Application of Scalable Solver Techniques to Magnetized Plasma Problems in 2D and 3D

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Organization of Presentation

- Previous solver results for 2D MHD waves in a doubly periodic uniform plane
- New test problem: Magnetized Target Fusion, radially compressed compact toroid.
- Moving grid equations.
- Results for cylindrically compressed FRC.
- Status of solver.
- Future plans.

Physics-Based Preconditioning

Factorization and Schur Complement

Linear System

$$\mathsf{L}\mathbf{u} = \mathbf{r}, \quad \mathsf{L} \equiv \begin{pmatrix} \mathsf{L}_{11} & \mathsf{L}_{12} \\ \mathsf{L}_{21} & \mathsf{L}_{22} \end{pmatrix}, \quad \mathbf{u} = \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{pmatrix}, \quad \mathbf{r} = \begin{pmatrix} \mathbf{r}_1 \\ \mathbf{r}_2 \end{pmatrix}$$

Factorization

$$\mathsf{L} \equiv \begin{pmatrix} \mathsf{L}_{11} & \mathsf{L}_{12} \\ \mathsf{L}_{21} & \mathsf{L}_{22} \end{pmatrix} = \begin{pmatrix} \mathsf{I} & \mathbf{0} \\ \mathsf{L}_{21}\mathsf{L}_{11}^{-1} & \mathsf{I} \end{pmatrix} \begin{pmatrix} \mathsf{L}_{11} & \mathbf{0} \\ \mathbf{0} & \mathsf{S} \end{pmatrix} \begin{pmatrix} \mathsf{I} & \mathsf{L}_{11}^{-1}\mathsf{L}_{12} \\ \mathbf{0} & \mathsf{I} \end{pmatrix}$$

Schur Complement

$$\mathsf{S} \equiv \mathsf{L}_{22} - \mathsf{L}_{21}\mathsf{L}_{11}^{-1}\mathsf{L}_{12}$$

Exact and Approximate Inverse

Preconditioned Krylov Iteration

Inverse

$$\mathsf{L}^{-1} = \begin{pmatrix} \mathsf{I} & -\mathsf{L}_{11}^{-1}\mathsf{L}_{12} \\ \mathbf{0} & \mathsf{I} \end{pmatrix} \begin{pmatrix} \mathsf{L}_{11}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathsf{S}^{-1} \end{pmatrix} \begin{pmatrix} \mathsf{I} & \mathbf{0} \\ -\mathsf{L}_{21}\mathsf{L}_{11}^{-1} & \mathsf{I} \end{pmatrix}$$

Exact Solution

$$\mathbf{s}_1 = \mathsf{L}_{11}^{-1}\mathbf{r}_1, \quad \mathbf{s}_2 = \mathbf{r}_2 - \mathsf{L}_{21}\mathbf{s}_1$$

$$\mathbf{u}_2 = \mathsf{S}^{-1}\mathbf{s}_2, \quad \mathbf{u}_1 = \mathbf{s}_1 - \mathsf{L}_{11}^{-1}\mathsf{L}_{12}\mathbf{u}_2$$

Preconditioned Krylov Iteration

$$\mathsf{P} \approx \mathsf{L}^{-1}, \quad (\mathsf{LP})\left(\mathsf{P}^{-1}\mathbf{u}\right) = \mathbf{r}$$

Outer iteration preserves full nonlinear accuracy.
Need approximate Schur complement $\mathbf{S}$
and scalable solution procedure for $\mathbf{L}_{11}$ and $\mathbf{S}$.

Ideal MHD Waves

Linearized, Normalized Equations

$$\frac{\partial p}{\partial t} + \gamma \nabla \cdot \mathbf{v} = 0, \quad \frac{\partial \mathbf{b}}{\partial t} = \nabla \times (\mathbf{v} \times \mathbf{B})$$

$$\frac{\partial \mathbf{v}}{\partial t} + \nabla \cdot \mathsf{T} = 0, \quad \mathsf{T} = (\beta p + \mathbf{B} \cdot \mathbf{b})\,\mathsf{I} - \mathbf{B}\mathbf{b} - \mathbf{b}\mathbf{B}$$

