A fully implicit 3D extended MHD algorithm

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Outline

Motivation

Spatial discretization

Resistive MHD (mature)

Hall MHD (proof-of-principle)

Conclusions and future work

Motivation for an implicit MHD solver

- The MHD formalism is a nonlinear system of stiff equations:
  - Elliptic stiffness (transport).
  - Hyperbolic stiffness (linear waves: magnetosonic, Alfvén, sound, whistler,...).
- Explicit methods:
  - Straightforward but inefficient (numerical stability).
- Semi-implicit methods:
  - Popular, efficient, but potentially inaccurate (linearization, splitting, simplifications in semi-implicit operator).
- Implicit methods: accurate and efficient, but of difficult implementation:
  - Non-linear couplings in equations.
  - Ill-conditioned matrices due to elliptic operators and stiff waves.
- Here, a viable, scalable implicit strategy using Newton-Krylov methods is explored.
- At the core of the approach is the so-called physics-based preconditioning strategy.

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Properties of spatial discretization

L. Chacón, *Comput. Phys. Comm.*, 163 (3), 143-171 (2004)

- A cell-centered (collocated) difference scheme has been devised that:
  - Is conservative in particles and momentum (energy also if energy equation is chosen instead of temperature).
  - Is solenoidal in the magnetic field.
  - Is linearly (no red-black modes) and nonlinearly (no anti-diffusive terms) stable in the absence of physical and/or numerical dissipation.
  - Eliminates the “parallel force” problem of the conservative formulation of EOM.
  - Is suitable for curvilinear representations (as needed in fusion applications).
- While only 2D tests have been presented, all properties carry to 3D (the code is fully 3D capable).
- Crucial to the scheme is the so-called ZIP differencing, which satisfies very desirable properties such as:
  - Being conservative.
  - Mimics the chain rule of derivatives exactly.
  - Modified equation (truncation error) contains no anti-diffusive terms.

Implicit *resistive* MHD solver

Resistive MHD model equations

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

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

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

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

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

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

Jacobian-Free Newton-Krylov Methods

- Objective: solve nonlinear system $\vec{G}(\vec{x}^{n+1}) = \vec{0}$ efficiently.
- 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!

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Concept of physics-based preconditioning

- Developing AN implicit Newton-Krylov MHD solver is "EASY":

JUST BUILD NONLINEAR FUNCTION EVALUATION ROUTINE!

- Developing an EFFICIENT Newton-Krylov MHD solver is "HARD": need SCALABLE preconditioning.
  - Elliptic and parabolic systems: use scalable MG methods. Usually OK.
  - Hyperbolic systems: diagonally submissive, not amenable to MG. HARD!
- Physics-based preconditioning: technique to develop effective, SCALABLE preconditioners for hyperbolic systems. Based on two concepts:
  - SEMI-IMPLICIT approximations: limit level of implicitness based on physical insight.
  - PARABOLIZATION: from hyperbolic to parabolic: a MG-friendly formulation.

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Parabolization and Schur complement: an example

- PARABOLIZATION EXAMPLE:

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

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

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

- 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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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:

$$J\delta\vec{x} = \left[\begin{array}{cc} M & U \\ L & D_v \end{array}\right] \left(\begin{array}{c} \delta\vec{y} \\ \delta\vec{v} \end{array}\right)$$

$$\delta\vec{y} = \left(\begin{array}{c} \delta\rho \\ \delta T \\ \delta\vec{B} \end{array}\right) \;\; ; \;\; M = \left(\begin{array}{ccc} D_\rho & 0 & 0 \\ 0 & D_T & 0 \\ 0 & 0 & D_B \end{array}\right)$$

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

Schur complement analysis of 2x2 block J yields:

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

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

- 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: SEMI-IMPLICIT approximation

- 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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Small flow PC

