Scalable Linear Solver in 3D MHD Simulation

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in collaboration with

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M3DP M3DC1 M3DK

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Extended MHD Equations:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\vec{V}) = 0$$
$$\frac{\partial(\vec{B})}{\partial t} = -\nabla \times \vec{E} \qquad \vec{J} = \nabla \times \vec{B}$$
$$nM_i(\frac{\partial \vec{V}}{\partial t} + \vec{V} \cdot \nabla \vec{V}) + \nabla p = \vec{J} \times \vec{B} - \nabla \cdot \Pi_{GV} + \mu \nabla^2 \vec{V}$$
$$\vec{E} + \vec{V} \times \vec{B} = \eta \vec{J} + \frac{1}{ne}(\vec{J} \times \vec{B} - \nabla p_e) - \lambda_H (\Delta x)^2 \nabla^2 \vec{J}$$
$$\frac{3}{2}\frac{\partial p_e}{\partial t} + \nabla \cdot (\frac{3}{2} p_e \vec{V}) = -p_e \nabla \cdot \vec{V} + \frac{\vec{J}}{ne} \cdot [\frac{3}{2}\nabla p_e - \frac{5}{2}\frac{p_e}{n}\nabla n] + \eta J^2 - \nabla \cdot q_e + Q_\Delta$$
$$\frac{3}{2}\frac{\partial p_i}{\partial t} + \nabla \cdot (\frac{3}{2} p_i \vec{V}) = -p_i \nabla \cdot \vec{V} + \mu |\nabla V|^2 - \nabla \cdot q_i - Q_\Delta$$

Ideal MHD

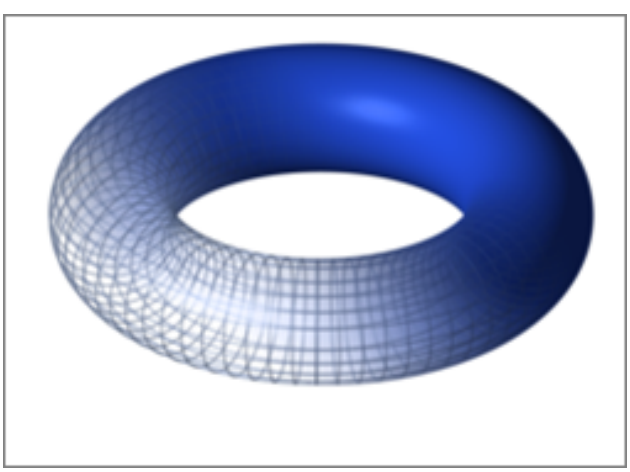
Resistive MHD

2-fluid Extended MHD

$$\vec{V} = \nabla U \times \hat{z} + \nabla_\perp \chi + V_z$$
$$\vec{B} = \nabla \psi \times \hat{z} + I\hat{z}$$

8 scalar variables: $\psi, I, U, \chi, V_z, n, p_e, p_i$

Δx **is typical element size**



Stiffness and Singularity

Temporal variation

Spatial variation

Fluid Dynamics Closure

$\rightarrow$ Stiff numerical problem

Preconditioning techniques

Implicit & Split Implicit Velocity Time-Advance

$$\begin{aligned}\{\rho - \theta^2(\delta t)^2 L\}V^{n+1} &= \{\rho - \theta^2(\delta t)^2 L\}V^n + \\ &\quad \delta t\{-\nabla p + \tfrac{1}{\mu_0}(\nabla \times B) \times B\}^{n+1/2}\end{aligned}$$

MHD operator

$$\begin{aligned}LV &\equiv \tfrac{1}{\mu_0}\{\nabla \times [\nabla \times (V \times B)]\} \times B + \\ &\quad \tfrac{1}{\mu_0}(\nabla \times B) \times \nabla \times (V \times B) + \\ &\quad \nabla(V \cdot \nabla p + \gamma p \nabla \cdot V)\end{aligned}$$

Operated by

$$\begin{bmatrix} \nabla\times \\ \vec{Z} \\ \nabla\cdot \end{bmatrix}$$

to separate fast wave, shear Alfven wave, and slow wave

corresponding to 3 sets of eigenvalues

$\Rightarrow$ reduce condition number.

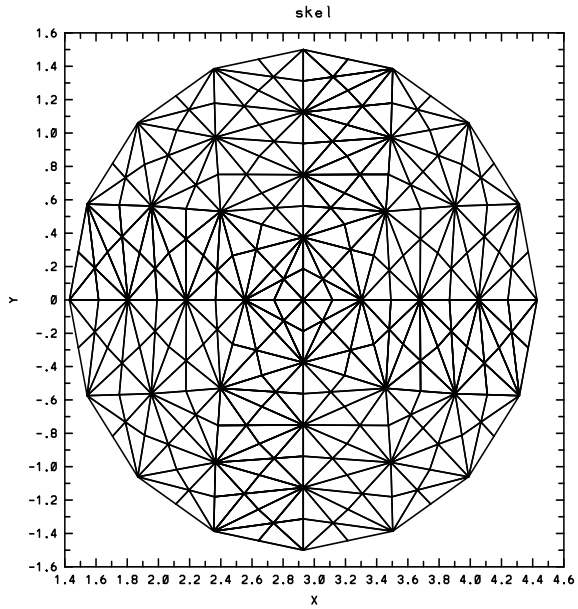
$$\begin{aligned}\lambda_1 &= (\rho_0 + sk_\parallel^2 B_0^2)k_\perp^2 \\ \lambda_2 &= (\rho_0 + sk_\parallel^2 p_0) \\ \lambda_3 &= -k_\parallel^2(\rho_0 + sk^2 B_0^2 + sk_\perp^2 \gamma p_0)\end{aligned}$$