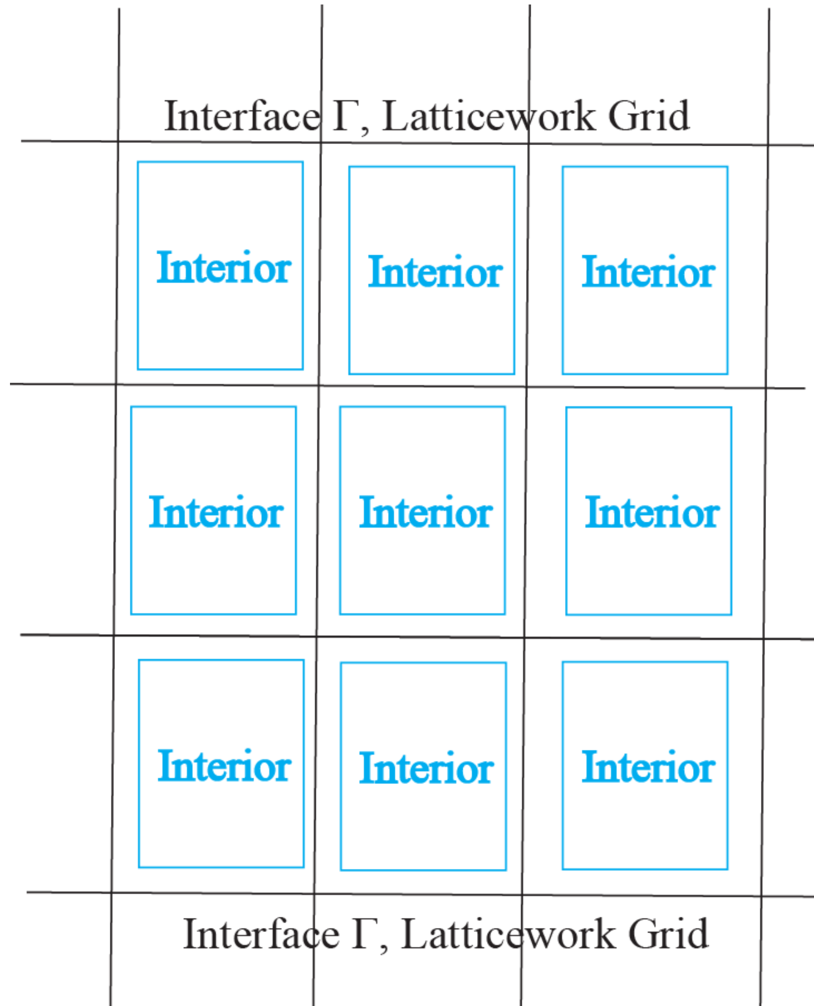
Approximate Schur Complement

$$\mathsf{S}\mathbf{v} = \mathbf{v} + \nabla \cdot \mathsf{T},$$

$$\mathsf{T} \equiv h^2\theta^2 \left\{ \left[\mathbf{B} \cdot \nabla \times (\mathbf{v} \times \mathbf{B}) - \gamma\beta \nabla \cdot \mathbf{v} \right] \mathsf{I} - \mathbf{B} \nabla \times (\mathbf{v} \times \mathbf{B}) - \nabla \times (\mathbf{v} \times \mathbf{B})\, \mathbf{B} \right\}$$

