A Newton-Krylov solver for fully implicit 3D extended MHD

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In collaboration with B. Philip (LANL), J. Shadid, R. Pawlowski, J. Banks (SNL)

2007 OASCR PI MEETING

MAY 22-24, 2007

LIVERMORE, CA, USA

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Outline

- Motivation: XMHD and the tyranny of scales
- Parabolization of XMHD: key for SCALABILITY
- Resistive MHD
- Hall MHD
- Migration to unstructured FE: status report (with SNL)
- Spatial adaptivity: Implicit + AMR (with B. Philip, LANL LDRD)

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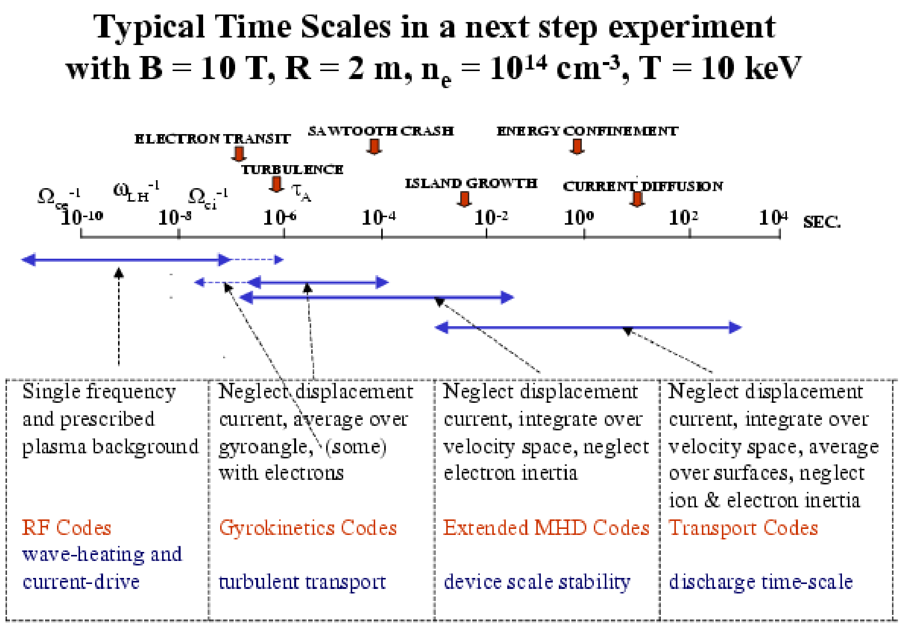
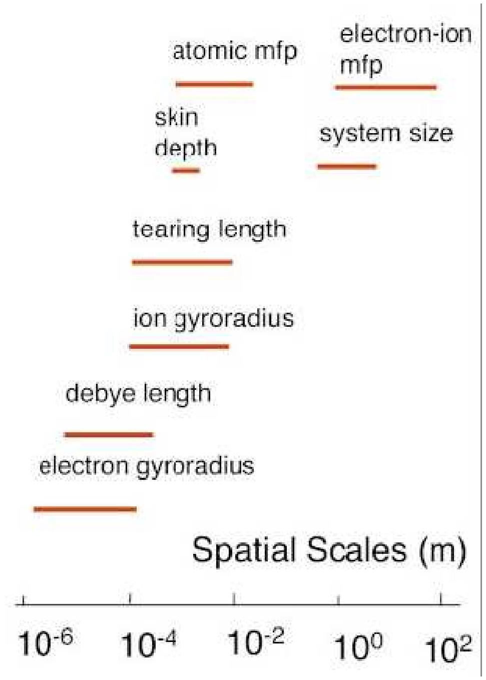
“The tyranny of scales” (SBES report, 2006)



(a) Time scales in fusion plasmas (FSP report)



(b) Length scales in a typical fusion plasma (Tang, *Phys. Plasmas*, 9 (5), 2002)

"The tyranny of scales will not be simply defeated by building bigger and faster computers" (SBES report, p. 30)

Algorithmic challenges in XMHD

- XMHD has mixed character, with strongly hyperbolic and parabolic components.
- Numerically, XMHD is a nonlinear algebraic system of very stiff equations:
  - Elliptic stiffness (diffusion): $\kappa(J) \sim \frac{\Delta t\, D}{\Delta x^2} \gg 1$
  - Hyperbolic stiffness (linear and dispersive waves): $\kappa(J) \sim \Delta t\, \omega_{fast} \sim \frac{\Delta t}{\Delta t_{CFL}} \gg 1$
- Brute-force algorithms will not be able to cover the span between disparate time/length scales, regardless of computer power (SBES report).
- Key algorithmic requirement: SCALABILITY [$CPU \sim \mathcal{O}(N/n_p)$]!
  - Minimize number of degrees of freedom N: spatial adaptivity.
  - Follow slowest time scales (application dependent): implicit time stepping.
- Scalable implicit methods require MULTILEVEL approaches:

$$CPU \sim \mathcal{O}\left(\frac{N\ \log(N)}{np^{\beta}}\right)\ ,\ \beta \lesssim 1$$

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XMHD and multilevel approaches

- A fundamental component of iterative ML methods is the SMOOTHER.
- XMHD is strongly hyperbolic $\Rightarrow$ smoothing is a serious challenge (diagonally submissive for $\Delta t > \Delta t_{CFL}$).
  - Previous attempts to use multilevel methods (two-level NKS, MG-NKS) on XMHD have failed to demonstrate a scalable XMHD solver.

Our solution: parabolize XMHD! (multilevel-friendly)

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Parabolization and Schur complement: an example

PARABOLIZATION EXAMPLE:

$$\partial_t u = \partial_x v \ , \ \partial_t v = \partial_x u.$$

$$u^{n+1} = u^n + \Delta t \partial_x v^{n+1}, v^{n+1} = v^n + \Delta t \partial_x u^{n+1}.$$

$$\boxed{(I - \Delta t^2 \partial_{xx}) u^{n+1} = u^n + \Delta t \partial_x v^n}$$

- PARABOLIZATION via SCHUR COMPLEMENT:

$$\begin{bmatrix} D_1 & U \\ L & D_2 \end{bmatrix} = \begin{bmatrix} I & U D_2^{-1} \\ 0 & I \end{bmatrix} \begin{bmatrix} D_1 - U D_2^{-1} L & 0 \\ 0 & D_2 \end{bmatrix} \begin{bmatrix} I & 0 \\ D_2^{-1} L & I \end{bmatrix}.$$

Stiff off-diagonal blocks L, U now sit in diagonal via Schur complement $D_1 - U D_2^{-1} L$. The system has been "PARABOLIZED."

$$D_1 - U D_2^{-1} L = (I - \Delta t^2 \partial_{xx})$$

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Our approach to a successful fully implicit algorithm for XMHD

- Even if a smoother exists, MG is remarkably temperamental.
- Combination of Krylov methods and MG is optimal:
  - MG provides scalability (as a preconditioner)
  - Krylov provides robustness

> We seek to develop a successful algorithm for XMHD based on Newton-Krylov-MG

- Proof the concept in resistive MHD, and then move to XMHD.