Spatial Discretization

To be solved

- **in full 3D**
- **2D Planes with Fourier &**
  higher order finite difference decompositions
  in ϕ direction.

Using PETSc as an interface to access other preconditioners, such as Hypre, Superlu_dist, PDSLin, Mumps.



M3D, Solve as 2D Planes & Scalable Linear Solver

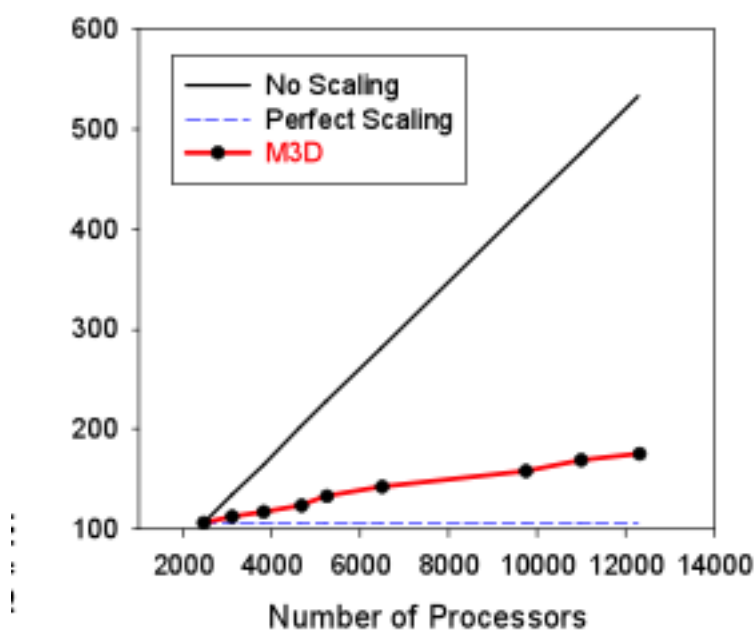
$$\begin{aligned} \nabla_\perp u &= f, \quad & (\nabla_\perp + \lambda)u &= f_\lambda \\ \nabla^\star u &= f^\star, \quad & (\nabla^\star + \lambda)u &= f^\star_\lambda \\ \nabla^\dagger u &= f^\dagger, \quad & (\nabla^\dagger + \lambda)u &= f^\dagger_\lambda \end{aligned}$$

with Dirichlet, Neumann boundary conditions, where

$$\begin{aligned} \nabla_\perp &= \frac{\partial^2}{\partial R^2} + \frac{\partial^2}{\partial R^2} \\ \nabla_\star &= \nabla_\perp - \frac{1}{R}\frac{\partial}{\partial R} \\ \nabla_\dagger &= \nabla_\perp + \frac{1}{R}\frac{\partial}{\partial R} \end{aligned}$$

Using BoomerAMG proconditioned CG through PETSc interface

Since the stiffness matices are symmetric non-negative defined.