Static Condensation

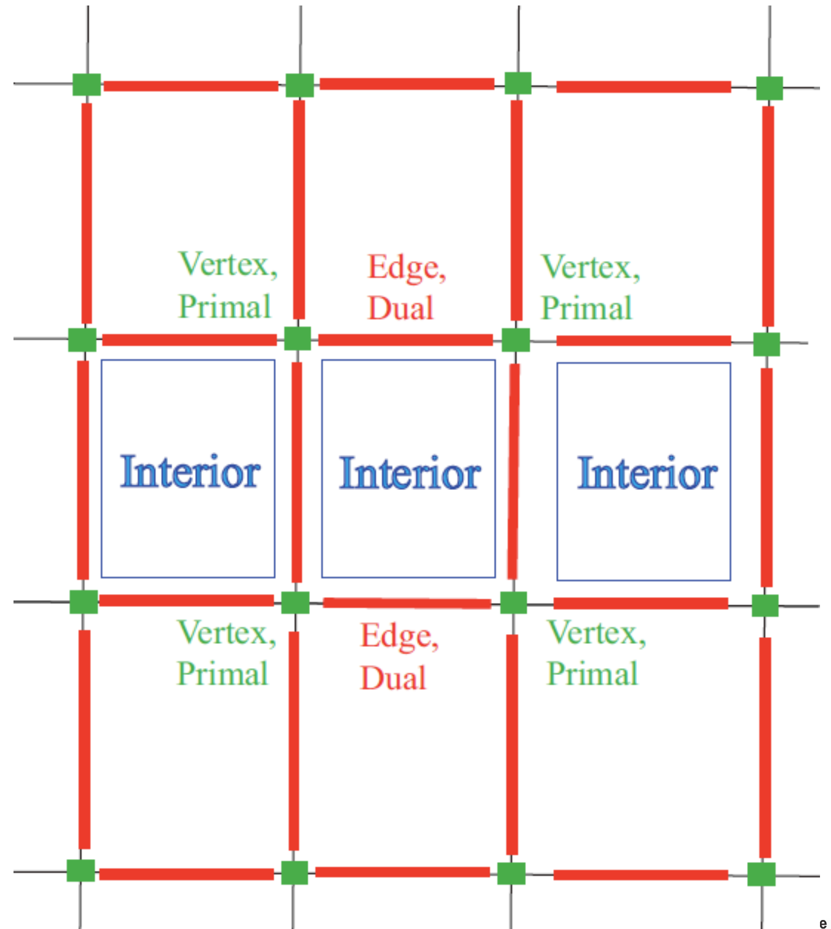
- Implicit time step requires linear system solution: **L u = r**.
- Direct solution time grows as n^3.
- Break up large matrix into smaller pieces: Interiors + Interface.
- Small direct solves for interior.
- Interface solve by CG or GMRES, precoditioned with LU or ILU(k) on each processor, with Schwarz overlap between processors.
- Substantially reduces solution time, condition number.



FETI-DP

Finite Element Tearing and Interconnecting, Dual-Primal

- Break up large matrix into three pieces: interior + dual + primal.
- Small direct solves for interior.
- Parallel direct solve for primal points.
- Matrix-free preconditioned GMRES for dual points.
- Primal solve provides information to dual problem about coarse global conditions, providing scalability.
- Interior preconditioner accelerates convergence of dual solve.