- 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

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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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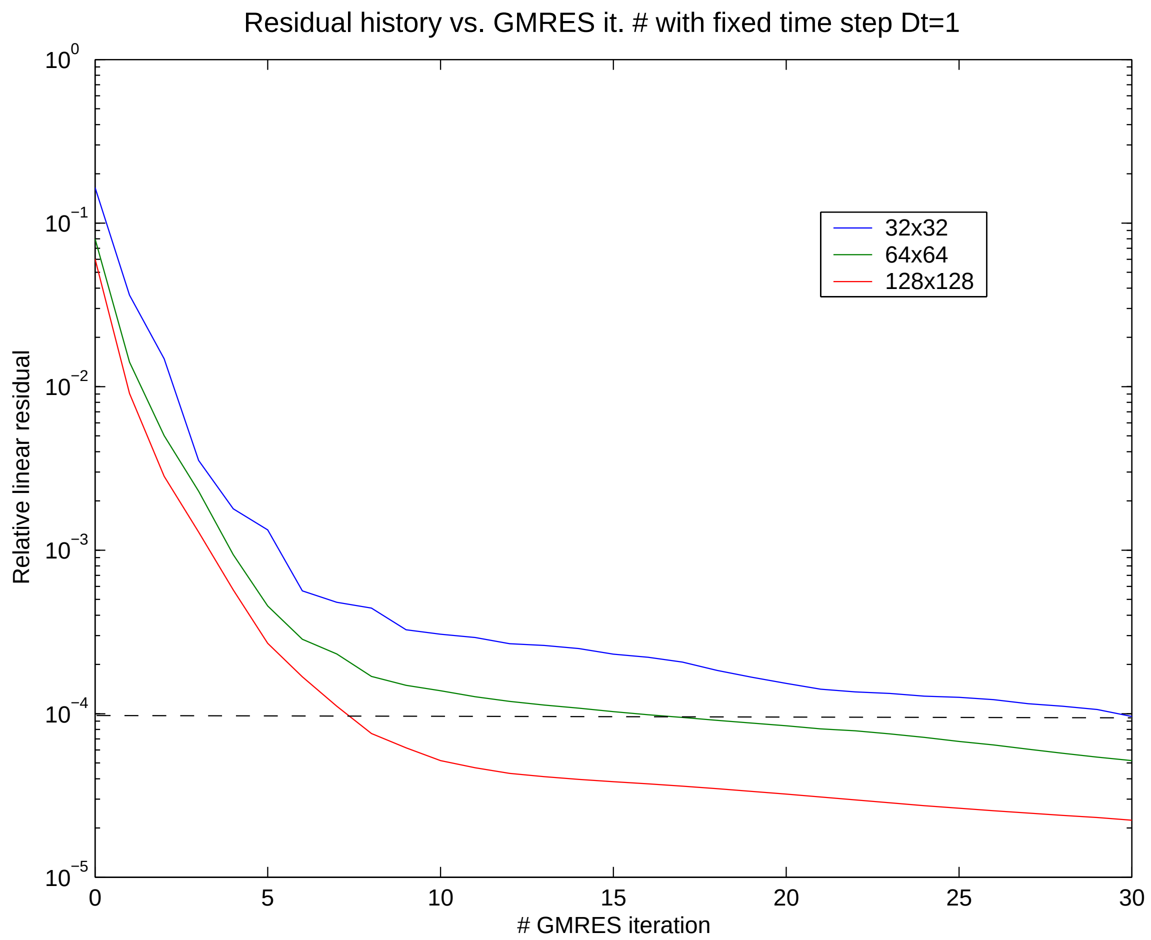
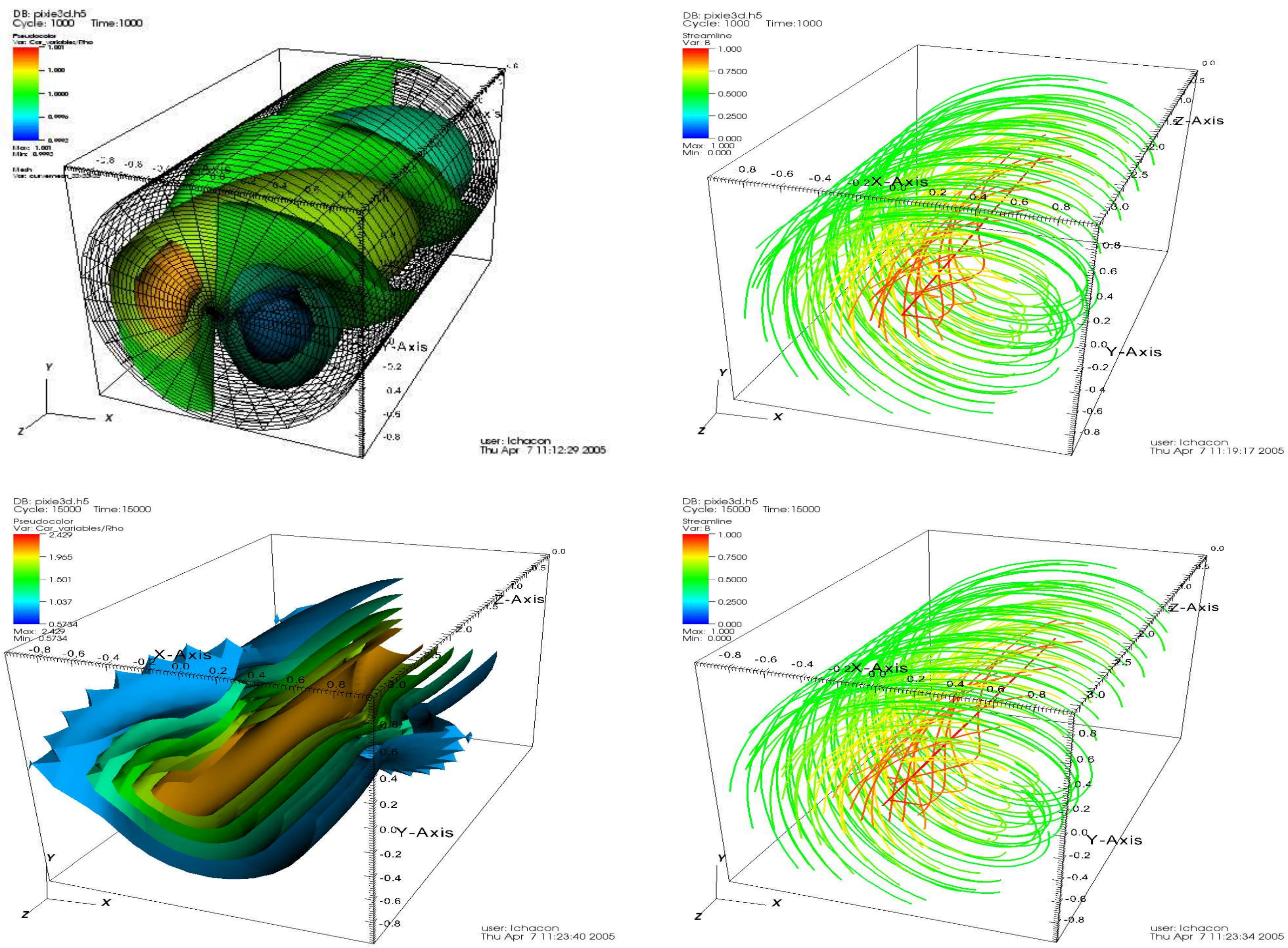
Effect of spatial truncation error



