PIXIE3D: A Parallel, Implicit, eXtended MHD 3D Code

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Outline

Introduction/motivation

Spatial discretization:
ZIP average

Temporal discretization:
Newton-Krylov
Physics-based preconditioning: 2D, 3D

Concluding remarks

Introduction

Motivation and goals

- PIXIE3D is a project in progress. This is a progress report.
- GOAL: to demonstrate the path for fully implicit MHD in general geometries, using state-of-the-art scalable solver technology (NK-MG), and exploiting massively parallel computing environments.
- Desired features of implicit solver:
  - Fully implicit and nonlinear: Newton-Krylov.
  - Parallel: PETSC.
  - Scalable in mesh and time step size: PHYSICS-BASED PRECONDITIONING.
- Desired features of spatial representation:
  - Conservative.
  - Solenoidal in the magnetic field (no divergence cleaning).
  - Arbitrary geometry (curvilinear grids).
  - Numerically stable without physical or numerical dissipation.

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Some perspective on finite-volume implicit MHD

Author (year)	TS	Cons	Solen	Geom	Dim	Spatial rep	Other
Lindemuth (73)	lin. ADI	NO	NO	Cyl.	2D	Cell-cent.	–
Schnack (80)	lin. ADI	YES	NO	Orth.	2D	Cell-cent.	–
Finan (81)	nl. ADI	NO	NO	Orth.	3D	Cell-cent.	NL unst.
Schnack (87)	SI	NO	YES	Cyl.	3D	Stagg.	–
Jones (97)	SI (ADI)	YES	NO	Cart.	2D	Cell-cent.	Shock
Amari (99)	SI (P-C)	NO	YES	Cart.	2D	Stagg.	–
PIXIE3D	*NK*	*YES*	*YES*	*Curv.*	*3D*	*Cell-cent.*	*Parallel*

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MHD model equations

$$\begin{aligned}
\frac{\partial \rho}{\partial t} &+ \nabla \cdot (\rho \vec{v}) = 0, \\
\frac{\partial \vec{B}}{\partial t} &+ \nabla \times \vec{E} = 0, \\
\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot \left[\rho \vec{v}\vec{v} - \frac{\vec{B}\vec{B}}{\mu_0} \right. &- \left. \rho \nu(T) \nabla \vec{v} + \overleftrightarrow{I}(p + \frac{B^2}{2\mu_0}) \right] = 0, \\
\frac{\partial T}{\partial t} + \vec{v} \cdot \nabla T &+ (\gamma - 1) T \nabla \cdot \vec{v} = 0,
\end{aligned}$$

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

$$\vec{E} = -\vec{v} \times \vec{B} + \frac{\eta(T)}{\mu_0} \nabla \times \vec{B}$$

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Spatial discretization

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

Properties of spatial discretization

- Features of spatial representation:
  - Conservative.
  - Solenoidal in the magnetic field (no divergence cleaning).
  - Arbitrary geometry (curvilinear grids).
  - Numerically stable without physical or numerical dissipation.
- Equations are discretized on logical grid ($\vec{\xi}$) (uniform and logically rectangular).
- Non-staggered (cell-centered) representation (advantageous for MG treatment).
- However, conservation requires fluxes to be defined at faces $\Rightarrow$ Interpolation is needed.

THE CHOICE OF INTERPOLATION IS CRUCIAL
TO AVOID NONLINEAR (ANTI-DIFFUSION) INSTABILITIES.

- The ZIP average was proposed by Hirt[1] to avoid antidiffusive nonlinear instabilities.
  1. ZIP is exactly conservative and second-order
  2. ZIP satisfies the chain rule numerically
  3. ZIP is nonlinearly stable (no antidiffusion), and
  4. ZIP is linearly stable (no red-black modes).