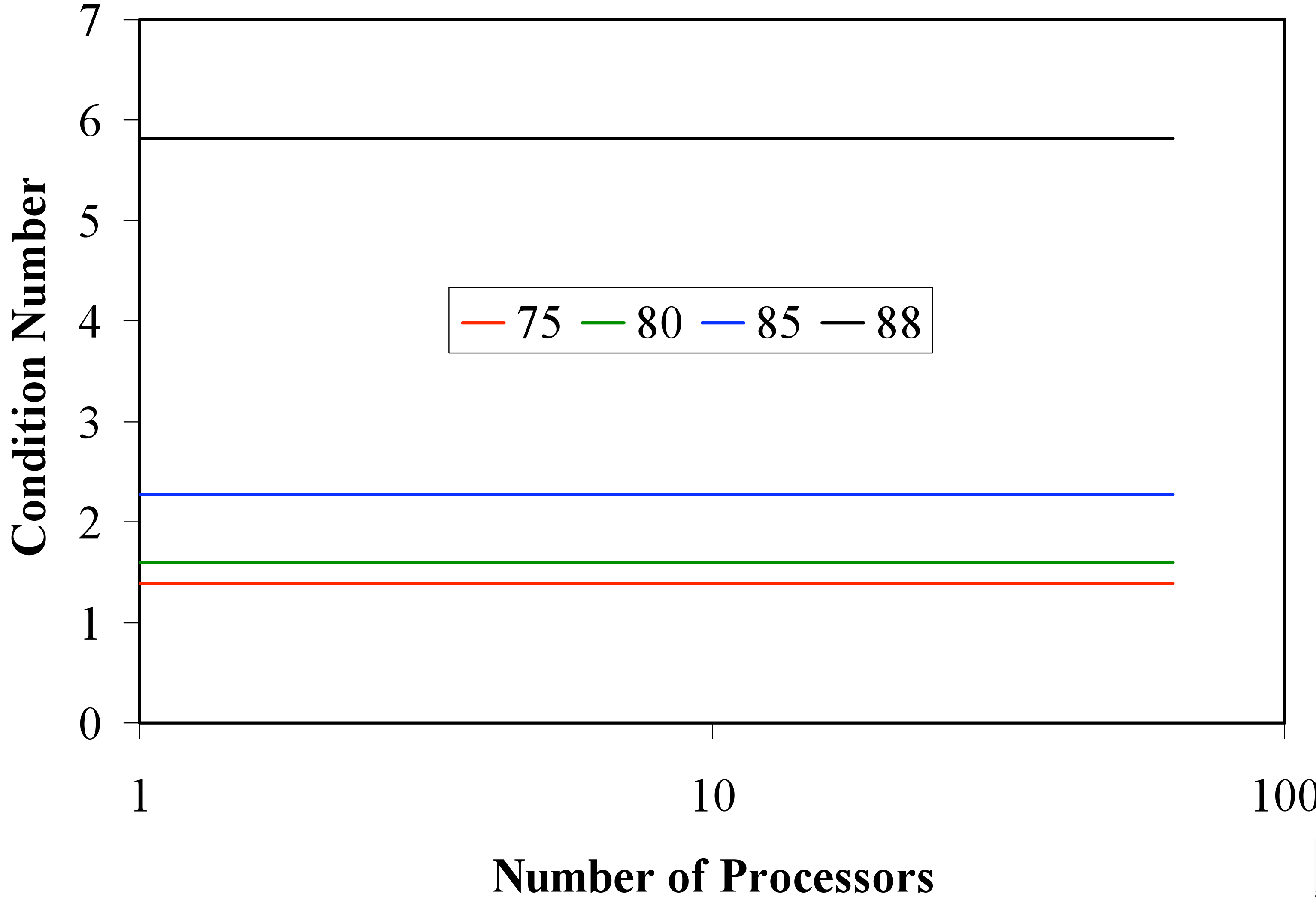


Weak Scaling Test Problem

- Ideal or Hall MHD waves in a doubly periodic uniform plane.
- 2D **k** vector in computational plane, 3D **B** vector specified by spherical angles about normal to plane. Continuous control of angle θ between **k** and **B.**
- Initialize to pure eigenvector: fast (whistler), shear (kinetic Alfven), or slow wave.
- Unit cell: (knx, kny) full wavelengths.
- Two test cases:
  1. Each processor has one unit cell. Scale up unit cells with nproc. Hold (nx,ny,np) fixed in each unit cell.
  2. One unit cell held fixed, scale up (nx,ny) with nproc. Splits wave length among multiple processors.
- 1 – 64 processors on bassi debug queue.
- Largest test problem size: 16 x 16 wavelengths, 64 processors, 589,824 spatial locations, 6 physical degrees of freedom, 3,538,944 variables, 2 large time steps, CFL number ~100, 1 jacobian evaluation, wallclock time ~30 seconds.