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Jacobian-Free Newton-Krylov Methods

- Objective: solve nonlinear system $\vec{G}(\vec{x}^{n+1}) = \vec{0}$ efficiently (scalably).
- Converge nonlinear couplings using Newton-Raphson method: $\left.\frac{\partial \vec{G}}{\partial \vec{x}}\right|_k \delta \vec{x}_k = -\vec{G}(\vec{x}_k)$.
- Jacobian-free implementation: $\left(\frac{\partial \vec{G}}{\partial \vec{x}}\right)_k \vec{y} = J_k \vec{y} = \lim_{\epsilon \to 0} \frac{\vec{G}(\vec{x}_k + \epsilon \vec{y}) - \vec{G}(\vec{x}_k)}{\epsilon}$
- Krylov method of choice: GMRES (nonsymmetric systems).
- Right preconditioning: solve equivalent Jacobian system for $\delta y = P_k \delta \vec{x}$:

$$J_k P_k^{-1} \underbrace{P_k \delta \vec{x}}_{\delta \vec{y}} = -\vec{G}_k$$

APPROXIMATIONS IN PRECONDITIONER DO NOT AFFECT ACCURACY OF CONVERGED SOLUTION; THEY ONLY AFFECT EFFICIENCY!

Implicit *resistive* MHD solver

Resistive MHD model equations

$$\begin{aligned}
\frac{\partial \rho}{\partial t} &+ \nabla \cdot (\rho \vec{v}) = 0, \\
\frac{\partial \vec{B}}{\partial t} &+ \nabla \times \vec{E} = 0, \\
\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot \Big[\rho \vec{v}\vec{v} - \vec{B}\vec{B} &- \rho \nu \nabla \vec{v} + \overleftrightarrow{I}(p + \frac{B^2}{2}) \Big] = 0, \\
\frac{\partial T}{\partial t} + \vec{v} \cdot \nabla T &+ (\gamma - 1) T \nabla \cdot \vec{v} = 0,
\end{aligned}$$

- Plasma is assumed polytropic $p \propto n^\gamma$.
- Resistive Ohm's law:

$$\vec{E} = -\vec{v} \times \vec{B} + \eta \nabla \times \vec{B}$$

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Resistive MHD Jacobian block structure

- The linearized resistive MHD model has the following couplings:

$$
\begin{aligned}
\delta\rho &= L_\rho(\delta\rho, \delta\vec{v}) \\
\delta T &= L_T(\delta T, \delta\vec{v}) \\
\delta\vec{B} &= L_B(\delta\vec{B}, \delta\vec{v}) \\
\delta\vec{v} &= L_v(\delta\vec{v}, \delta\vec{B}, \delta\rho, \delta T)
\end{aligned}
$$

- Therefore, the Jacobian of the resistive MHD model has the following coupling structure:

$$
J\delta\vec{x} = \begin{bmatrix} D_\rho & 0 & 0 & U_{v\rho} \\ 0 & D_T & 0 & U_{vT} \\ 0 & 0 & D_B & U_{vB} \\ L_{\rho v} & L_{Tv} & L_{Bv} & D_v \end{bmatrix} \begin{pmatrix} \delta\rho \\ \delta T \\ \delta\vec{B} \\ \delta\vec{v} \end{pmatrix}
$$

- Diagonal blocks contain advection-diffusion contributions, and are “easy” to invert using MG techniques. Off diagonal blocks L and U contain all hyperbolic couplings.

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PARABOLIZATION: Schur complement formulation

- We consider the block structure:

$$J\delta\vec{x} = \left[\begin{array}{cc} M & U \\ L & D_v \end{array}\right]\left(\begin{array}{c} \delta\vec{y} \\ \delta\vec{v} \end{array}\right) \quad ; \quad \delta\vec{y} = \left(\begin{array}{c} \delta\rho \\ \delta T \\ \delta\vec{B} \end{array}\right) \quad ; \quad M = \left(\begin{array}{ccc} D_\rho & 0 & 0 \\ 0 & D_T & 0 \\ 0 & 0 & D_B \end{array}\right)$$

- M is "easy" to invert (advection-diffusion, MG-friendly).

Schur complement analysis of 2x2 block J yields:

$$\left[\begin{array}{cc} M & U \\ L & D_v \end{array}\right]^{-1} = \left[\begin{array}{cc} I & 0 \\ -LM^{-1} & I \end{array}\right]\left[\begin{array}{cc} M^{-1} & 0 \\ 0 & P_{Schur}^{-1} \end{array}\right]\left[\begin{array}{cc} I & -M^{-1}U \\ 0 & I \end{array}\right],$$

$$P_{Schur} = D_v - LM^{-1}U.$$

- EXACT Jacobian inverse only requires M^{-1} and P_{Schur}^{-1}.
- Schur complement formulation is fundamentally unchanged in Hall MHD!

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Physics-based preconditioner (I)

- The Schur complement analysis translates into the following 3-step EXACT inversion algorithm:

$$
\begin{aligned}
\text{Predictor} &: \quad \delta\vec{y}^* = -M^{-1}G_y \\
\text{Velocity update} &: \quad \delta\vec{v} = P_{Schur}^{-1}[-G_v - L\delta\vec{y}^*], \;\; P_{Schur} = D_v - LM^{-1}U \\
\text{Corrector} &: \quad \delta\vec{y} = \delta\vec{y}^* - M^{-1}U\delta\vec{v}
\end{aligned}
$$

- MG treatment of P_{Schur} is impractical due to M^{-1}.

> Need suitable simplifications (SEMI-IMPLICIT)!

- We consider the small-flow-limit case: $M^{-1} \approx \Delta t$
- This approximation is equivalent to splitting flow in original equations.

