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)

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

Typical Time Scales in a next step experiment
with $B = 10$ T, $R = 2$ m, $n_e = 10^{14}$ cm$^{-3}$, $T = 10$ keV

(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): \( \kappa(J) \sim \Delta t \omega_{\text{fast}} \sim \frac{\Delta t}{\Delta t_{\text{CFL}}} \gg 1 \)
- 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 \([CPU \sim O(N/n_p)]\):
  - Minimize number of degrees of freedom \(N\): spatial adaptivity.
  - Follow slowest time scales (application dependent): implicit time stepping.
- Scalable implicit methods require MULTILEVEL approaches:

\[
CPU \sim O\left(\frac{N \log(N)}{n \beta}ight), \quad \beta \lesssim 1
\]
XMHD and multilevel approaches

- A fundamental component of iterative ML methods is the SMOOTHER.
- XMHD is strongly hyperbolic ⇒ 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)
Parabolization and Schur complement: an example

PARABOLIZATION EXAMPLE:

\[ \partial_t u = \partial_x v, \quad \partial_t v = \partial_x u. \]

\[ u^{n+1} = u^n + \Delta t \partial_x v^{n+1}, \quad v^{n+1} = v^n + \Delta t \partial_x u^{n+1}. \]

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

- PARABOLIZATION via SCHUR COMPLEMENT:

\[
\begin{bmatrix}
D_1 & U \\
L & D_2
\end{bmatrix} =
\begin{bmatrix}
I & UD_2^{-1} \\
0 & I
\end{bmatrix}
\begin{bmatrix}
D_1 - UD_2^{-1}L & 0 \\
0 & D_2
\end{bmatrix}
\begin{bmatrix}
I & 0 \\
D_2^{-1}L & I
\end{bmatrix}.
\]

Stiff off-diagonal blocks \( L, U \) now sit in diagonal via Schur complement \( D_1 - UD_2^{-1}L \).

The system has been “PARABOLIZED.”

\[ D_1 - UD_2^{-1}L = (I - \Delta t^2 \partial_{xx}) \]
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.
Jacobian-Free Newton-Krylov Methods

- **Objective:** solve nonlinear system $\tilde{G}(\bar{x}^{n+1}) = 0$ efficiently (scalably).

- Converge nonlinear couplings using Newton-Raphson method:

  $$\frac{\partial \tilde{G}}{\partial \bar{x}}|_k \delta \bar{x}_k = -\tilde{G}(\bar{x}_k)$$

- Jacobian-free implementation:

  $$\left( \frac{\partial \tilde{G}}{\partial \bar{x}} \right)_k \delta \bar{y} = J_k \delta \bar{y} = \lim_{\epsilon \to 0} \frac{\tilde{G}(\bar{x}_k + \epsilon \delta \bar{y}) - \tilde{G}(\bar{x}_k)}{\epsilon}$$


- Right preconditioning: solve equivalent Jacobian system for $\delta y = P_k \delta \bar{x}$:

  $$J_k P_k^{-1} P_k \delta \bar{x} = -\tilde{G}_k$$

**Approximations in preconditioner do not affect accuracy of converged solution; they only affect efficiency!**

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Implicit *resistive* MHD solver
Resistive MHD model equations

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0, \]

\[ \frac{\partial \vec{B}}{\partial t} + \nabla \times \vec{E} = 0, \]

\[ \frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot \left[ \rho \vec{v} \vec{v} - \vec{B} \vec{B} - \rho \nu \nabla \vec{v} + \overleftarrow{I} \left( p + \frac{B^2}{2} \right) \right] = 0, \]

\[ \frac{\partial T}{\partial t} + \vec{v} \cdot \nabla T + (\gamma - 1) T \nabla \cdot \vec{v} = 0, \]

- Plasma is assumed polytropic \( p \propto n^\gamma \).
- Resistive Ohm’s law:
  \[ \vec{E} = -\vec{v} \times \vec{B} + \eta \nabla \times \vec{B} \]
Resistive MHD Jacobian block structure

- The linearized resistive MHD model has the following couplings:

\[
\begin{align*}
\delta \rho &= L_\rho(\delta \rho, \delta \vec{v}) \\
\delta T &= L_T(\delta T, \delta \vec{v}) \\
\delta \vec{B} &= L_B(\delta \vec{B}, \delta \vec{v}) \\
\delta \vec{v} &= L_v(\delta \vec{v}, \delta \vec{B}, \delta \rho, \delta T)
\end{align*}
\]

