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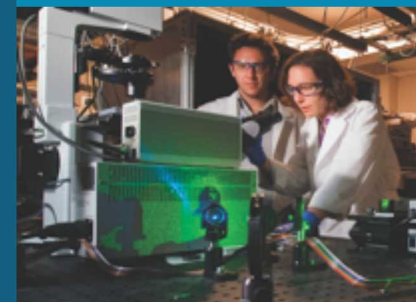
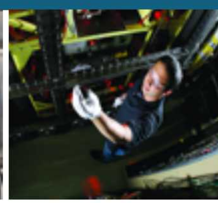


Benchmarking Fully-Implicit Discretization of Multi-fluid Plasma-electromagnetic Models for Pulsed Power Applications



PRESENTED BY

Kris Beckwith; Org. 1641 HEDP Theory

Work Performed in part under `Ultra-Scale and Fault-Resilient Algorithms: Mathematical Algorithms for Ultra-Parallel Computing`; Contract # FA9550-12-1-047; Program Managers: Drs. Fariba Fahroo & John W. Luginsland and Contract # FA9550-14-C-0004; Program Manager: Drs. Jason Marshall & John W. Luginsland and NASA Astrophysics Theory Program grant #NNX15AP39G

Multi-Fluid Plasma-Electromagnetic Models

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot [\rho_i U_i] = 0;$$

$$\frac{\partial \rho_i U_i}{\partial t} + \nabla \cdot [\rho U_i U_i + P_i] = R_i + n_i q_i E + J_i \times B;$$

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$$\frac{\partial E}{\partial t} - c^2 \nabla \times B = -\frac{\sum_i J_i}{\epsilon_0}; \quad \frac{\partial B}{\partial t} + \nabla \times E = 0$$

Target:

- multi-species fluid-plasma problems

Fundamental model:

- **hydrodynamics:** Navier-Stokes
- **multiple species:** ions, electrons and neutrals
- **coupling:** chemistry, collisions, and EM

Different species have different timescales:

- Ions, neutrals: slow
- Electrons: fast
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Simplify physics:

- Electrostatic: multiple species, but no EM waves
- MHD: single fluid, no light waves

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$\nabla^2 \phi(x,y,z) = \varrho(x,y,z)$

Electrostatic case: still need good preconditioning for Poisson +electrons

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Example Pulsed Power Application: Plasma Opening Switch

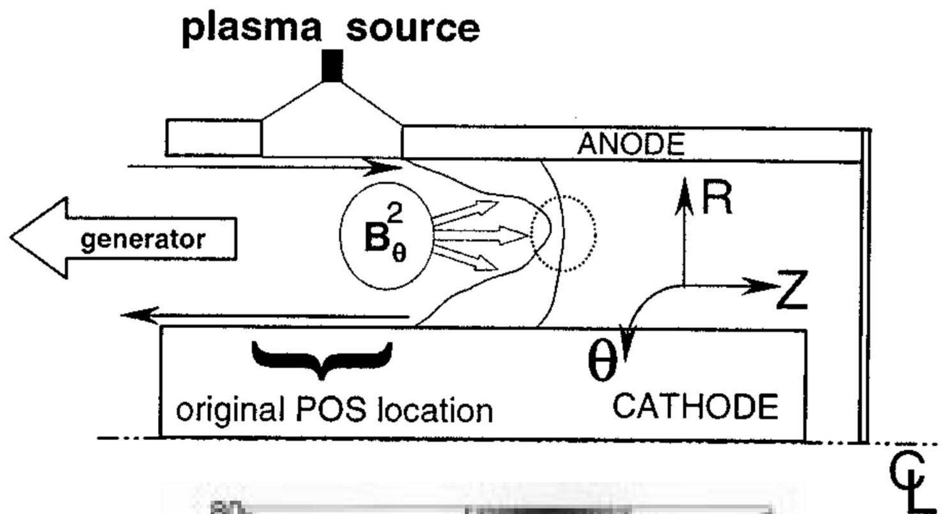
Plasma Opening Switch (**Schumer et al., 2001**):