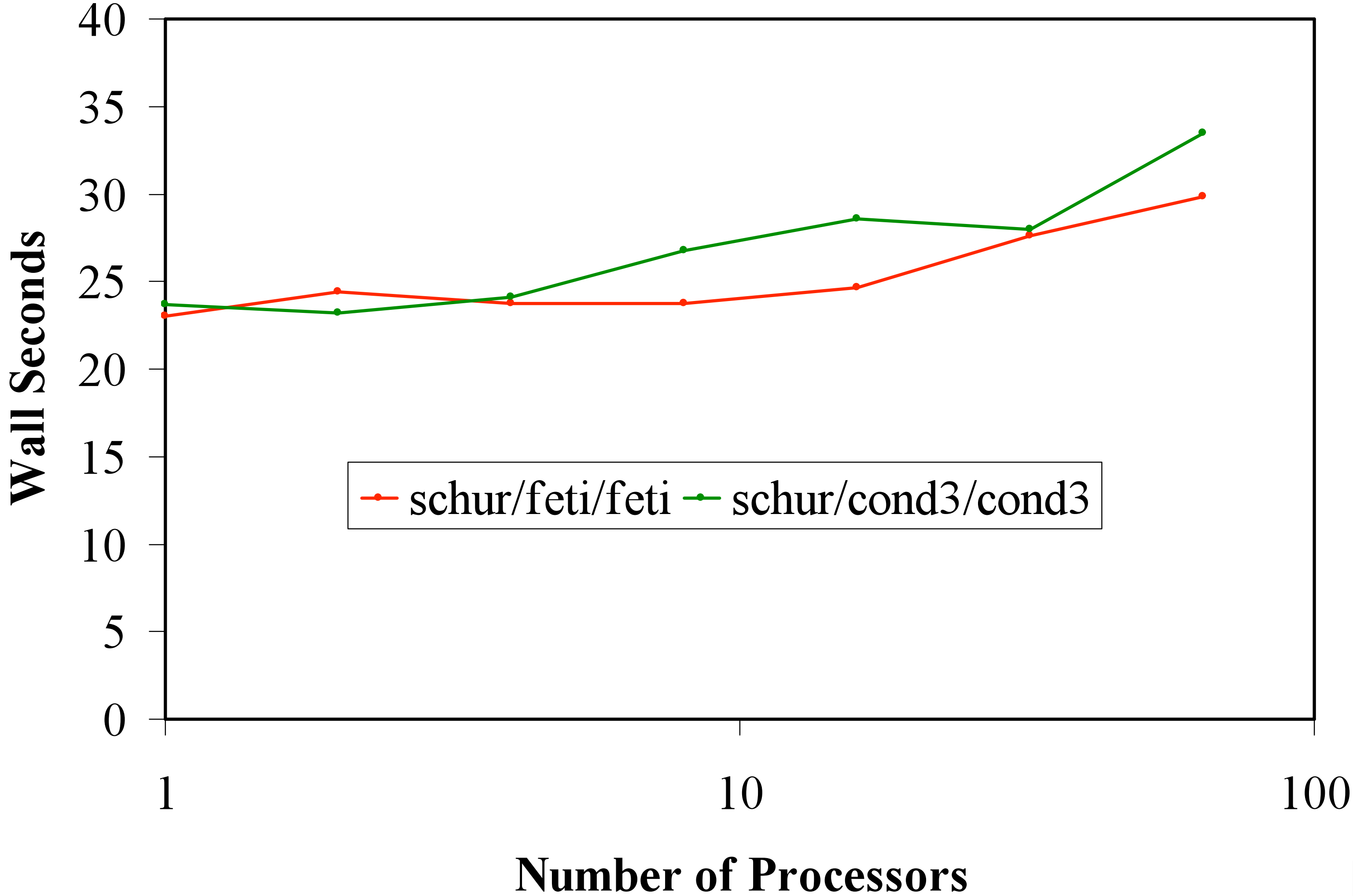
FETI-DP Dual Condition Number

MHD Slow Wave, Various k-B Angle θ, Degrees



Wallclock Time to Solution

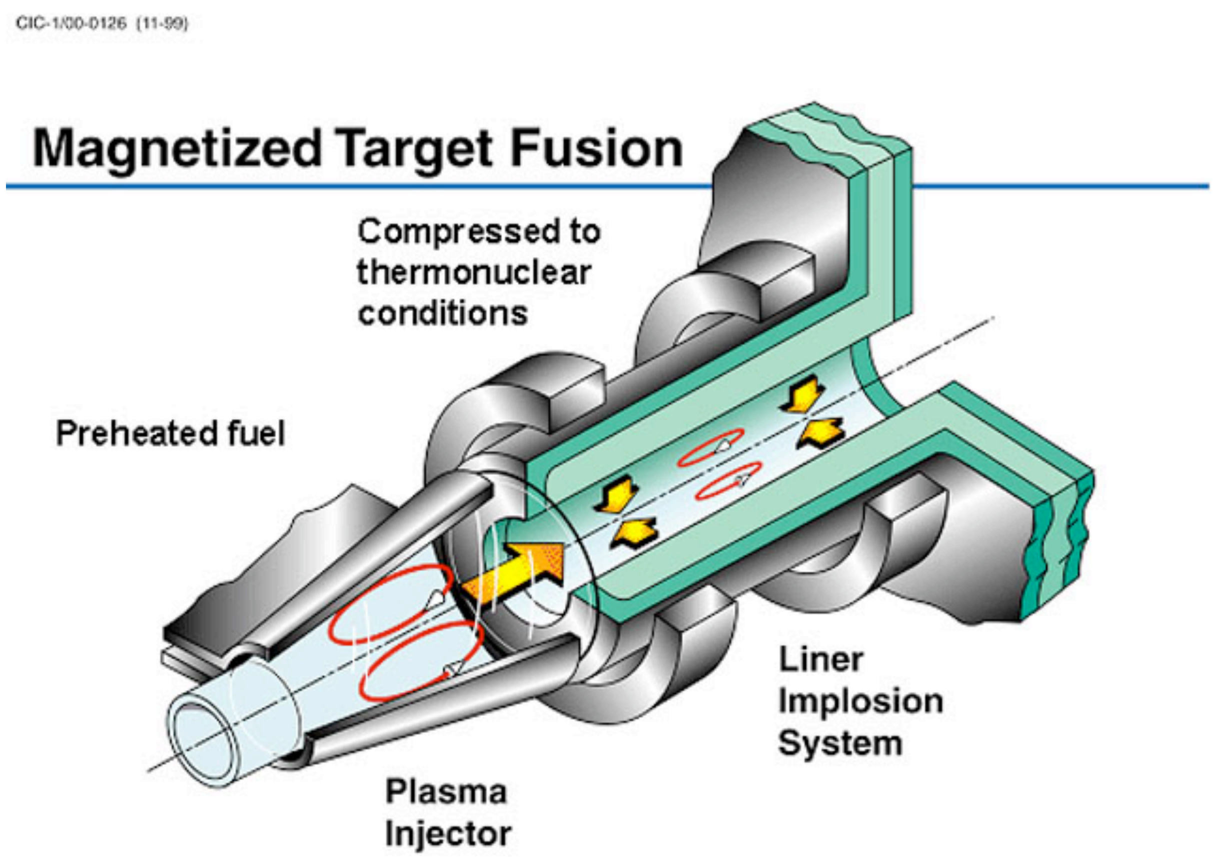
MHD Slow Wave, $\theta = 75^o$, FETI-DP vs. Static Condensation