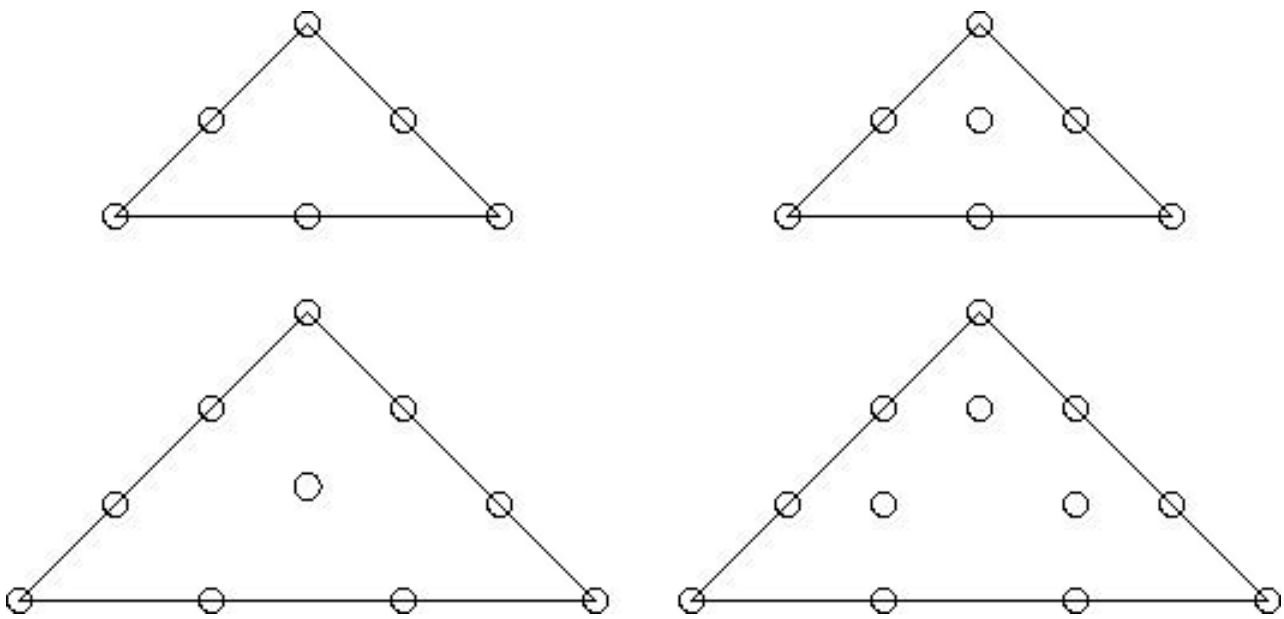


Higher Order Elements & Scalable Linear Solver

Lump higher order elements: 2nd & 3rd order

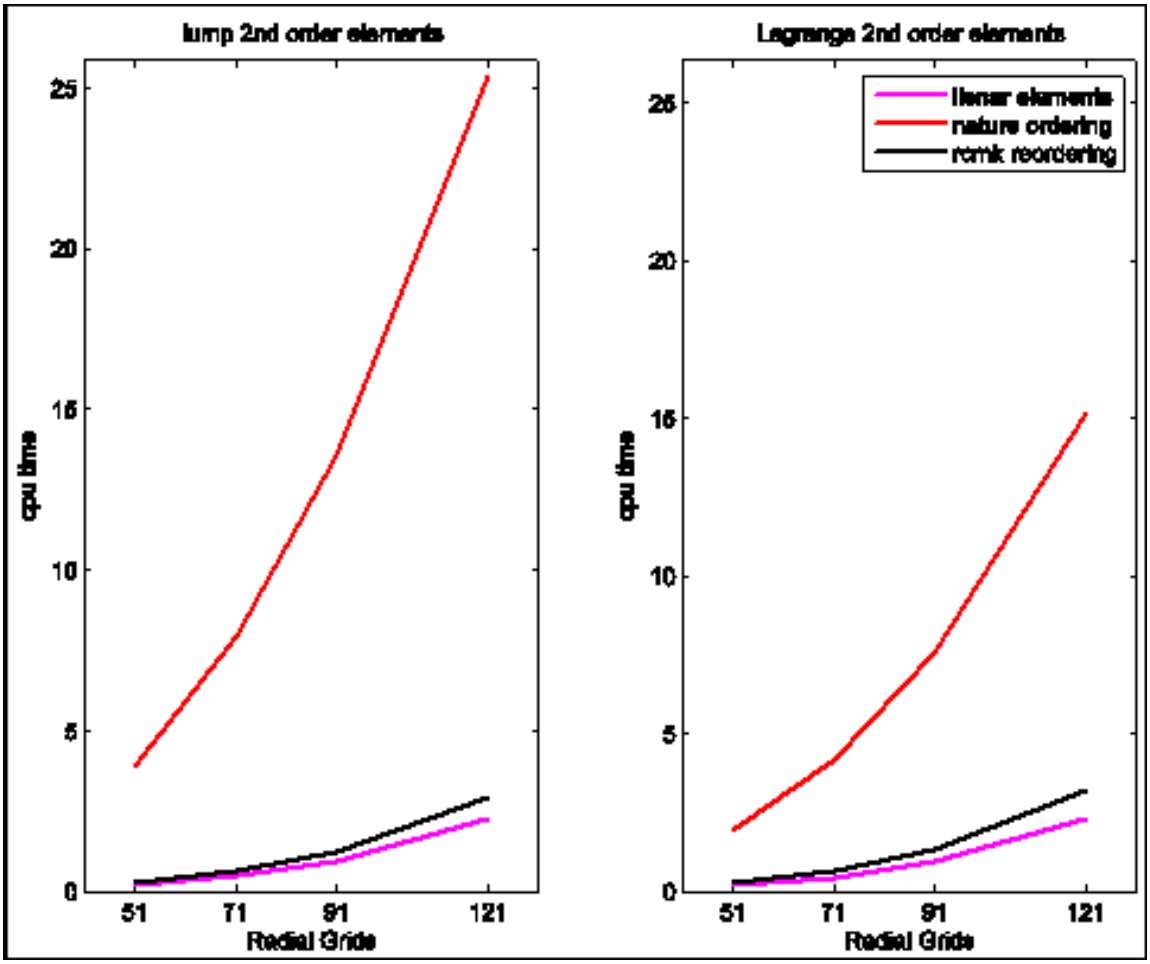
scales as well as linear elements:

- **Mass matrix lumping capable;**
- **RCMK (Reverse Cuthill-McKee) reordering stiffness matrices.**
- **BoomerAMG proconditioned CG through PETSc interface**