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Physics-based preconditioner (II)

- Small flow approximation: $M^{-1} \approx \Delta t$ in steps 2 & 3 of Schur algorithm:

$$\begin{aligned} \delta\vec{y}^* &= -M^{-1} G_y \\ \delta\vec{v} &\approx P_{SI}^{-1}\left[-G_v - L\delta\vec{y}^*\right] \; ; \; P_{SI} = D_v - \Delta t L U \\ \delta\vec{y} &\approx \delta\vec{y}^* - \Delta t U \delta\vec{v} \end{aligned}$$

where:

$$\boxed{P_{SI} = \rho^n \left[\overleftrightarrow{I}/\Delta t + \theta(\vec{v}_0 \cdot \nabla \overleftrightarrow{I} + \overleftrightarrow{I} \cdot \nabla\vec{v}_0 - \nu^n \nabla^2 \overleftrightarrow{I})\right] + \Delta t \theta^2 W(\vec{B}_0, p_0)}$$

$$W(\vec{B}_0, p_0) = \vec{B}_0 \times \nabla \times \nabla \times [\overleftrightarrow{I} \times \vec{B}_0] - \vec{j}_0 \times \nabla \times [\overleftrightarrow{I} \times \vec{B}_0] - \nabla[\overleftrightarrow{I} \cdot \nabla p_0 + \gamma p_0 \nabla \cdot \overleftrightarrow{I}]$$

- P_{SI} is block diagonally dominant by construction!
- We employ multigrid methods (MG) to approximately invert P_{SI} and M: 1 V(4,4) cycle

Efficiency: Δt scaling (2D tearing mode)

32×32

Δt	Newton/Δt	GMRES/Δt	CPU (s)	CPU_{exp}/CPU	$\Delta t/\Delta t_{CFL}$
2	5.9	20.9	115	3.1	354
3	5.9	25.6	139	3.8	531
4	6.0	30.5	163	4.3	708
6	6.0	34.7	184	5.8	1062

128×128

Δt	Newton/Δt	GMRES/Δt	CPU (s)	CPU_{exp}/CPU	$\Delta t/\Delta t_{CFL}$
0.5	4.9	8.4	764	8.0	380
0.75	5.7	10.2	908	10.0	570
1.0	5.0	11.5	1000	12.7	760
1.5	5.6	14.7	1246	14.6	1140

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Efficiency: grid scaling

$\Delta t \approx 1100\Delta t_{CFL}$, 10 time steps

Grid	Δt	Newton/Δt	GMRES/Δt	CPU	$\widehat{CPU}$
32x32	6	6.0	34.7	184	5.3
64x64	3	5.8	22.9	468	20.4
128x128	1.5	5.6	14.8	1246	84.2

Why does GMRES/Δt decrease with resolution?

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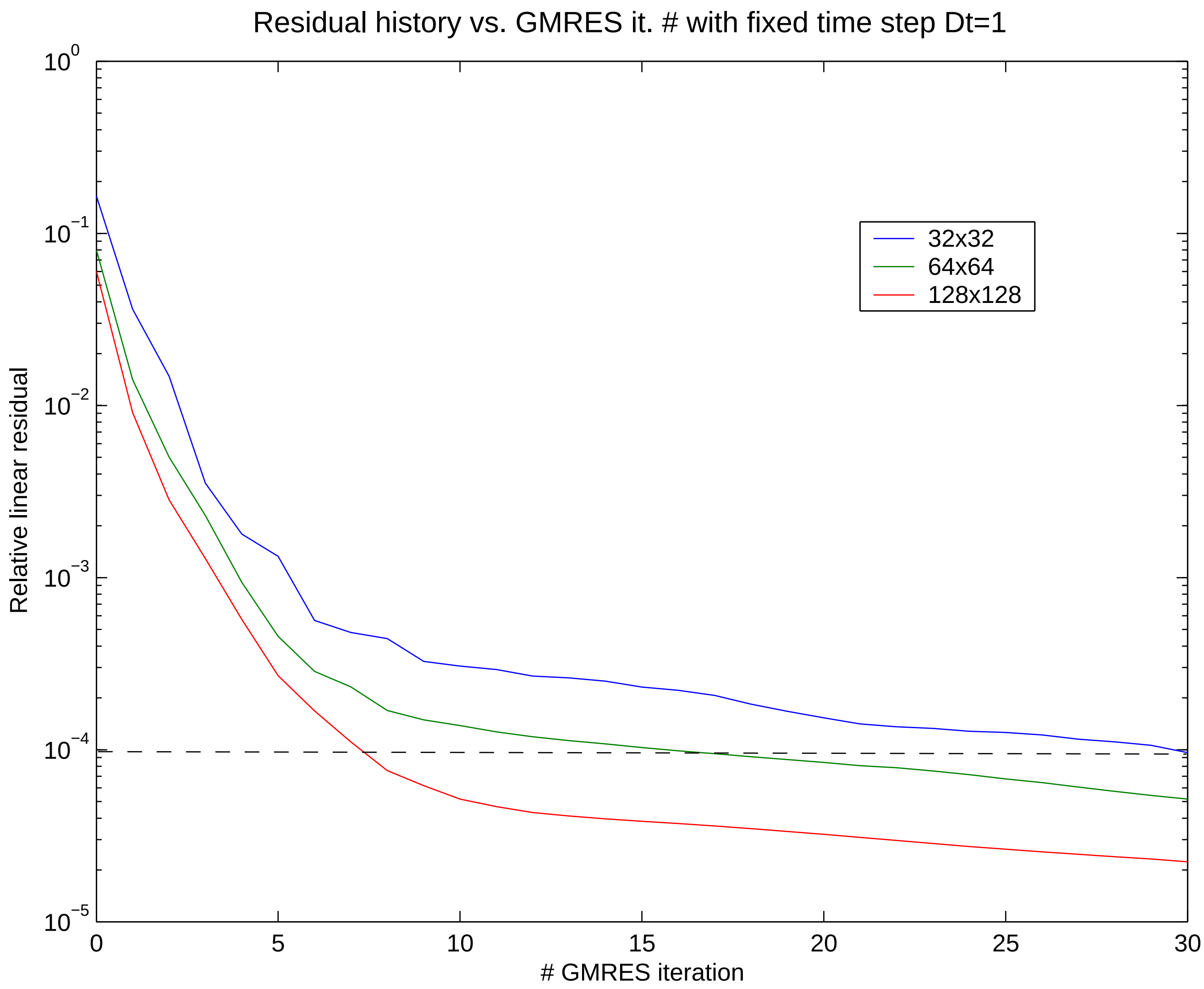
Effect of spatial truncation error