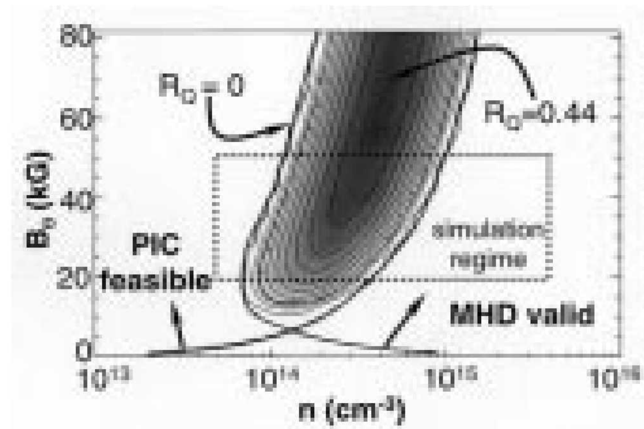
Largest scales, pulsed power requirements:

- Size of device: 10cm
- Operation timescale: 10^{-6}s

Smallest scales, plasma physics:

- Plasma density: 10^{12} - 10^{16} cm^{-3}
- Length scale: 10^{-5}cm (Debye)
- Timescale: 10^{-12}s (Plasma Freq.)





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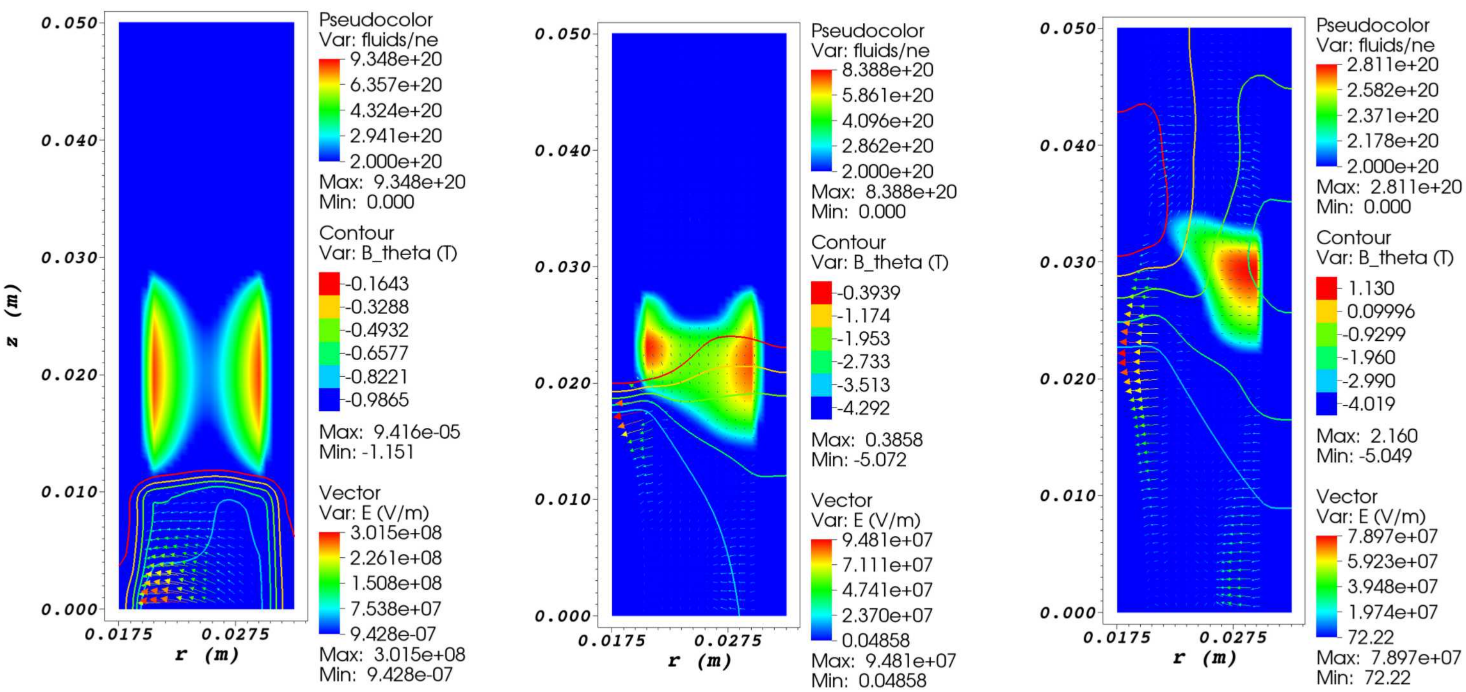