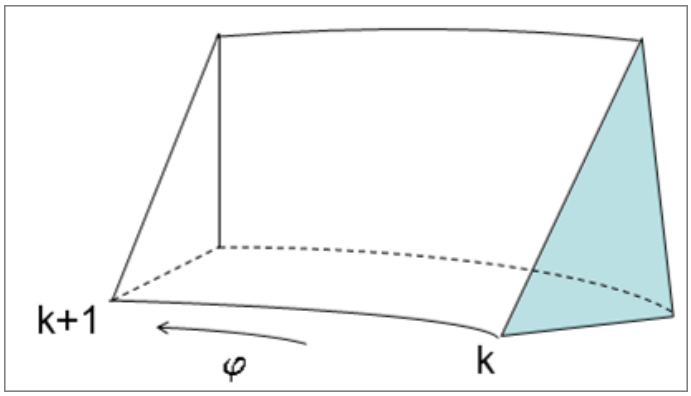


Lagrange elements **Lump elements**

Higher Order Elements & Scalable Linear Solver



M3D, Solve as Full 3D & Scalable Linear Solver



3D finite element: Each ϕ plane has two Hermite cubic functions associated with it

$$\Phi_1(x) = (|x|-1)^2(2|x|+1) \quad \Phi_2(x) = (|x|-1)^2(x)$$

$$\begin{aligned} U(R,Z,\phi) = \textstyle\sum_{j=1}^{18} v_j(R,Z)[\ & U^1_{j,k}\Phi_1(\phi/h)+ \\ & U^2_{j,k}\Phi_2(\phi/h)+ \\ & U^1_{j,k+1}\Phi_1(\phi/h-1)+ \\ & U^2_{j,k+1}\Phi_2(\phi/h-1)] \end{aligned}$$

On each plane, we use 5th order reduced quintic triangular with C^1 continuity across elements.

The Reduced Quintic Triangular Finite Element

- **All data is at nodes: function + first 5 derivatives (6 dofs)**

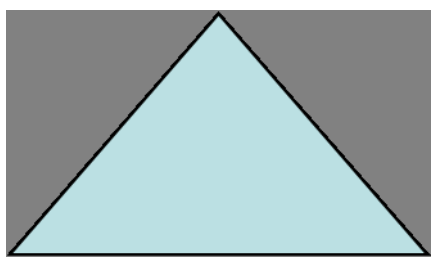
  $\Phi, \Phi_x, \Phi_y, \Phi_{xx}, \Phi_{xy}, \Phi_{yy}$

- **Complete quintic polynomial has 21 coefficients**

- **18 values come from the 3 nodes (3 x 6)**

  If we locally number the unknowns $\phi, \phi_x, \phi_y, \phi_{xx}, \phi_{xy}, \phi_{yy}$ **at** P_1 **at** $\Phi_1 - \Phi_6$**, at** P_2 **at** $\Phi_7 - \Phi_{12}$**, and at** P_3 **at** $\Phi_{13} - \Phi_{18}$**,**

  The general expression for the unknown function ϕ**:**



  $\phi(\xi, \eta) = \sum_{j=1}^{j=18} v_j \Phi_j$

  where $\Phi(R, \phi, Z) = \sum_{q=0}^{5} \sum_{p=0}^{q} \Phi_{p.q}(\phi) R^{q-p} Z^p$

- **3 values come from requirement that the normal derivative along each edge be only a (univariate) cubic, Leads to** C^1 **continuity**

- **Contains a complete Taylor series through** 4th **order in space without introducing auxiliary variables**

  error $\sim h^5$

The Sparse Linear System for Velocity Variables

$$\begin{bmatrix} S^v_{11} & S^v_{12} & S^v_{13} \\ S^v_{21} & S^v_{22} & S^v_{23} \\ S^v_{31} & S^v_{32} & S^v_{33} \end{bmatrix} \cdot \begin{bmatrix} U \\ \omega \\ \chi \end{bmatrix}^{n+1} = \begin{bmatrix} D^v_{11} & D^v_{12} & D^v_{13} \\ D^v_{21} & D^v_{22} & D^v_{23} \\ D^v_{31} & D^v_{32} & D^v_{33} \end{bmatrix}^{n+1} \cdot \begin{bmatrix} U \\ \omega \\ \chi \end{bmatrix}^{n} + \begin{bmatrix} R^v_{11} & R^v_{12} & R^v_{13} \\ R^v_{21} & R^v_{22} & R^v_{23} \\ R^v_{31} & R^v_{32} & R^v_{33} \end{bmatrix} \cdot \begin{bmatrix} \Psi \\ f \\ F \end{bmatrix}^{n+1/2}$$

corresponding to projections of the operator equation

Also contains 2 non-trivial sub-systems (reduced MHD) that conserve appropriate energy and are numerically stable

$$[S^v_{11}] \cdot [U]^{n+1} = [D^v_{11}] \cdot [U]^n + [R^v_{11}] \cdot [\Psi]$$

and

$$\begin{bmatrix} S^v_{11} & S^v_{12} \\ S^v_{21} & S^v_{22} \end{bmatrix} \cdot \begin{bmatrix} U \\ \omega \end{bmatrix}^{n+1} = \begin{bmatrix} D^v_{11} & D^v_{12} \\ D^v_{21} & D^v_{22} \end{bmatrix}^{n+1} \cdot \begin{bmatrix} U \\ \omega \end{bmatrix}^{n} + \begin{bmatrix} R^v_{11} & R^v_{12} \\ R^v_{21} & R^v_{22} \end{bmatrix} \cdot \begin{bmatrix} \Psi \\ f \end{bmatrix}^{n+1/2}$$