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Implicit *extended* MHD solver

Extended MHD model equations

$$\begin{aligned}
\frac{\partial \rho}{\partial t} &+ \nabla \cdot (\rho \vec{v}) = 0, \\
\frac{\partial \vec{B}}{\partial t} &+ \nabla \times \vec{E} = 0, \\
\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot \left[\rho \vec{v}\vec{v} - \vec{B}\vec{B} \right. &- \left. \rho \nu \nabla \vec{v} + \overleftrightarrow{I}(p + \frac{B^2}{2}) \right] = 0, \\
\frac{\partial T_e}{\partial t} + \vec{v} \cdot \nabla T_e &+ (\gamma - 1) T_e \nabla \cdot \vec{v} = 0,
\end{aligned}$$

- Plasma is assumed polytropic $p \propto n^\gamma$.
- We assume cold ion limit: $T_i \ll T_e \Rightarrow \boxed{p \approx p_e}$.
- Generalized Ohm's law:

$$\boxed{\vec{E} = -\vec{v} \times \vec{B} + \eta \nabla \times \vec{B} - \frac{d_i}{\rho}(\vec{j} \times \vec{B} - \nabla p_e)}$$

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Extended MHD Jacobian block structure

- The linearized extended MHD model has the following couplings:

$$
\begin{aligned}
\delta\rho &= L_\rho(\delta\rho, \delta\vec{v}) \\
\delta T &= L_T(\delta T, \delta\vec{v}) \\
\delta\vec{B} &= L_B(\delta\vec{B}, \delta\vec{v}, \delta\rho, \delta T) \\
\delta\vec{v} &= L_v(\delta\vec{v}, \delta\vec{B}, \delta\rho, \delta T)
\end{aligned}
$$

- Jacobian coupling structure:

$$
J\delta\vec{x} = \begin{bmatrix} D_\rho & 0 & 0 & U_{v\rho} \\ 0 & D_T & 0 & U_{vT} \\ L_{\rho B} & L_{TB} & D_B & U_{vB} \\ L_{\rho v} & L_{Tv} & L_{Bv} & D_v \end{bmatrix} \begin{pmatrix} \delta\rho \\ \delta T \\ \delta\vec{B} \\ \delta\vec{v} \end{pmatrix}
$$

- We have added off-diagonal couplings.

Extended MHD Jacobian block structure (cont.)

- The coupling structure can be substantially simplified if we note $(p \approx p_e)$:

$$\frac{1}{\rho}(\vec{j} \times \vec{B} - \nabla p_e) \approx \frac{D\vec{v}}{Dt}$$

and therefore:

$$\vec{E} \approx -\vec{v} \times \vec{B} + \frac{\eta(T)}{\mu_0}\nabla \times \vec{B} - d_i \frac{D\vec{v}}{Dt}$$

- This transforms jacobian coupling structure to:

$$J\delta\vec{x} \approx \begin{bmatrix} D_\rho & 0 & 0 & U_{v\rho} \\ 0 & D_T & 0 & U_{vT} \\ 0 & 0 & D_B & U_{vB}^R + U_{vB}^H \\ L_{\rho v} & L_{Tv} & L_{Bv} & D_v \end{bmatrix} \begin{pmatrix} \delta\rho \\ \delta T \\ \delta\vec{B} \\ \delta\vec{v} \end{pmatrix}$$

We can therefore reuse ALL resistive MHD PC framework!

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Extended MHD preconditioner

- Use same Schur complement approach.
- M block contains ion scales only! Approximation $M^{-1} \approx \Delta t$ is very good in extended MHD (ion scales do NOT contribute to numerical stiffness).
- Additional block U_{vB}^{H} results, after the Schur complement treatment, in systems of the form:

$$\partial_t \delta\vec{v} - d_i \vec{B}_0 \times (\nabla \times \nabla \times \delta\vec{v}) = rhs$$

- This system supports dispersive waves $\omega \sim k^2$!
- We have shown analytically that damped JB is a smoother for these systems!

We can use classical MG!

Preliminary efficiency results (2D tearing mode)

$d_i = 0.05$

1 time step, $\Delta t = 1.0$, V(3,3) cycles, mg_tol=1e-2

Grid	Newton/Δt	GMRES/Δt	CPU (s)	CPU_{exp}/CPU	$\Delta t/\Delta t_{exp}$
32x32	5	22	25	0.44	110
64x64	5	12	66	1.4	238
128x128	5	8	164	6.2	640
256x256	4	7	674	30	3012

Again, GMRES/Δt decreases with resolution!