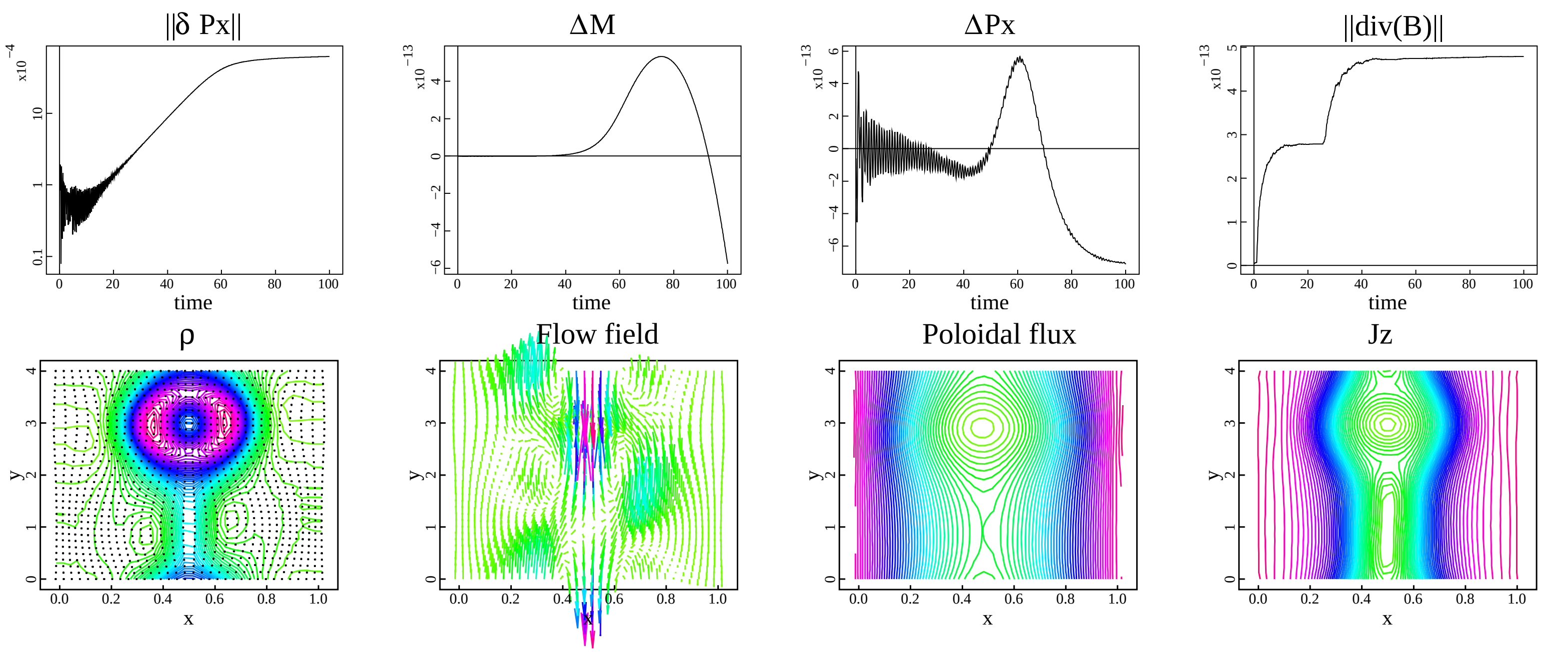
[1] Hirt, JCP 2 (1968)

Numerical test I: Resistive tearing mode in sinusoidal grid

- Equilibrium: $B_{x0}(y) = \tanh(y/\lambda)$ ($\lambda = 0.2$), uniform density, pressure; no flow.
- 2D domain of 4x1, 32x32 grid, $\eta = 10^{-2}$, $\nu = 10^{-3}$, $\gamma = 5/3$.
- Sinusoidal grid defined as perturbation of Cartesian grid:

$$x = \xi_1 - \epsilon \sin(\frac{2\pi}{L_x}\xi_1)\sin(\frac{2\pi}{L_y}\xi_2)\ ,\ \ y = \xi_2 - \epsilon \sin(\frac{2\pi}{L_x}\xi_1)\sin(\frac{2\pi}{L_y}\xi_2)\ ,\ \ \epsilon = 0.05$$

- Linear growth rate $\gamma_{EV} = 0.098$; implicit solver: $\gamma_{32\times32} = 0.089$, $\gamma_{64\times64} = 0.097$.