3D Nonlinear Scalable Solver

Leads to block triangular structure

$$\begin{bmatrix} B_1 & C_1 & & & & & \\ \cdot & \cdot & \cdot & & & & \\ & \cdot & \cdot & \cdot & & & \\ & & A_i & B_i & C_1 & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & \cdot & \cdot & \cdot \\ & & & & & A_N & N_N \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ x_i \\ \cdot \\ \cdot \\ x_N \end{bmatrix} = \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ y_i \\ \cdot \\ \cdot \\ y_N \end{bmatrix}$$

$$\begin{bmatrix} S_{11} \end{bmatrix}$$

$$\begin{bmatrix} S^v_{11} & S^v_{12} \\ S^v_{21} & S^v_{22} \end{bmatrix}$$

$$\begin{bmatrix} S^v_{11} & S^v_{12} & S^v_{13} \\ S^v_{21} & S^v_{22} & S^v_{23} \\ S^v_{31} & S^v_{32} & S^v_{33} \end{bmatrix}$$

Ill Conditioned,
Block-Jacobi preconditioned GMRES, SuperLU_Dist, Mumps, PDSLin solves
The 3 sets of eigenvalues correspond to

3D Nonlinear Scalable Solver

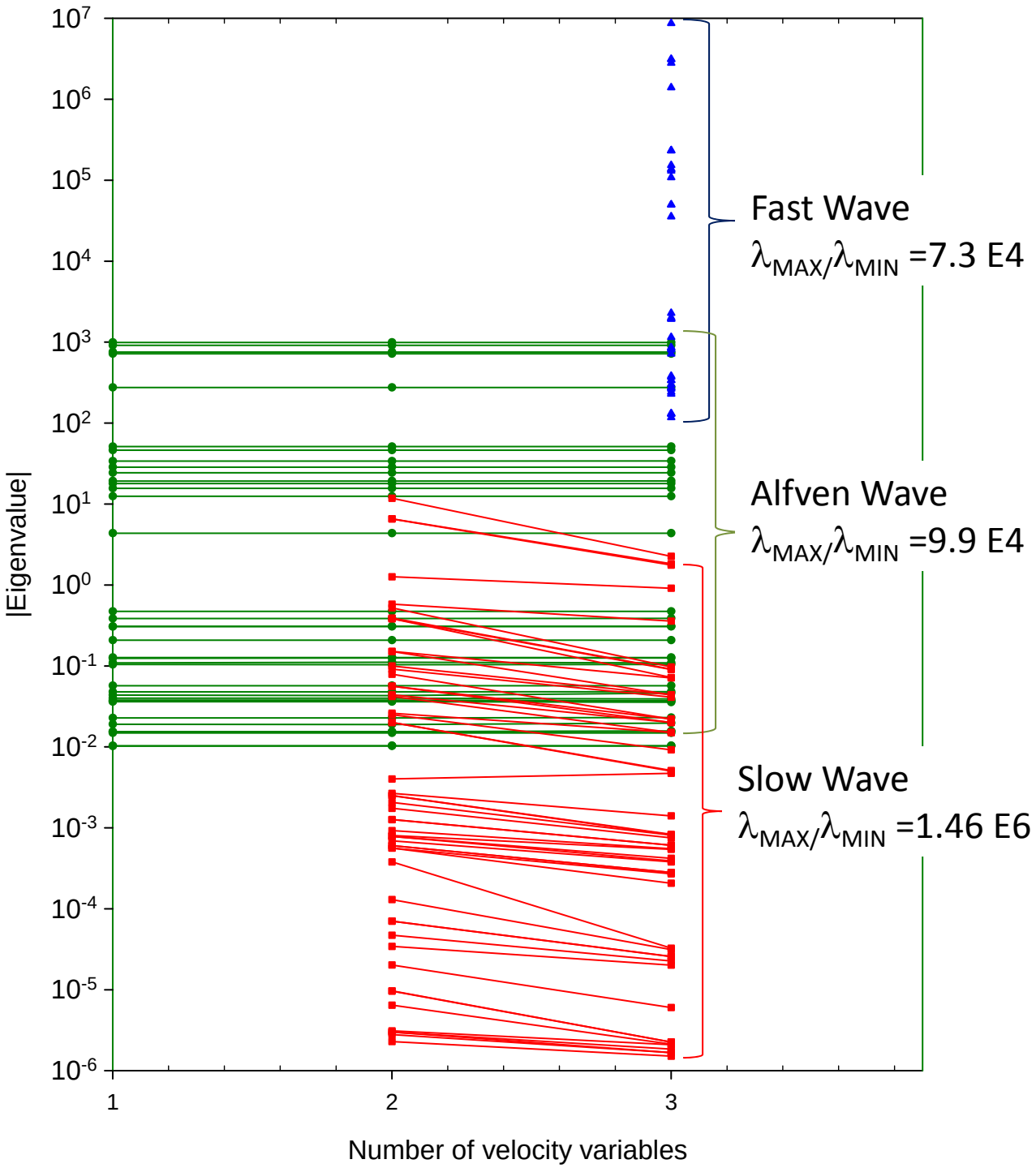
Calculate the eigenvalues:
Use SLEPc, EPS (Eigenvalue Problem Solvers)