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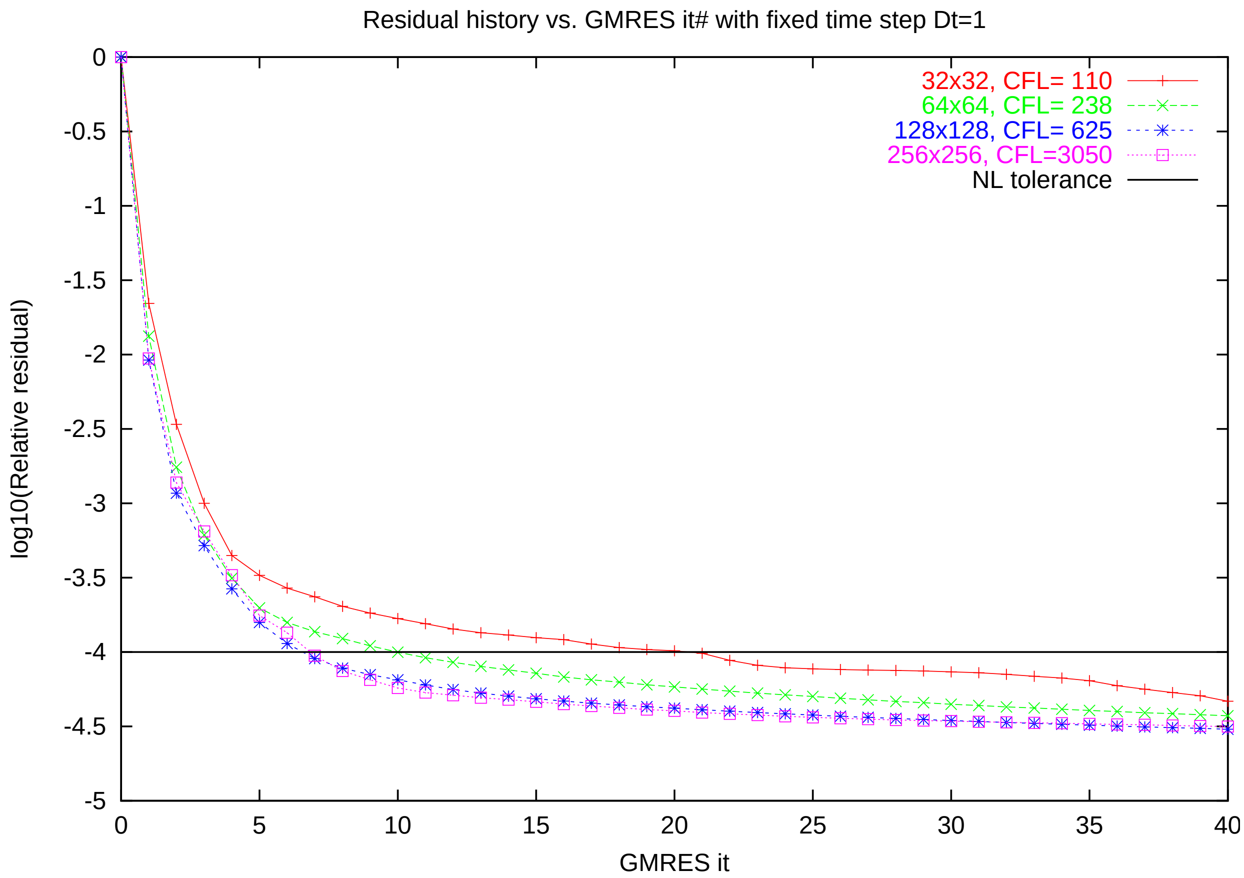
Effect of spatial truncation error



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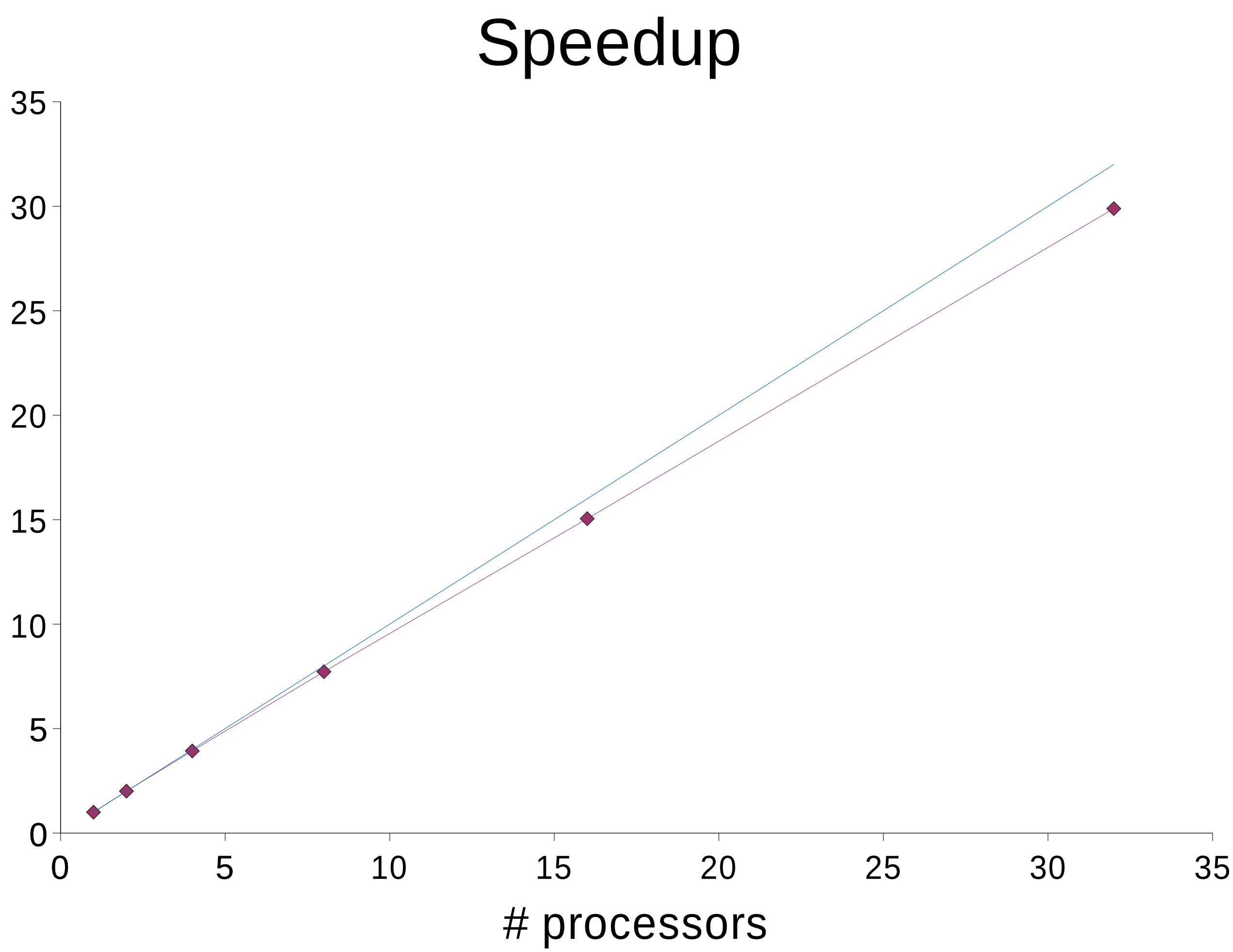
Parallel performance with PETSc Toolkit
(unpreconditioned, 3D, weak scaling with 32^3 nodes per processor)



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Migration to unstructured FE

(In collaboration with J. Shadid, R. Pawlowski, J. Banks, SNL)