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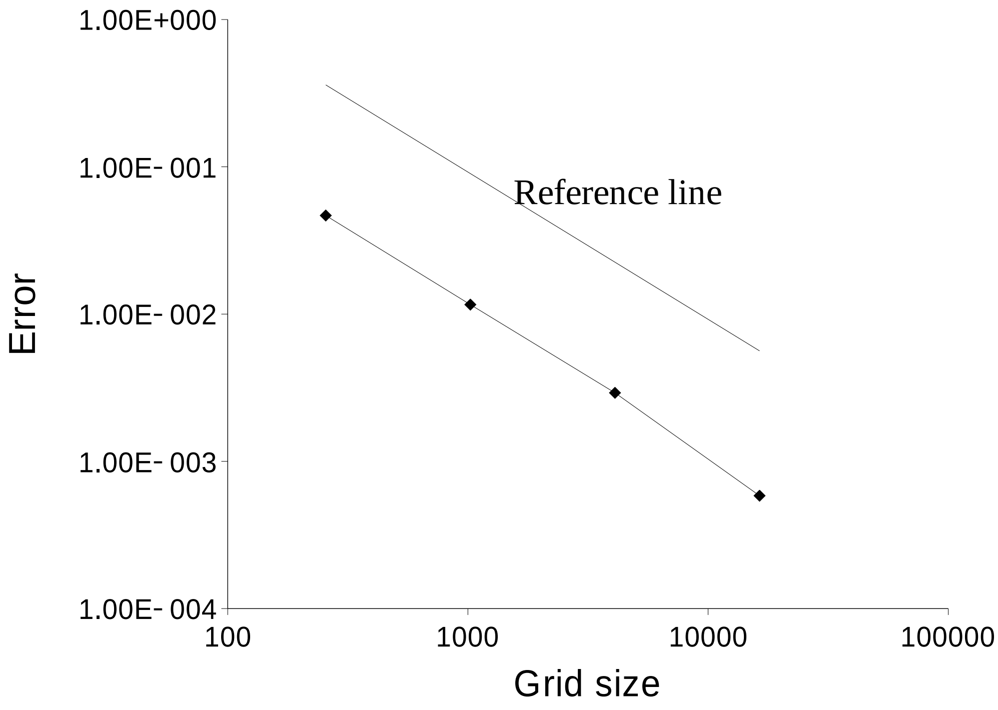
Resistive tearing mode in sinusoidal grid (cont)

- Grid convergence study with sinusoidal grid demonstrates second-order accurate discretization:



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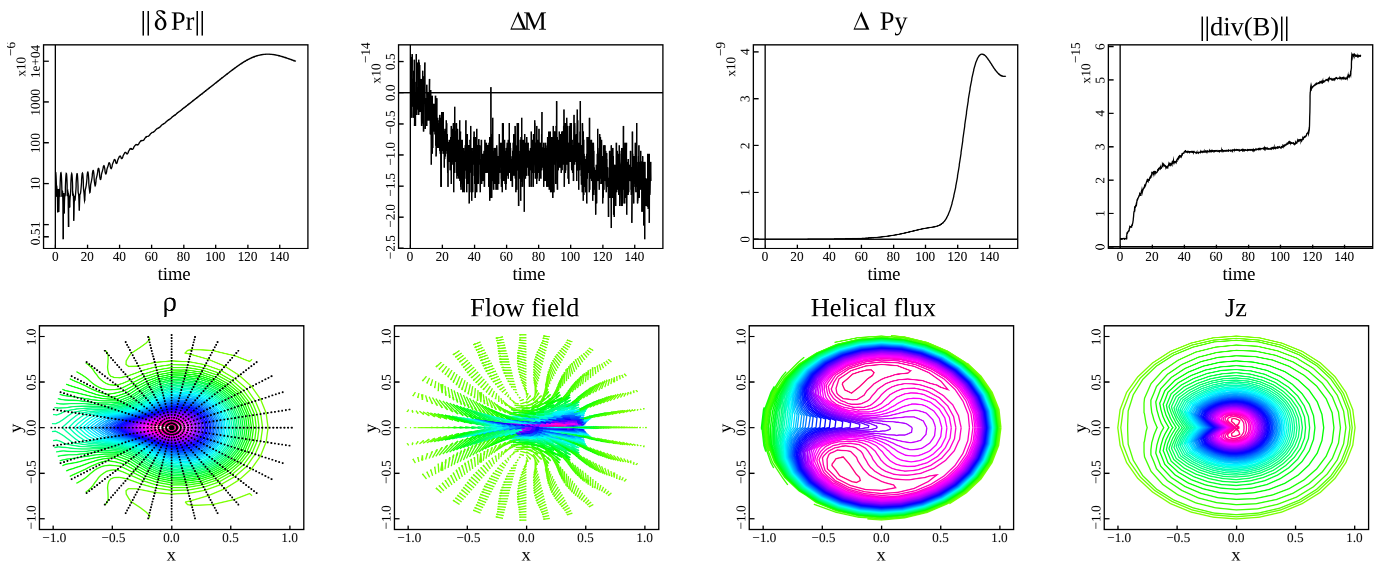
Numerical test II: Screw pinch, m=1 (kink) mode