PETSc based Scalable Library for Eigenvalue Problem

Developed by Jose E Roman, Eloy Romero, Andres Tomas

At www.grycap.upv.es/slepc

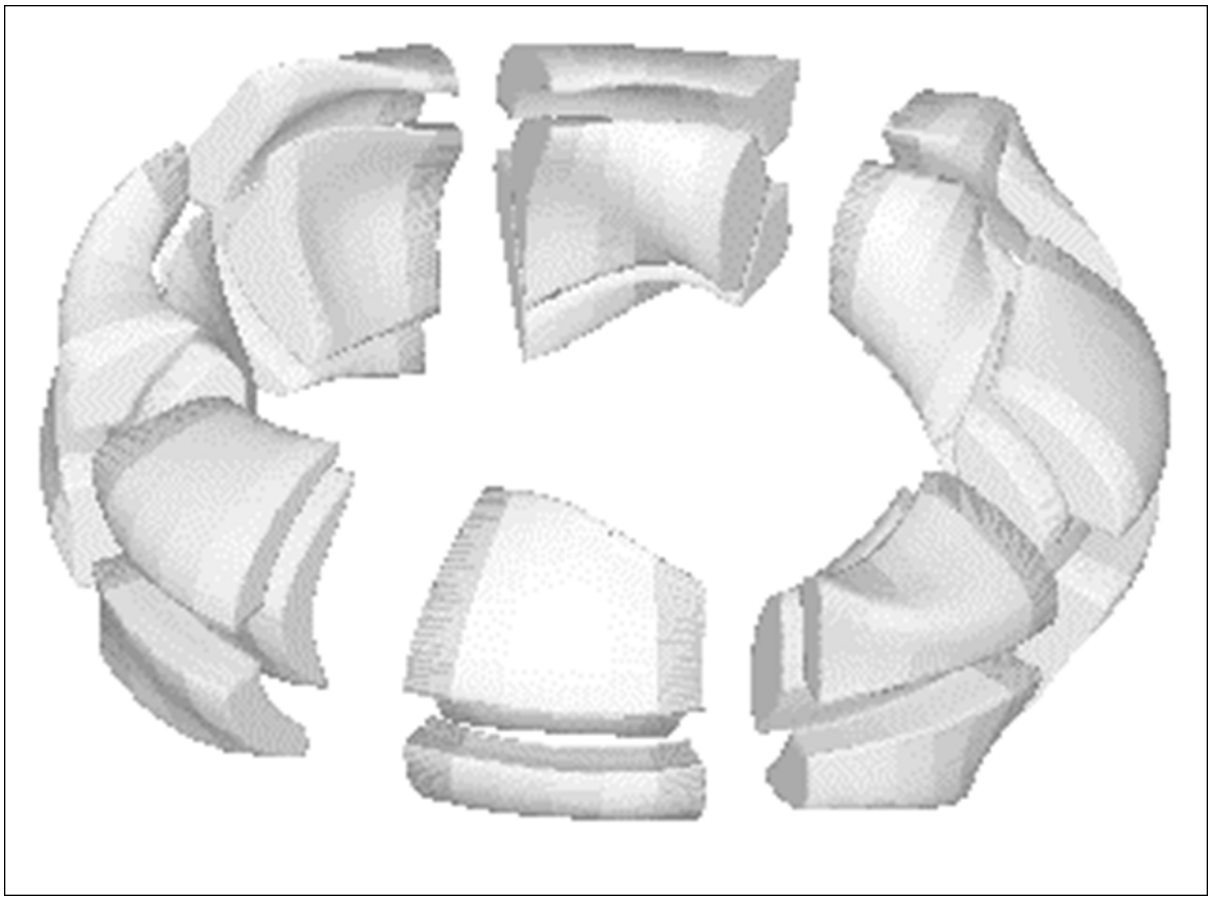
3D Nonlinear Scalable Solver



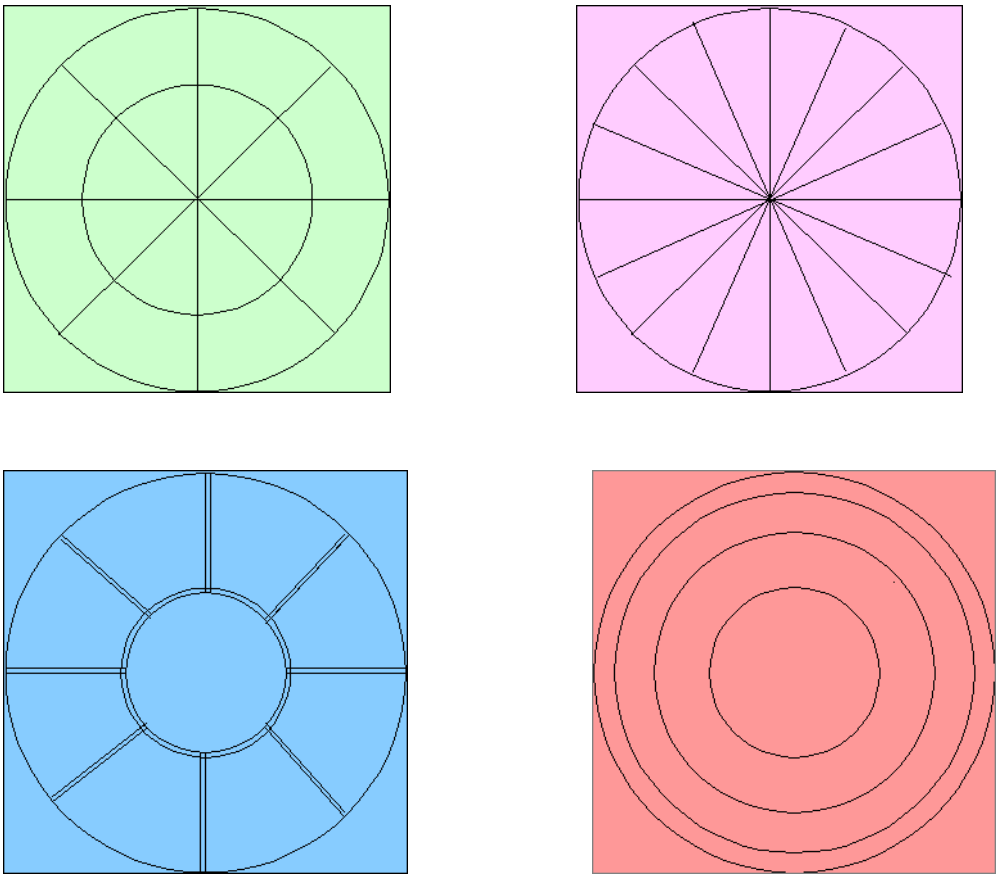
Scalability Studies

- **implicit time advance as physics preconditioning**
- **separate fast wave, shear alfven wave, compressive alfven, slow wave to further reduce condition number**
- **Jacobi preconditioning to reduce the condition number by a factor of 3**