Currently: Initial Single Fluid Resistive MHD Unstructured FE Formulation

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \bullet \mathbf{F} + \mathbf{S} = \mathbf{0}$$

$$E = e + \frac{1}{2}\|\mathbf{v}\|^2$$

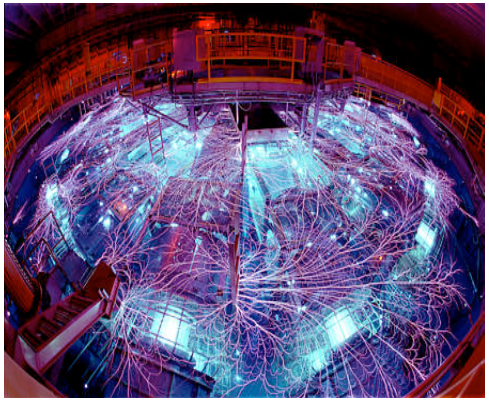
$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho\mathbf{v} \\ \Sigma_{tot} \\ \mathbf{B} \end{bmatrix} \quad \mathbf{F} = \begin{bmatrix} \rho\mathbf{v} \\ \rho\mathbf{v}\otimes\mathbf{v} - \frac{1}{\mu_0}\mathbf{B}\otimes\mathbf{B} - \mathbf{T} + \frac{1}{2\mu_0}\|\mathbf{B}\|^2\mathbf{I} \\ \rho E\mathbf{v} - \mathbf{T}\cdot\mathbf{v} + \mathbf{E}\times\mathbf{B} + \mathbf{q} \\ \mathbf{v}\otimes\mathbf{B} - \mathbf{B}\otimes\mathbf{v} - \frac{\eta}{\mu_0}\left(\nabla\mathbf{B} - \nabla\mathbf{B}^T\right) \end{bmatrix} \quad \mathbf{S} = \begin{bmatrix} 0 \\ \mathbf{0} \\ Q^{rad} + Q \\ \mathbf{0} \end{bmatrix}$$

$$\Sigma_{tot} = \rho E + \frac{1}{2\mu_0}\|\mathbf{B}\|^2$$

$$\mathbf{E} = -\mathbf{v}\times\mathbf{B} + \eta\mathbf{J} + \underbrace{\frac{1}{en}(\mathbf{J}\times\mathbf{B} - \nabla\mathbf{P}_e)}_{\text{Hall}} + \underbrace{\frac{m_e}{e^2 n_e}\frac{d\mathbf{J}}{dt}}_{\text{Inertia}}.$$

Project Goals:

- **Develop stable, accurate, physics compatible, scalable and efficient fully-implicit computational formulations for xMHD and PTR (e.g. SNL Cray XT3 12.5K nodes, 25K cores)**
- **Develop and evaluate scalable physics-based preconditioners, based on multi-level methods**
- **Produce comprehensive accuracy, convergence, stability and scalability studies employing challenging prototype problems.**
- **Produce first-of-a-kind large-scale computational demonstrations on selected science / technology problems**
  - **Science**
    - **Magnetic Reconnection Studies**
    - **Hydro-Magnetic Rayleigh-Taylor (e.g. Z-pinch [HEDP])**
  - **Technology (e.g. advanced materials processing)**
    - **Plasma arc jet CVD, Plasma CVD/ Etching**



(J. N. Shadid, R. P. Pawlowski, J. W. Banks - SNL)

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Currently:

- **2D & 3D Incompressible Resistive MHD**
- **Unstructured Stabilized Finite Elements**
- **2D Vector Potential; 2D&3D Projection Method;**
- **Fully-implicit 1st & 2nd order (BE, TR, BDF2);**
- **Direct to Steady State; Continuation;**
- **Parallel Newton-Krylov:**
    - **Additive Schwarz DD w/ Variable Overlap;**
    - **Aggressive Coarsening Block AMG for Systems (w/ R. Tuminaro, P. Lin -SNL);**

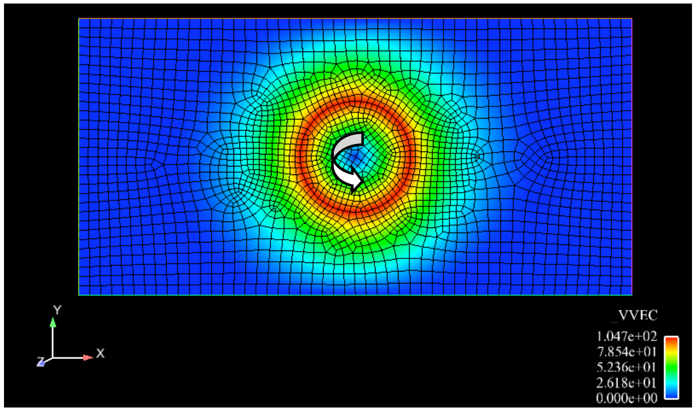
Soon:

- **Physics Based Preconditioning (w/ L. Chacon LANL)**
- **Compressible Resistive / Extended MHD**
- **Monotone Hyperbolic Solver (FE-TVD/FCT)**
- **Compatible Discretizations (e.g De Rham complex - w/ P. Bochev SNL)**

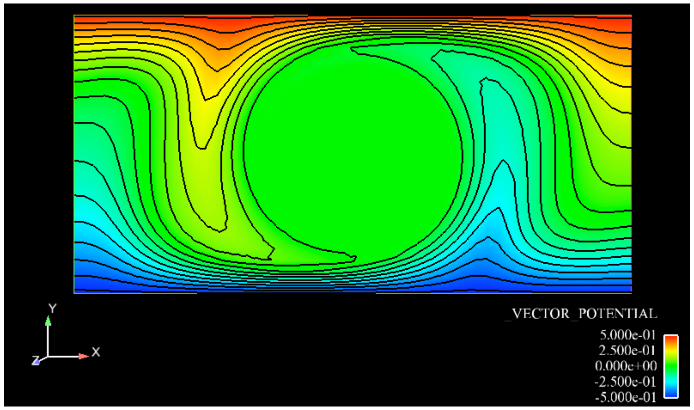
Example Unstructured Mesh Solutions

Flux Expulsion Rotating Cyl. 5000 RPM (steady state)