Solver Conclusions, Ideal MHD Waves

- **Physics-Based Preconditioning**
  - Reduces matrix order requiring solution
  - Improves condition number and diagonal dominance.
  - Similar to time step split, but maintains full nonlinear accuracy.
- **FETI-DP**
  - Provides scalable solver for SPD preconditioning equations, i.e. ideal MHD.
  - Computational results verify analytical scalability theorem.
  - Requires extension to non-SPD problems, such as Hall MHD.
  - Primal solve requires minor modifications to achieve true scalability.
  - 3D primal constraints require research.
- **Static Condensation**
  - Appears to be as scalable as FETI-DP on 1-64 processors.
  - No increase in condition number and time as theta approache 90 degrees.
  - Requires no extension for non-SPD problems.
  - Already implemented for the 3D HiFi spectral element code (Sato).

More Interesting Test Problem for Solver Development



Fast radial compression of a compact toroid.

FRC Equations

Dependent Variables

$$\mathbf{u} = (u_1, u_2, u_3, u_4, u_5, u_6) = (\rho, -A_\phi, p, \rho v_z, \rho v_r, J_\phi)$$

Interior Equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \quad \frac{3}{2}\frac{\partial p}{\partial t} + \nabla \cdot \left(\frac{5}{2} p \mathbf{v} - \kappa \cdot \nabla T\right) = \eta J_\phi^2 + \pi : \nabla \mathbf{v}$$

$$\frac{\partial}{\partial t}(-A_\phi) = v_r B_z - v_z B_r + \eta J_\phi, \quad J_\phi = \frac{A_\phi}{r^2} - \nabla^2 A_\phi$$

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v}\mathbf{v} + p\mathbf{I} + \pi) = \mathbf{J} \times \mathbf{B}$$

Spitzer-Chodura resistivity η, Braginskii $\kappa_{\parallel}$ and $\kappa_{\perp}$.

Top Boundary Conditions, $r = R$

$$\rho \text{ natural}, \quad \frac{\partial A_\phi}{\partial t} = 0, \quad \frac{\partial}{\partial r}\left(\frac{p}{\rho}\right) = 0, \quad v_z = 0, \quad v_r = \dot{R}, \quad J_\phi = 0$$

Bottom Boundary Conditions, $r = 0$

$$\frac{\partial \rho}{\partial r} = \frac{\partial p}{\partial r} = \frac{\partial \rho v_z}{\partial r} = A_\phi = \rho v_r = J_\phi = 0$$

z periodic

Moving Grid

Rescaling Transformation

$$\mathbf{x}(\mathbf{y},t) \equiv \mathsf{T}(t)\cdot\mathbf{y}, \quad \mathbf{y}(\mathbf{x},t) \equiv \mathsf{T}^{-1}(t)\cdot\mathbf{x}, \quad u(\mathbf{x}(\mathbf{y},t),t) = u(\mathsf{T}(t)\cdot\mathbf{y},t)$$