Semi-Implicit two-fluid simulation of plasma opening switch:

- Stiff source terms for multi-fluid model computed using operator split, semi-implicit method
- Simulation demonstrate penetration of electromagnetic field into the plasma and opening of the switch

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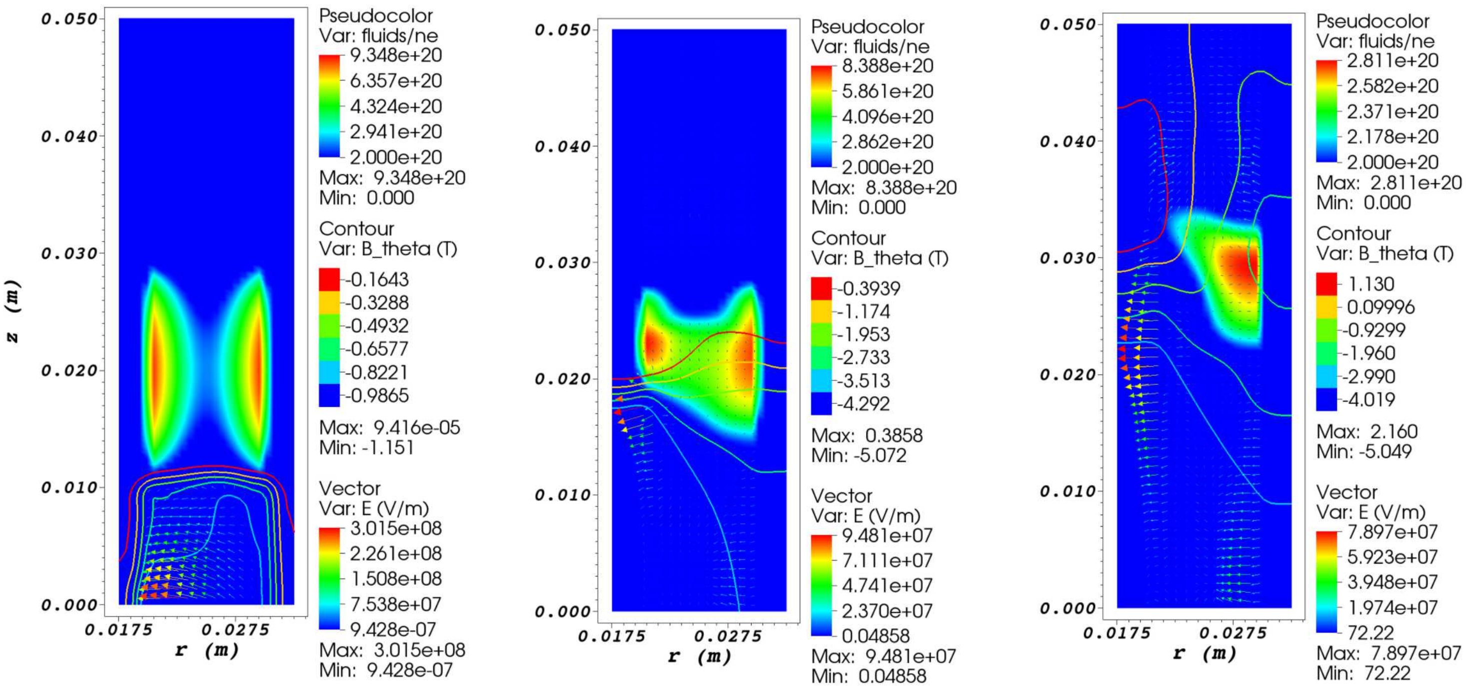