Sample 3D results: Screw pinch in 3D



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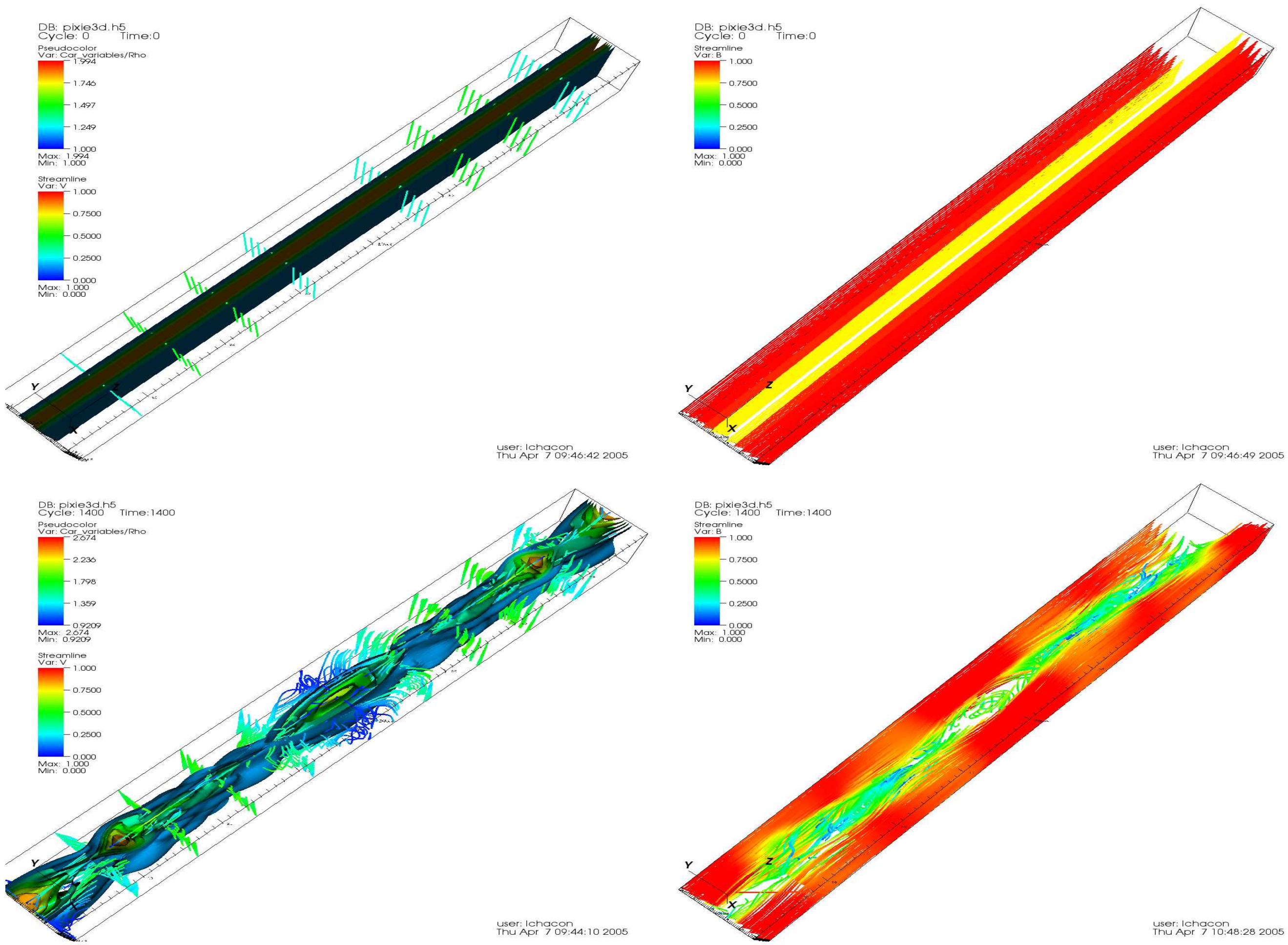
Sample 3D results: 3D KHI

Knoll and Brackbill, Phys. Plasmas 9 (9) 2002



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Implicit *extended* MHD solver

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Extended MHD model equations

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

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

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

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

- 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!