- 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.
PARABOLIZATION: Schur complement formulation

• We consider the block structure:

\[
J\delta\vec{x} = \begin{bmatrix} M & U \\ L & D_v \end{bmatrix} \begin{bmatrix} \delta\vec{y} \\ \delta\vec{v} \end{bmatrix} ; \quad \delta\vec{y} = \begin{bmatrix} \delta\rho \\ \delta T \\ \delta\vec{B} \end{bmatrix} ; \quad M = \begin{bmatrix} D_\rho & 0 & 0 \\ 0 & D_T & 0 \\ 0 & 0 & D_B \end{bmatrix}
\]

• \(M\) is “easy” to invert (advection-diffusion, MG-friendly).

\[
\text{Schur complement analysis of 2x2 block } J \text{ yields:}
\]

\[
\begin{bmatrix} M & U \\ L & D_v \end{bmatrix}^{-1} = \begin{bmatrix} I & 0 \\ -LM^{-1} & I \end{bmatrix} \begin{bmatrix} M^{-1} & 0 \\ 0 & P_{Schur}^{-1} \end{bmatrix} \begin{bmatrix} I & -M^{-1}U \\ 0 & I \end{bmatrix},
\]

\[
P_{Schur} = D_v - LM^{-1}U.
\]

• 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:

  Predictor : \( \delta \vec{y}^* = -M^{-1}G_y \)

  Velocity update : \( \delta \vec{v} = P_{Schur}^{-1}[-G_v - L\delta \vec{y}^*], \quad P_{Schur} = D_v - LM^{-1}U \)

  Corrector : \( \delta \vec{y} = \delta \vec{y}^* - M^{-1}U\delta \vec{v} \)

- 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.
Physics-based preconditioner (II)

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

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

where:

\[
P_{SI} = \rho^n \left[ \frac{\vec{I}}{\Delta t} + \theta (\vec{v}_0 \cdot \nabla \vec{I} + \vec{I} \cdot \nabla \vec{v}_0 - \nu^n \nabla^2 \vec{I}) \right] + \Delta t \theta^2 W(\vec{B}_0, p_0)
\]
\[
W(\vec{B}_0, p_0) = \vec{B}_0 \times \nabla \times \nabla \times [\vec{I} \times \vec{B}_0] - j_0 \times \nabla \times [\vec{I} \times \vec{B}_0] - \nabla [\vec{I} \cdot \nabla p_0 + \gamma p_0 \nabla \cdot \vec{I}]
\]

- $P_{SI}$ is block diagonally dominant by construction!
- We employ multigrid methods (MG) to approximately invert $P_{SI}$ and $M$: 1 V(4,4) cycle
### Efficiency: $\Delta t$ scaling (2D tearing mode)

#### 32 $\times$ 32

<table>
<thead>
<tr>
<th>$\Delta t$</th>
<th>Newton/$\Delta t$</th>
<th>GMRES/$\Delta t$</th>
<th>CPU (s)</th>
<th>$CPU_{exp}/CPU$</th>
<th>$\Delta t/\Delta t_{CFL}$</th>
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#### 128 $\times$ 128

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<th>GMRES/$\Delta t$</th>
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<td>12.7</td>
<td>760</td>
</tr>
<tr>
<td>1.5</td>
<td>5.6</td>
<td>14.7</td>
<td>1246</td>
<td>14.6</td>
<td>1140</td>
</tr>
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</table>
Efficiency: grid scaling

\[ \Delta t \approx 1100 \Delta t_{CFL}, \ 10 \ \text{time steps} \]

<table>
<thead>
<tr>
<th>Grid</th>
<th>( \Delta t )</th>
<th>Newton/( \Delta t )</th>
<th>GMRES/( \Delta t )</th>
<th>CPU</th>
<th>( \overline{CPU} )</th>
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<td>14.8</td>
<td>1246</td>
<td>84.2</td>
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</tbody>
</table>

Why does GMRES/\( \Delta t \) decrease with resolution?