Semi-Implicit two-fluid simulation of plasma opening switch:

- Penetration of EM field into the plasma controlled by non-linear electron MHD shear instability (Richardson et al., 2016)
- Boundary conditions play a key role.

Example Application: Dense Plasma Focus

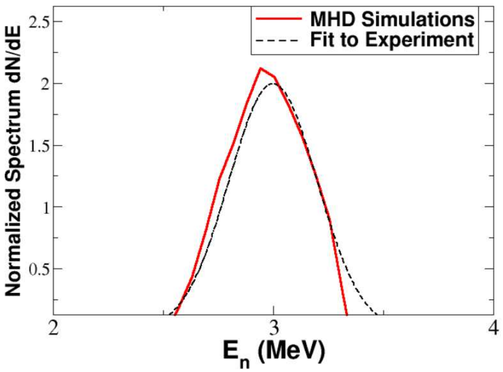
Mechanisms for pinch formation, ion acceleration and subsequent neutron production in Dense Plasma Focus are not well-understood

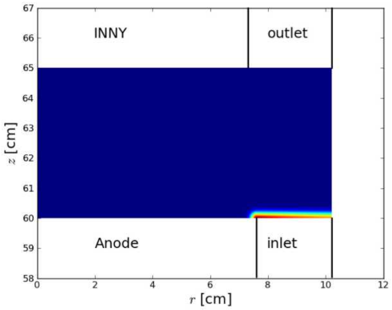
Li et al. (LANL report, 2016):

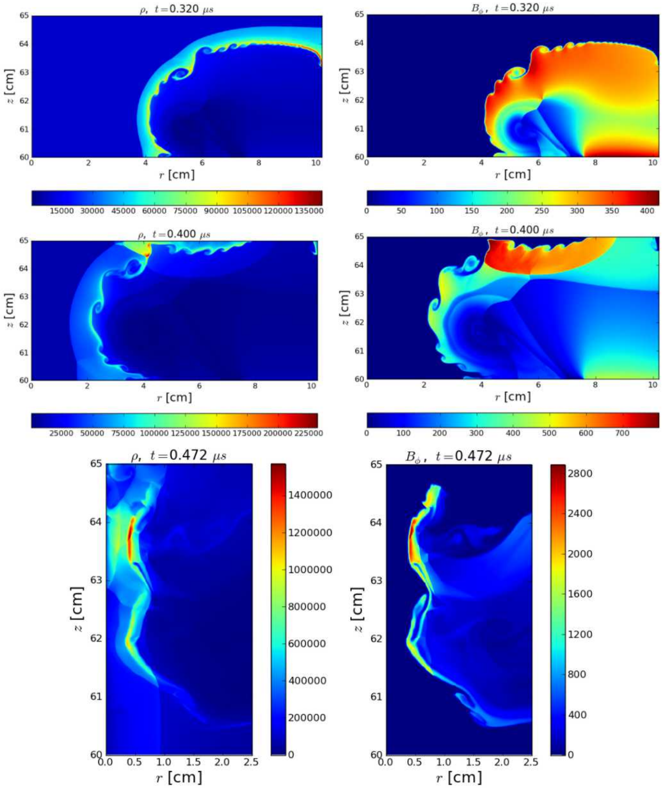
- Report high fidelity MHD simulations of a DPF geometry
- Shear layer between the magnetized region and unmagnetized region drives the onset of a Kelvin-Helmholtz-type instability
- Ions are accelerated by local electromotive forces according to:

$$\frac{d\phi_n}{dE_n}(r,t) = \frac{1}{2\pi}\int dz \int_0^{V_{max}(t)} dE_b \frac{d\phi_B(r,z,t)}{dE_B} n_2(r,z,t)\sigma(E_B)\delta(E_n - \varepsilon(E_b))$$