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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

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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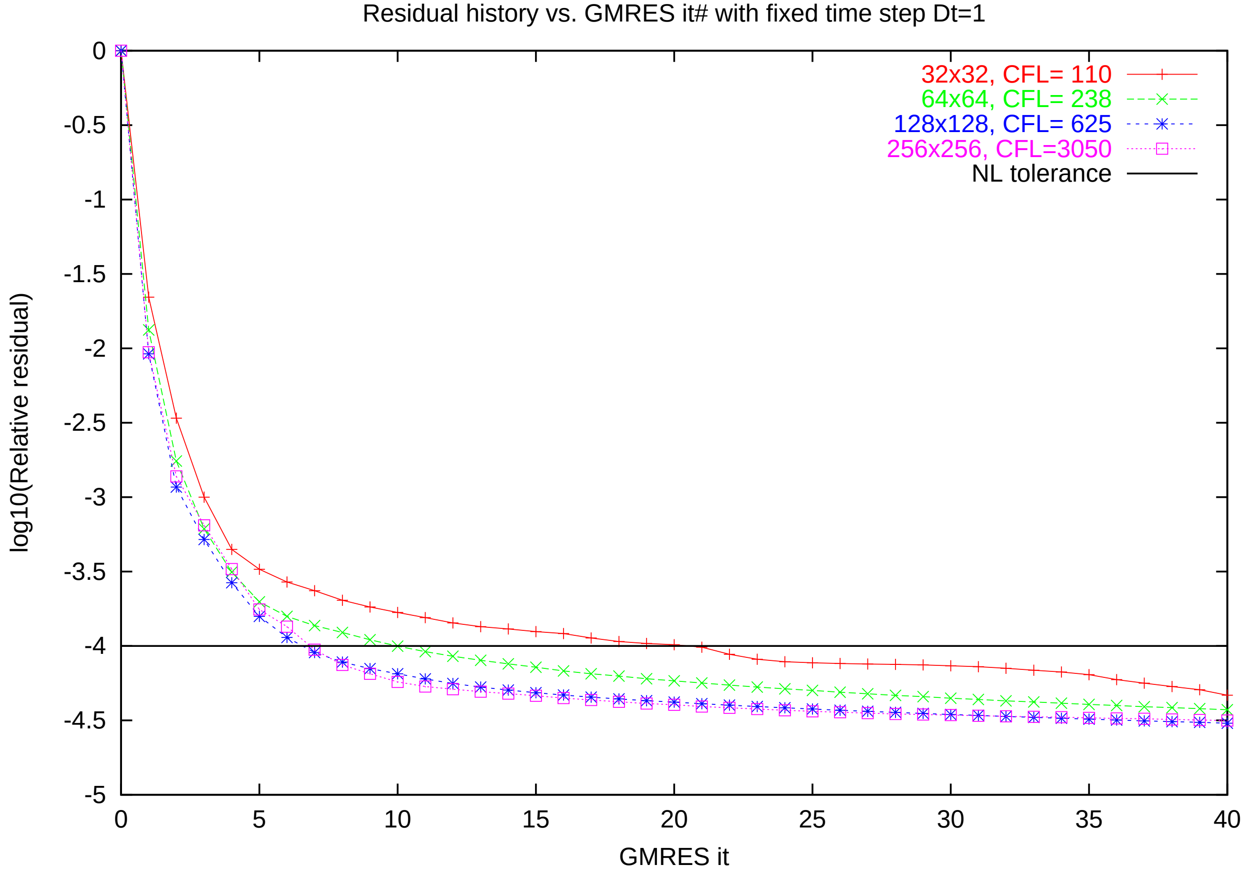
Effect of spatial truncation error