Decomposition in ϕ direction



Decomposition in (R, Z) plane



ghost nodes communication optimization

Architecture: HOPPER at NERSC

NERSC's first peta-flop system

a Cray XE6, with 153,216 compute cores

217 TB of memory and 2PB of disk

5 on the November 2010 Top500 Supercomputer list.

Compute Node Configuration

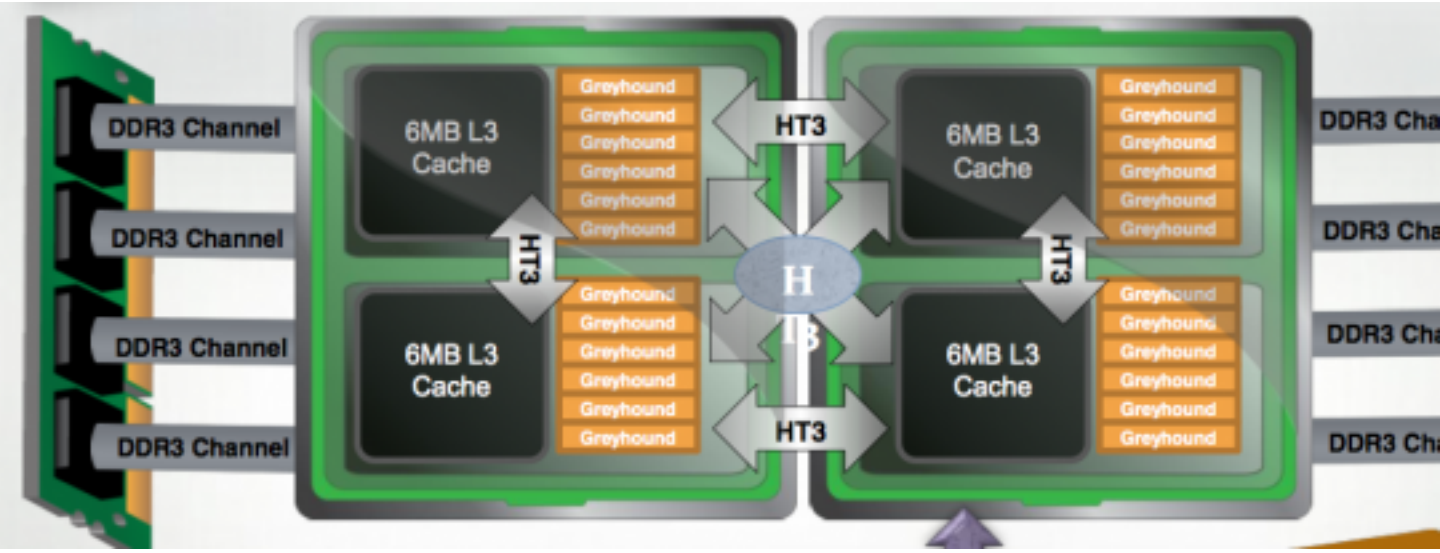
6384 nodes

2 twelve-core AMD 'MagnyCours' 2.1 GHz processors per node

24 cores per node (153,216 total cores)