- Predicted neutron distribution…







Prototype Pulsed-Power Problem: Plasma Shear Instabilities

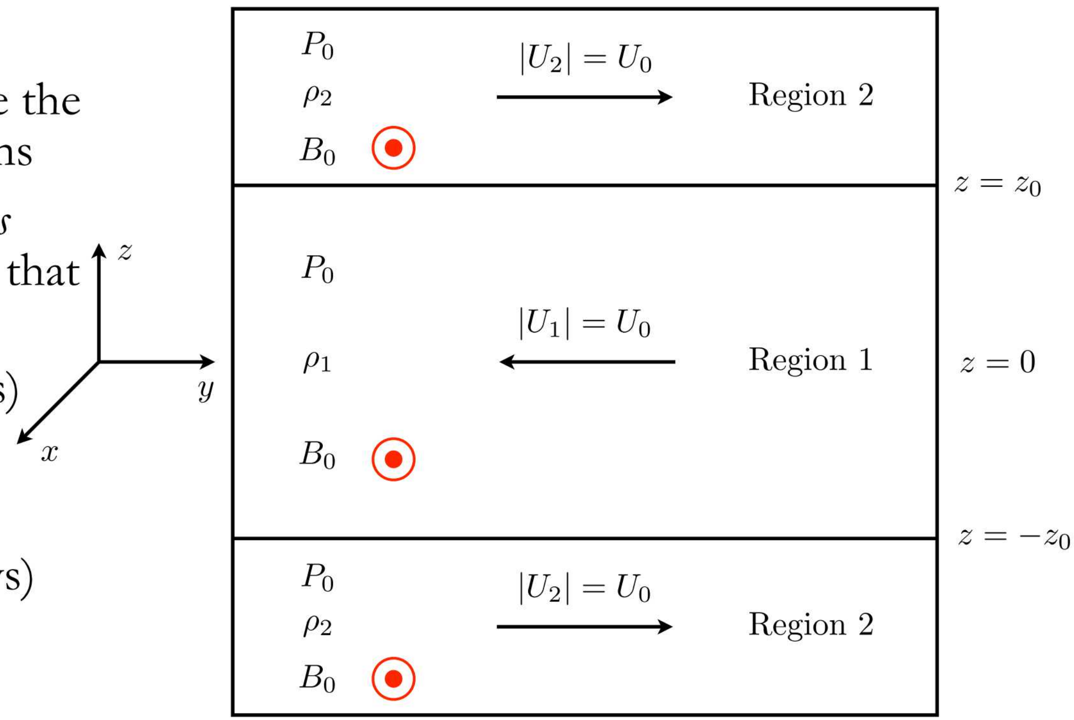
Understanding *how* the electromagnetic field penetrates into the plasma is a key aspect of understanding the operation of the plasma opening switch

- By studying this as a prototype problem physics, we can remove the influence of boundary conditions

Allows us to probe different *physics* using an *well-understood* problem so that we can investigate:

- Compressibility (transonic flows)
- Magnetic field amplification & turbulent energy cascades
- Dynamo activity (two-fluid flows)
  - Electrons can be KHI *unstable* when ions are *stable*
- Relativistic (finite Lorentz factor) effects

Salvesen et al. (2014)



$\rho_1 = 2\rho_2$; $U_0 = 0.1c_{s1}$; $B_0 = 2P_0$

Implicit Solution Stategy: Preconditioned JFNK

We have built a JFNK solver into a pre-existing plasma modeling code

- Based on existing infrastructure from Sandia National Lab available in the *Trilinos* package.
- Distributed linear algebra: *EPETRA*
- JFNK Solvers: *Nonlinear Object-Orientated Solutions*
- GMRES Solvers: *AztecOO*
- AMG Preconditioners: *ML*