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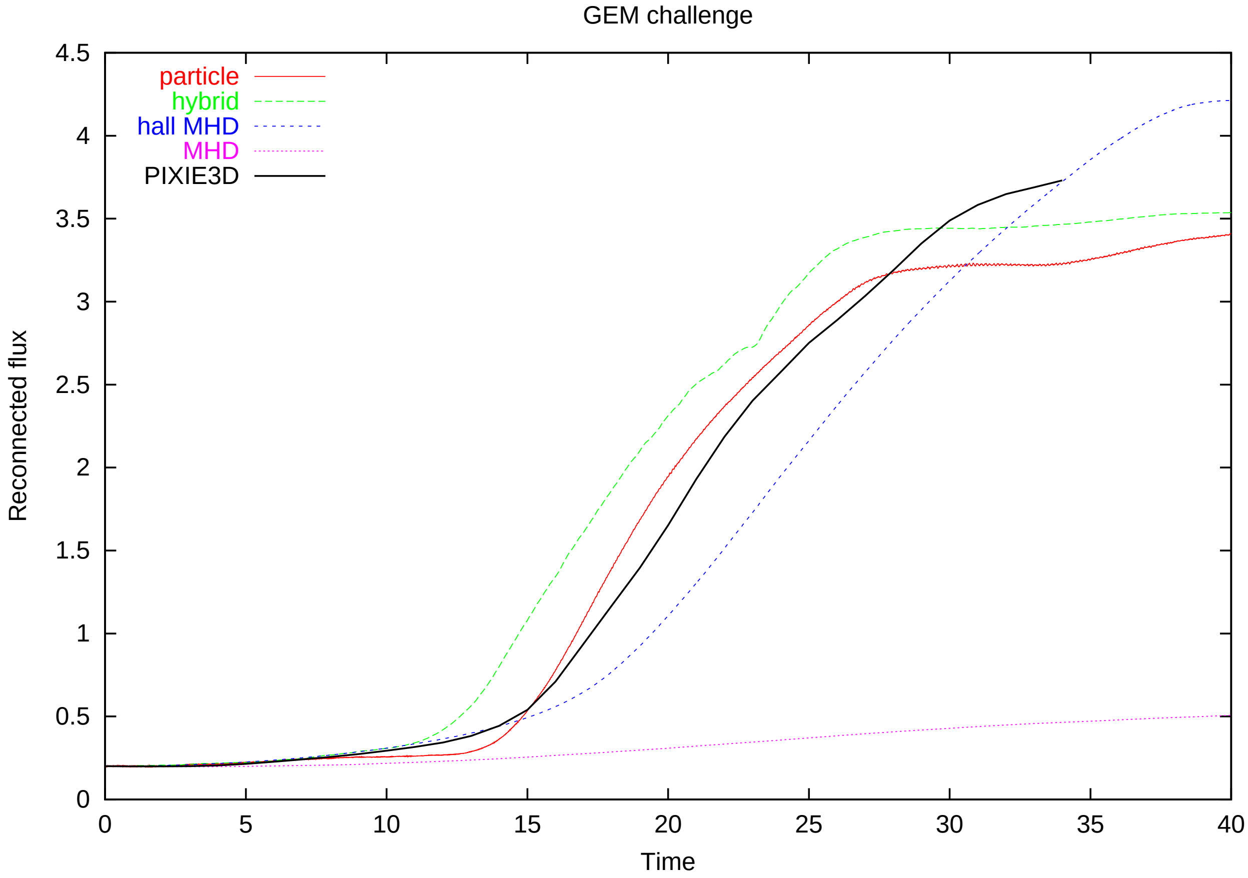
GEM Challenge