Each core has their own L1 and L2 caches

6 MB L3 cache shared between 6 cores on the MagnyCours processor



Scalability Studies

Grid MPI COMM Configuration

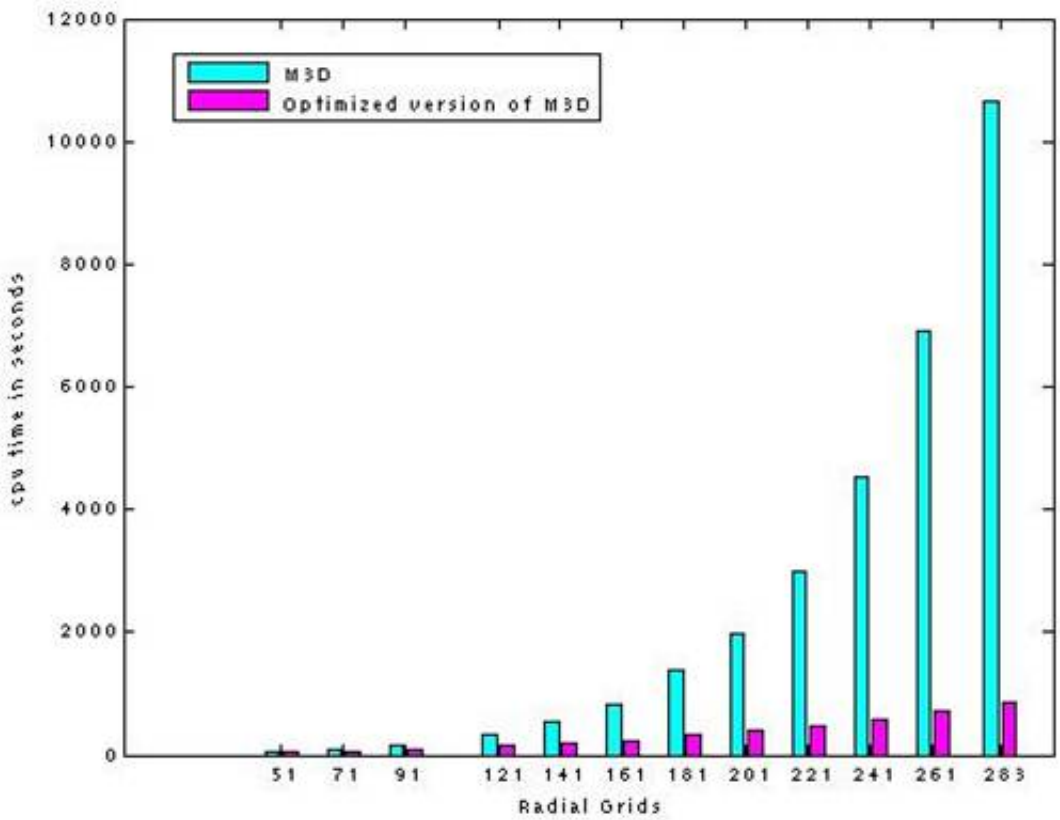
$Case\#$	A	B	C	D	E	F
1	168	84	170	2	5	5
2	192	96	190	2	6	8
3	216	108	203	2	7	11
4	240	120	213	2	8	14
5	272	136	220	2	9	17
6	296	148	225	2	10	20
7	320	160	229	2	11	23
8	344	172	233	2	12	26
9	368	184	236	2	13	29
10	$4l6$	208	241	2	15	35
11	440	220	242	2	16	38
12	464	232	244	2	17	41
13	512	256	247	2	19	47

A. Total number of planes in toroidal direction.
B. Number of CPUs in toroidal direction (B¡=A).
C. Number of grids in minor radial direction.
D. Number of CPUs in radial direction.
E. Number of mesh partitions in theta direction (E¿=3).
F. Number of CPUs in theta direction.

Scalability Studies

Total number of nodes:
$(1 + \frac{B(B-1)}{2} \times A$

Total number of CPUs:
$D > 1 : B \times E \times D^2$
$D = 1 : B \times F$



Summary & Future Development

Scalable Linear & Nonlinear Solver on multicore & GPU clusters

- **Physics based preconditioning for the whole MHD system**
- **Spatial Discretization related preconditioning**
  - **Scalable higher order element (Lump elements)**
  - **Separate spectrum with different spatial scales**
- **Matrix related preconditioning**
- **Scalable parallel I/O**

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