Fluid Velocity Magnitude

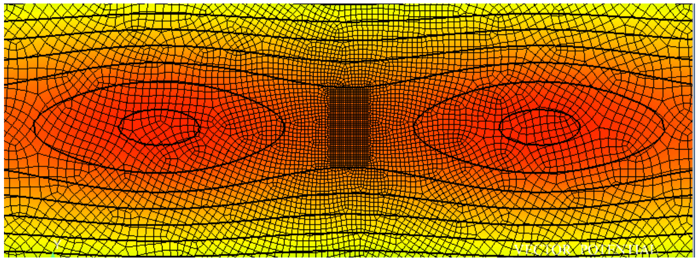


Vector Potential

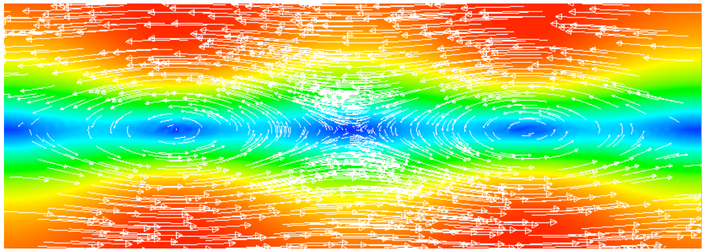


Island Coalescence Forced Equil. Solution

Vector Potential



B-Vector



Implicit NK-AMR

B. Philip, M. Pernice, and L. Chacón, *Lecture Notes in Computational Science and Engineering*, accepted (2006).

Current-Vorticity Formulation of Reduced Resistive MHD[1]

$$\begin{aligned}
(\partial_t + \mathbf{u}\cdot\nabla - \eta\Delta)\, J + \Delta E_0 &= \mathbf{B}\cdot\nabla\omega + \{\Phi,\Psi\} \\
(\partial_t + \mathbf{u}\cdot\nabla - \nu\Delta)\, \omega + S_\omega &= \mathbf{B}\cdot\nabla J \\
\Delta\Phi &= \omega \\
\Delta\Psi &= J
\end{aligned}$$

$$\mathbf{u} = \vec{z}\times\nabla\Phi \ , \ \mathbf{B} = \vec{z}\times\nabla\Psi$$

$$\{\Phi,\Psi\} = 2[\Phi_{xy}(\Psi_{xx}-\Psi_{yy}) - \Psi_{xy}(\Phi_{xx}-\Phi_{yy})]$$

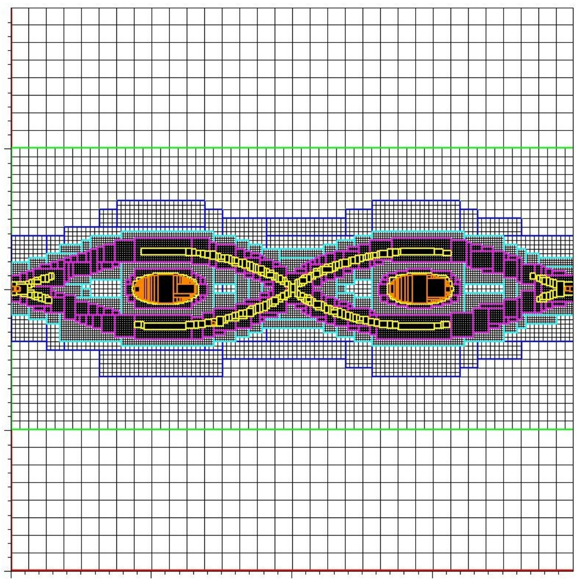
Preconditioner is an extension of

Chacón, Knoll and Finn, JCP, **178** (2002).

[1] Strauss and Longcope, JCP, **147**, 1998

Implicit Structured Adaptive Mesh Refinement (SAMRAI-PETSc-*hypre*)

- *Structured* adaptive mesh refinement (SAMR) represents a locally refined mesh as a union of logically rectangular meshes.



- The mesh is organized as a hierarchy of refinement levels.
- Each refinement level defines a region of uniform resolution.
- Each refinement level is the union of logically rectangular patches.

AMR-grids and multilevel methods are fundamentally compatible approaches!

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Performance (tearing mode)

- Generalized 2D reduced MHD PC [Chacon et al., JCP (2002)] for SAMR (MG⇒FAC).

	NNI					NLI				
Levels	1	2	3	4	5	1	2	3	4	5
32×32	1.5	2.0	2.0	2.1	2.5	3.4	7.9	12.0	19.3	33.7
64×64	1.8	2.0	2.0	2.4	–	6.5	11.7	19.1	33.2	–
128×128	1.8	2.0	2.4	–	–	12.5	20.1	27.2	–	–
256×256	1.9	2.0	–	–	–	19.9	27.5	–	–	–
512×512	1.9	–	–	–	–	26.3	–	–	–	–

$\Delta t = 1$ (fixed), $\eta_k = 0.1$, $\epsilon_{rel} = \epsilon_{abs} = 10^{-7}$, 2 SI iterations, V(3,3) cycles

- Fixed implicit time step (problem gets harder with refinement)
- Performance does not degrade with grid-refinement levels

