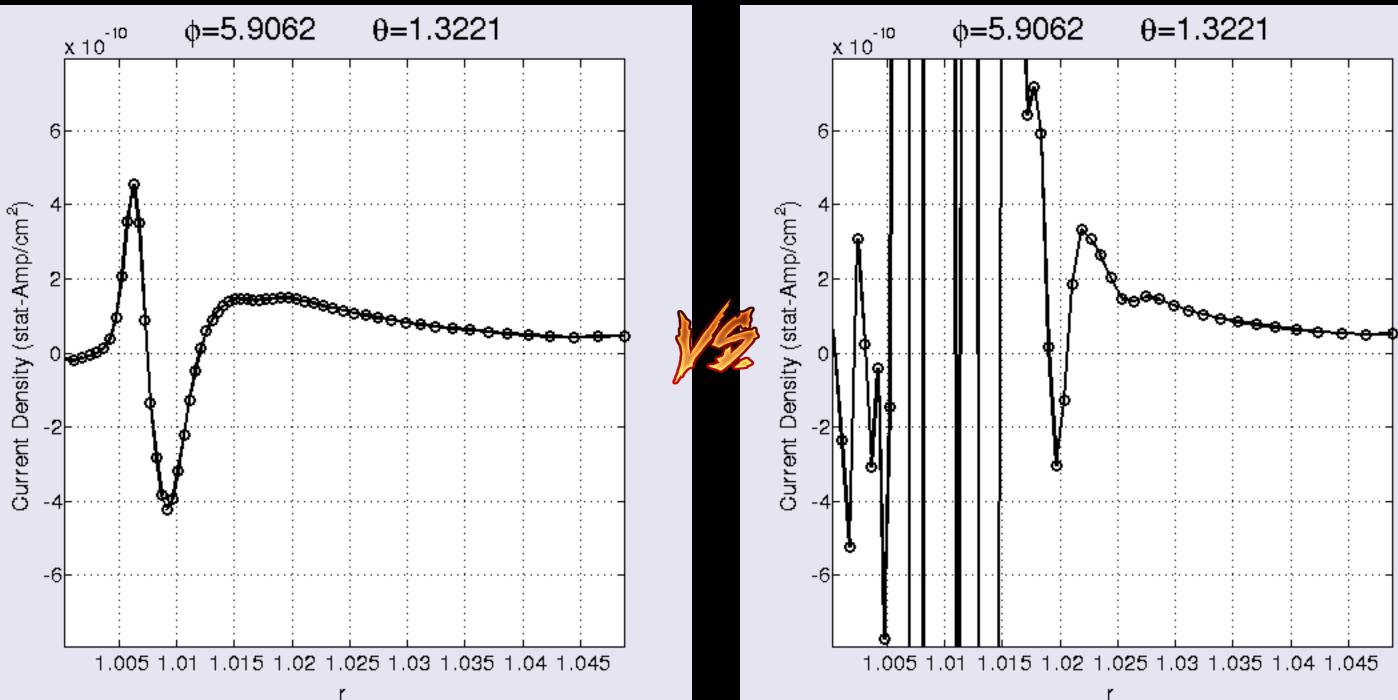
Validation

- First we compare Ψ BE+PCG2 versus RKL2 for thermal conduction only – match!
- Turning on RKL2 for Ψ viscosity has overall match (as seen in movies) but seems to have problems with the current density
- Maybe initial relaxation Ψ too violent? Try capping wave CFL to 200...
- Where is this Ψ happening?





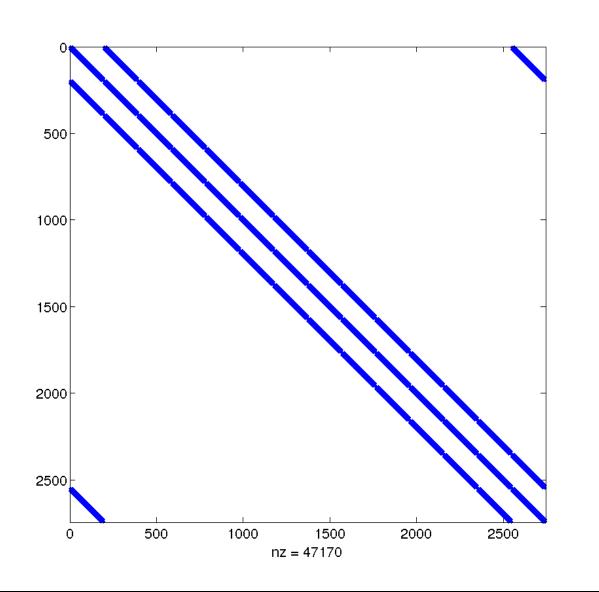
Validation

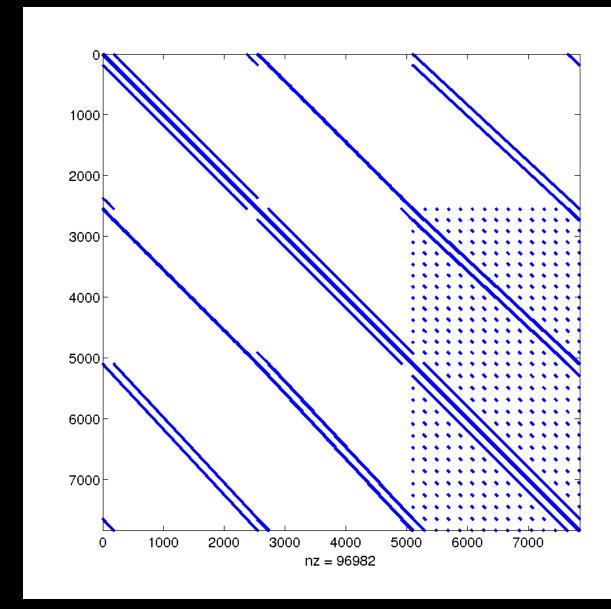


Thermal Conduction

Viscosity

Validation





Euler dt estimate: Euler dt estimate w/o pole bc: 0.0033

0.0018