$$\left.\frac{\partial u}{\partial \mathbf{x}}\right|_t = \frac{\partial}{\partial \mathbf{x}}\mathbf{y}\cdot\left.\frac{\partial u}{\partial \mathbf{y}}\right|_t = \mathsf{T}^{-1}\cdot\left.\frac{\partial u}{\partial \mathbf{y}}\right|_t, \quad \left.\frac{\partial u}{\partial t}\right|_x = \left.\frac{\partial u}{\partial t}\right|_y - \mathbf{V}\cdot\frac{\partial u}{\partial \mathbf{x}}, \quad \mathbf{V} \equiv \left.\frac{\partial \mathbf{x}}{\partial t}\right|_y = \dot{\mathsf{T}}\cdot\mathbf{y}$$

Transformation of Flux-Source Form

$$A\left.\frac{\partial u}{\partial t}\right|_x + \frac{\partial}{\partial \mathbf{x}}\cdot\left.\mathbf{F}\right|_t = S$$

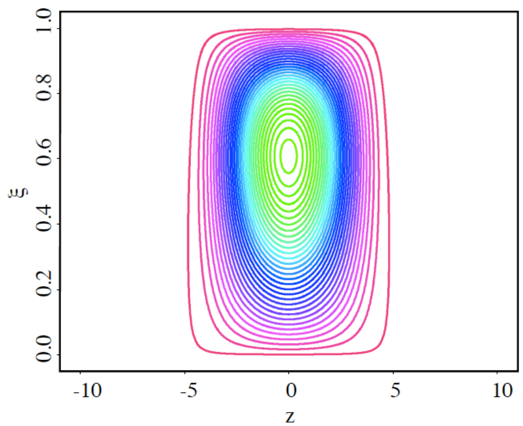
$$A\left.\frac{\partial u}{\partial t}\right|_y - A\mathbf{V}\cdot\frac{\partial u}{\partial \mathbf{x}} + \frac{\partial}{\partial \mathbf{x}}\cdot\mathbf{F} = S$$

$$A\left.\frac{\partial u}{\partial t}\right|_y - A\left(\dot{\mathsf{T}}\cdot\mathbf{y}\right)\cdot\left(\mathsf{T}^{-1}\cdot\frac{\partial u}{\partial \mathbf{y}}\right) + \frac{\partial}{\partial \mathbf{y}}\cdot\left(\mathbf{F}\cdot\mathsf{T}^{-1}\right) = S$$

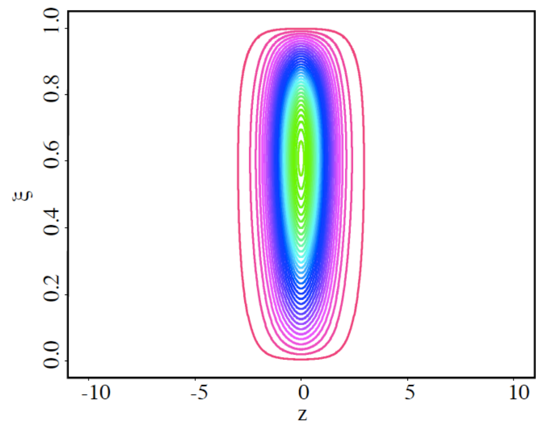
$$A\left.\frac{\partial u}{\partial t}\right|_y + \frac{\partial}{\partial \mathbf{y}}\cdot\left.\mathbf{F}'\right|_t = S', \quad \mathbf{F}' \equiv \mathbf{F}\cdot\mathsf{T}^{-1}, \quad S' = S + A\left(\dot{\mathsf{T}}\cdot\mathbf{y}\right)\cdot\left(\mathsf{T}^{-1}\cdot\frac{\partial u}{\partial \mathbf{y}}\right)$$