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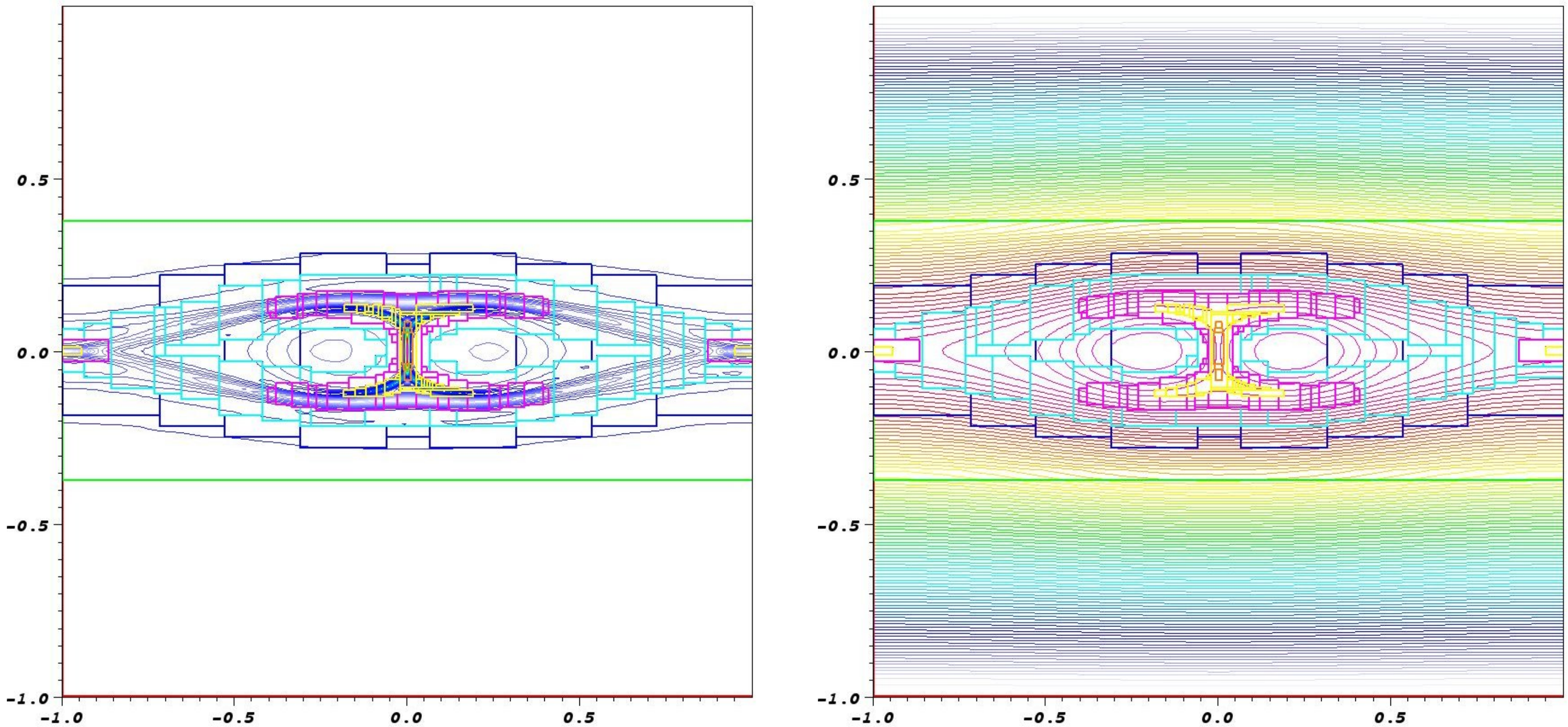
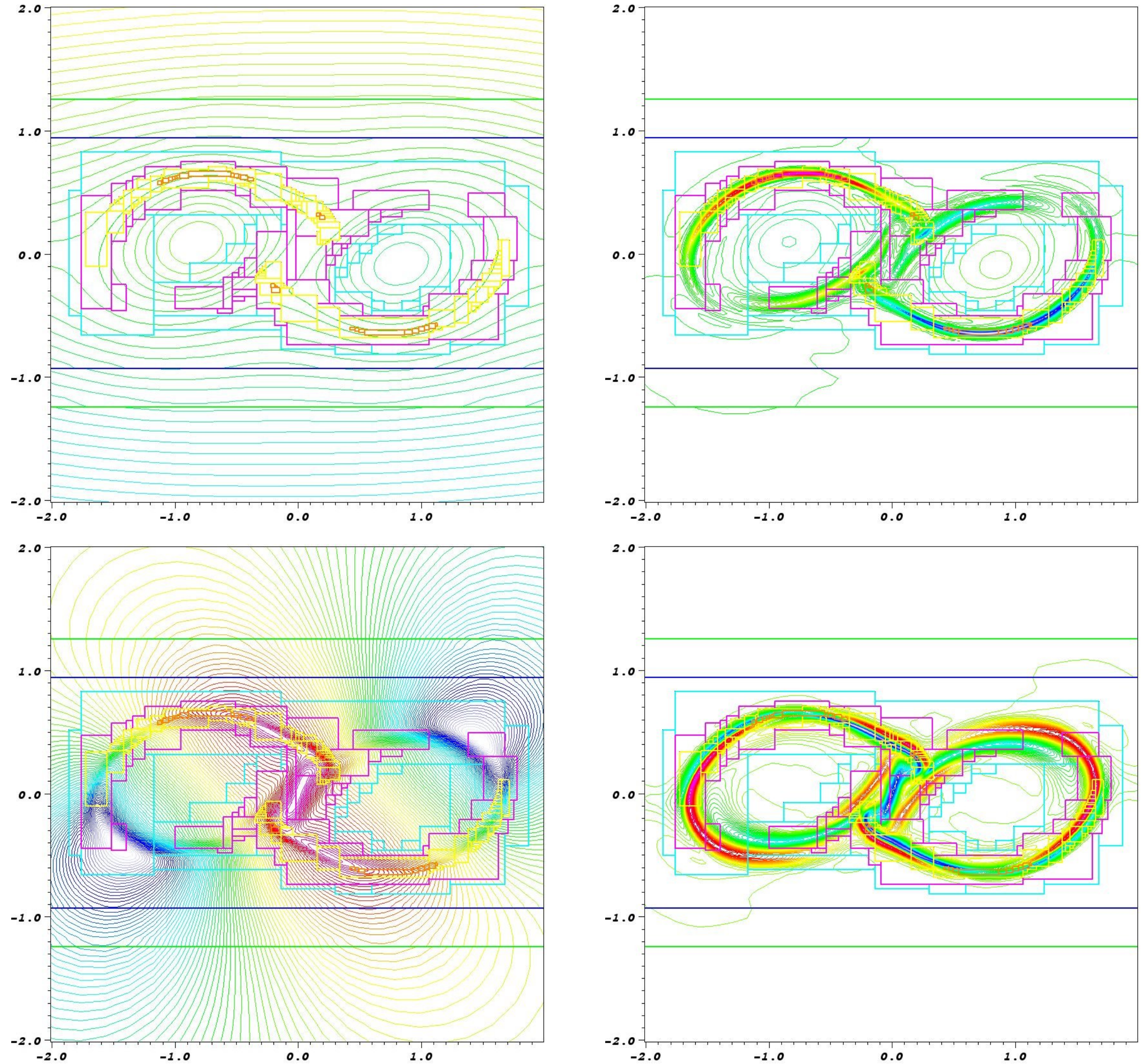
Island Coalescence Results at t=8



Tilt Instability Results at t=7



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Conclusions

- Developed a scalable, multilevel-based, fully implicit NK-MG solver for XMHD.

  Key algorithmic breakthrough: PARABOLIZATION + MG.

- Equivalence between parabolization and the Schur decomposition:
  - Provides a rigorous foundation for the parabolization step.
  - Provides a path to generalize approach when more complete XMHD models are considered.
- Demonstrated algorithmic viability of implicit AMR by generalizing single-grid preconditioning approaches for MHD.
- Future work:
  - Massively parallel test of 3D resistive MHD algorithm (NERSC).
  - Bring Hall MHD to production stage (high-order dissipation required).
  - Implicit AMR on 3D resistive MHD (B. Philip).
  - Multilevel-based PC on unstructured FE (SNL).

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