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Effect of spatial truncation error

Residual history vs. GMRES it. # with fixed time step Dt=1

Relative linear residual vs. # GMRES iteration

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Implicit extended MHD solver
Extended MHD model equations

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0, \]

\[ \frac{\partial \vec{B}}{\partial t} + \nabla \times \vec{E} = 0, \]

\[ \frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot \left[ \rho \vec{v} \vec{v} - \vec{B} \vec{B} - \rho \nu \nabla \vec{v} + \vec{T} \left( p + \frac{B^2}{2} \right) \right] = 0, \]

\[ \frac{\partial T_e}{\partial t} + \vec{v} \cdot \nabla T_e + (\gamma - 1) T_e \nabla \cdot \vec{v} = 0, \]

- Plasma is assumed polytropic \( p \propto n^\gamma \).
- We assume cold ion limit: \( T_i \ll T_e \Rightarrow p \approx p_e \).
- Generalized Ohm’s law:

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

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Extended MHD Jacobian block structure

- The linearized extended MHD model has the following couplings:

\[
\begin{align*}
\delta \rho &= L_\rho (\delta \rho, \delta \vec{v}) \\
\delta T &= L_T (\delta T, \delta \vec{v}) \\
\delta \vec{B} &= L_B (\delta \vec{B}, \delta \vec{v}, \delta \rho, \delta T) \\
\delta \vec{v} &= L_v (\delta \vec{v}, \delta \vec{B}, \delta \rho, \delta T)
\end{align*}
\]

- 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!
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:

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

- 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!

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Preliminary efficiency results (2D tearing mode)

\[ d_i = 0.05 \]

1 time step, \( \Delta t = 1.0 \), \( V(3,3) \) cycles, \( mg_{tol}=1e-2 \)

<table>
<thead>
<tr>
<th>Grid</th>
<th>Newton/( \Delta t )</th>
<th>GMRES/( \Delta t )</th>
<th>CPU (s)</th>
<th>( CPU_{exp}/CPU )</th>
<th>( \Delta t/\Delta t_{exp} )</th>
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</tbody>
</table>

Again, GMRES/\( \Delta t \) decreases with resolution!

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Effect of spatial truncation error

Residual history vs. GMRES it# with fixed time step Dt=1

NL tolerance

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

Speedup

# processors

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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

\[
\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F} + S = 0
\]

\[
\begin{bmatrix}
\rho \\
\rho \mathbf{v} \\
\Sigma_{\text{rot}} \\
\mathbf{B}
\end{bmatrix}

F =

\begin{bmatrix}
\rho \mathbf{v} \\
\rho \mathbf{v} \otimes \mathbf{v} - \frac{1}{\rho_0} \mathbf{B} \otimes \mathbf{B} - \mathbf{T} + \frac{1}{2 \rho_0} \|\mathbf{B}\|^2 \mathbf{I} \\
\rho \mathbf{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}{\rho_0} (\nabla \mathbf{B} - \nabla \mathbf{B}^T)
\end{bmatrix}

S =

\begin{bmatrix}
0 \\
0 \\
Q^{\text{reed}} + Q \\
0
\end{bmatrix}

\[
E = \epsilon + \frac{1}{2} \|\mathbf{v}\|^2
\]

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

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)
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)
Implicit NK-AMR

Current-Vorticity Formulation of Reduced Resistive MHD

\[
(p_t + \mathbf{u} \cdot \nabla - \eta \Delta) J + \Delta E_0 = \mathbf{B} \cdot \nabla \omega + \{\Phi, \Psi\}
\]
\[
(p_t + \mathbf{u} \cdot \nabla - \nu \Delta) \omega + S_\omega = \mathbf{B} \cdot \nabla J
\]
\[
\Delta \Phi = \omega
\]
\[
\Delta \Psi = J
\]

\[
\mathbf{u} = \hat{z} \times \nabla \Phi, \quad \mathbf{B} = \hat{z} \times \nabla \Psi
\]

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

Preconditioner is an extension of
Chacón, Knoll and Finn, JCP, 178 (2002).

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

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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).

<table>
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<tr>
<th>Levels</th>
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<th>3</th>
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<td></td>
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<td>20.1</td>
<td>27.2</td>
<td>–</td>
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<td></td>
<td>1.9</td>
<td>2.0</td>
<td>–</td>
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<td>19.9</td>
<td>27.5</td>
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<tr>
<td>512 × 512</td>
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<td>1.9</td>
<td>–</td>
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<td>–</td>
<td>26.3</td>
<td>–</td>
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</tbody>
</table>

Δt = 1 (fixed), η_k = 0.1, \( \varepsilon_{rel} = \varepsilon_{abs} = 10^{-7} \), 2 SI iterations, V(3,3) cycles

- Fixed implicit time step (problem gets harder with refinement)
- Performance does not degrade with grid-refinement levels
Island Coalescence Results at t=8

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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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