J. Birn et al., *J. Geophys. Res.*, 106 (A3), p.3715-19 (2001)



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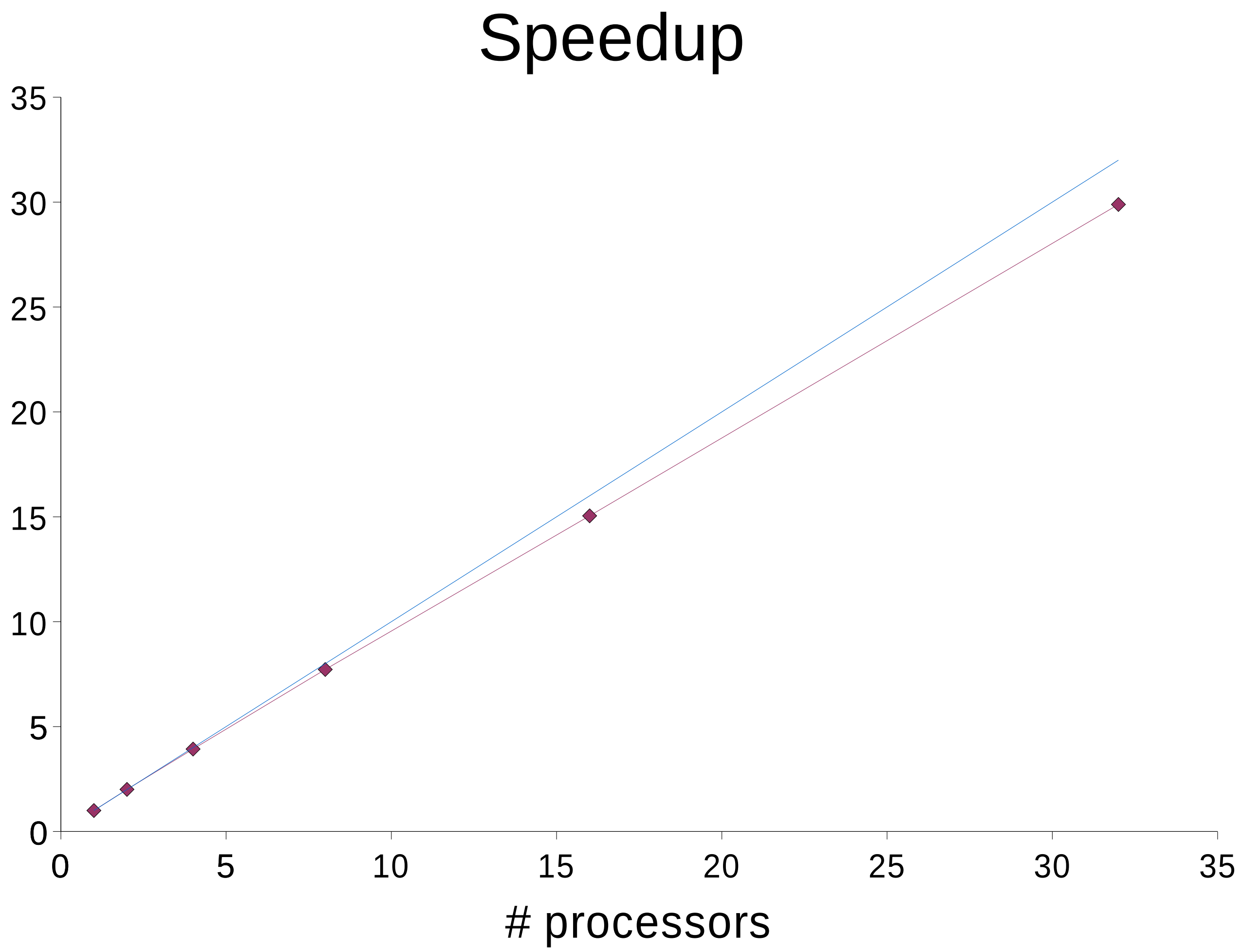
Parallel performance with PETSc Toolkit (unpreconditioned)



Conclusions and future work

- Physics-based preconditioning for hyperbolic systems: parabolization, semi-implicit approximation.
- Parabolization: Schur decomposition.
- Semi-implicit approximation: appropriate simplification of exact Schur decomposition.
- Concept tested for MHD stiff waves, in both resistive (mature), Hall (proof-of-principle) primitive variables formulations.
- Highlights:
  - SCALABILITY: $CPU \sim \mathcal{O}(N)$ (MG based)
  - WINS OVER EXPLICIT METHODS: CPU speedup up to 30!.
- Future work:
  - Characterize Hall MHD more exhaustively.
  - Demonstrate preconditioning scalability in 3D.
  - Extend efficiency results to other geometries.
  - Parallelization: incorporate preconditioner in PETSc parallel version.

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