- Force-free equilibrium defined by ($x = r/\lambda$):

$$B_\theta = \frac{Bx}{1+x^2} \; ; \; B_z = \sqrt{1 - B^2\left[1-(1+x^2)^{-2}\right]} \; ; \; B = \frac{1+(a/\lambda)^2}{\sqrt{[1+(a/\lambda)^2]^2 - 1}}$$

  with: $\lambda = 0.5$, $a = 2$, $m = 1$, $k = -n/R = -2$, $\eta = \nu = 10^{-3}$, $T_0 = 10^{-5}$, $\gamma = 1$

- Helical coordinate system: $\xi_1 = r \; , \; \xi_2 = \theta + \frac{k}{m} z$
- Linear growth rate $\gamma_{EV} = 0.071$; implicit solver: $\gamma_{32\times 32} = 0.071$.



Progress in 3D primitive-variable MHD: PIXIE3D

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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!

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:

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

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

- M is "easy" to invert (advection-diffusion, MG-friendly).
- Schur complement analysis of 2x2 block J yields:

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

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

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

- MG treatment of P_{Schur} is impractical: need suitable simplifications (SEMI-IMPLICIT).
- Simplest simplification: $\boxed{M^{-1} \approx \Delta t}$ in steps 2 & 3:

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

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

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

- We employ multigrid methods (MG) to approximately invert P_{SI} and M: 2 V(4,4) cycles

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Efficiency: Δt scaling (2D Cartesian, uniform grid)

32×32

Δt	Newton/Δt	GMRES/Δt	CPU (s)	CPU_{exp}/CPU	$\Delta t/\Delta t_{CFL}$
2	3	21.4	780	1.5	400
3	3	26.6	630	1.9	600
4	3	34.5	580	2	800
6	3	36.9	420	2.8	1200

128×128

Δt	Newton/Δt	GMRES/Δt	CPU (s)	CPU_{exp}/CPU	$\Delta t/\Delta t_{CFL}$
0.5	3	15	12675	1.6	435
0.75	3	19.1	9984	2.0	650
1.0	3	21.6	7640	2.7	870
1.5	3	26.2	5678	3.6	1300

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Efficiency: grid scaling
(2D Cartesian, uniform grid)

$\Delta t = 1200\Delta t_{CFL}$, 10 time steps

Grid	Δt	Newton/Δt	GMRES/Δt	CPU	$\widehat{CPU}$
32x32	6	3	40	420	10.5
64x64	3	3	34.5	1375	40.5
128x128	1.5	3	26.2	5678	216

$\widehat{CPU} \sim \mathcal{O}(N)$ OPTIMAL SCALING!

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Conclusions

- 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.
  - Is suitable for curvilinear representations (as needed in fusion applications).
- A viable physics-based preconditioning has been developed for resistive MHD. Highlights:
  - SCALABILITY: $CPU \sim \mathcal{O}(N \times \Delta t^{-0.7})$
  - WINS OVER EXPLICIT METHODS: CPU speedup ~ 4 in Cartesian coordinates (will be much more in cylindrical/toroidal geometries).
- Future work:
  - 3D proof-of-principle efficiency results in Cartesian.
  - Extend efficiency results to other geometries: MG in curvilinear geometries
  - Incorporate preconditioner in PETSc parallel version.