Compressed FRC Results

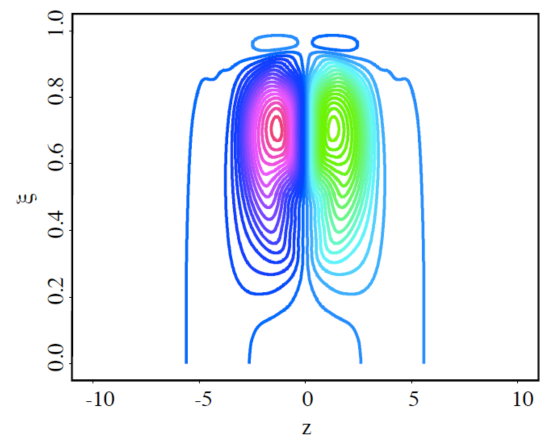
Initial ψ



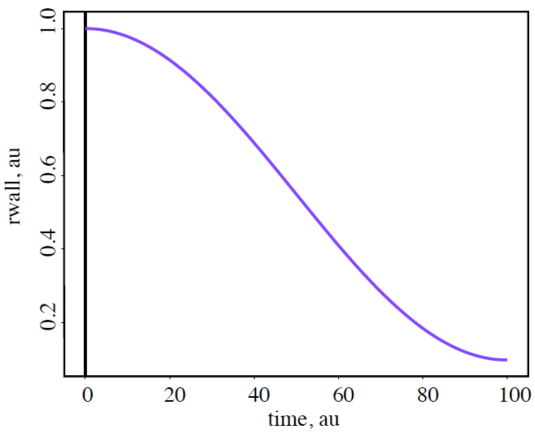
Final ψ



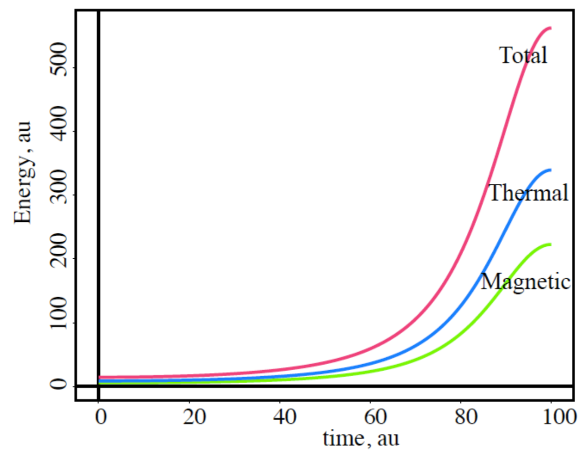
ρv_z



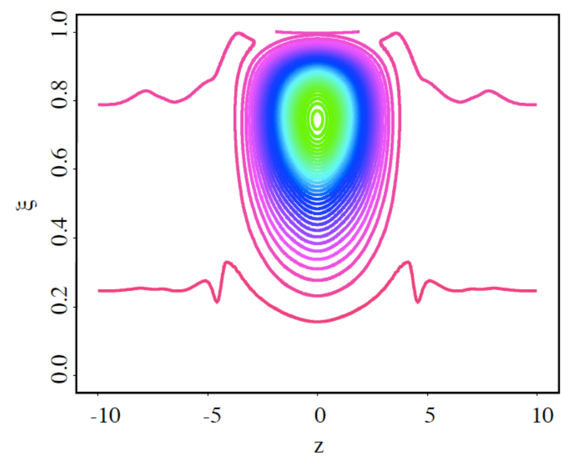
Wall Radius vs. Time



Energy vs. Time



ρv_r



Specs and Comments on Run

- Initial conditions:
  $n = 10^{17}$ cm^{-3}, $T = 100$ eV, $B = 10$ T, $\beta = 80\%$, $c_A = 1380$ km/s.
- Wall motion: $r_W = 20 \rightarrow 2$ cm, $v_W = 2$ km/s, $t_W = 100$ μs.
- Grid (nx,ny,np) = (64,32,8) , packed but not adaptive, nproc = 64.
- Walltime = 3.3 hr on new PSI Center SGI cluster.
- Falls short of fusion density and temperature; spheromak would make it.
- Magnetic vs. wall confinement, β < or > 1, problem of liner melting.
- Braginskii regime; will extend to include all.

Status of Solver Development

- Physics-based preconditioning reduces order of matrices and makes them more diagonally dominant.
- Schur complement:
  Ideal MHD force operator + ion viscosity + wall motion.
- Similar to time step split, but with outer Newton (PETSc/SNES) iteration to eliminate effects of approximation.
- SNES convergence tests for goodness of Schur complement.
- Schur complement requires further development to include nonuniformity, density variation, moving grid, boundary conditions.
- Once it works correctly, the next step is testing scalable solvers:
  FETI-DP, Static Condensation, GMRES, ILU(k), Hypre/BoomerAMG.
- New possibility:
  Schur complement + threshold ILU + GMRES in SuperLU 4.0.