Write non-linear system as a function:

- U^{n+1} is the vector of unknowns at time step $n+1$

Apply standard Newton's method to non-linear system

- Solve linear system at each substep using a Krylov method (either GMRES or BiCGStab)
- Krylov iterations can be accelerated via preconditioner
- Jacobian only appears in matrix vector products => only need the action

$$\mathcal{F}(U^{n+1}) = 0,$$

$$\delta U^k = -\left[\left(\frac{\partial \mathcal{F}}{\partial U}\right)^{n+1,k}\right]^{-1} \mathcal{F}$$

$$J(U^{n+1,k}) \equiv \left(\frac{\partial \mathcal{F}}{\partial U}\right)^{n+1,k}$$

$$\delta U^k \equiv U^{n+1,k+1} - U^{n+1,k},$$

$$J(U^k)\delta U^k \approx \frac{\mathcal{F}(U^{n+1,k} + \sigma \delta U^k) - \mathcal{F}(U^{n+1,k})}{\sigma},$$

Initial System: Two-Fluid Plasma-Electrostatic Models

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot [\rho_i U_i] = 0;$$

$$\frac{\partial \rho_i U_i}{\partial t} + \nabla \cdot [\rho U_i U_i + P_i] = R_i + n_i q_i E$$

$$\frac{\partial e_i}{\partial t} + \nabla \cdot [U_i \cdot (e_i + P_i)] = V \cdot R_i + Q_i + J_i \cdot E$$

$$V = \frac{\sum_i \rho_i U_i}{\sum_i \rho_i}; \quad R_i = -\sum_j n_i \mu_{ij} \tau_{ij}^{-1} \left(U_i - U_j\right);$$

$$Q_i = -\sum_j 3\,k\,n_i \left(\frac{\mu_{ij}}{m_i + m_j}\right) \tau_{ij}^{-1} \left(T_i - T_j\right)$$

$E = -\nabla \phi$

$\nabla^2 \phi(x,y,z) = \varrho(x,y,z)$

Electrostatic case: still need good preconditioning for Poisson +electrons

Target:

- multi-species fluid-plasma problems

Fundamental model:

- **hydrodynamics:** Navier-Stokes
- **multiple species:** ions, electrons and neutrals
- **coupling:** chemistry, collisions, and EM

Different species have different timescales:

- Ions, neutrals: slow
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- Maxwell: really fast

Simplify physics:

- Electrostatic: multiple species, but no EM waves
- MHD: single fluid, no light waves

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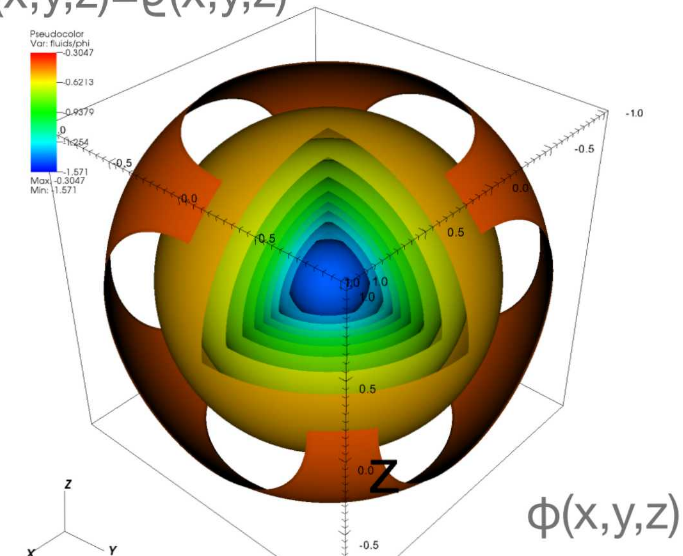

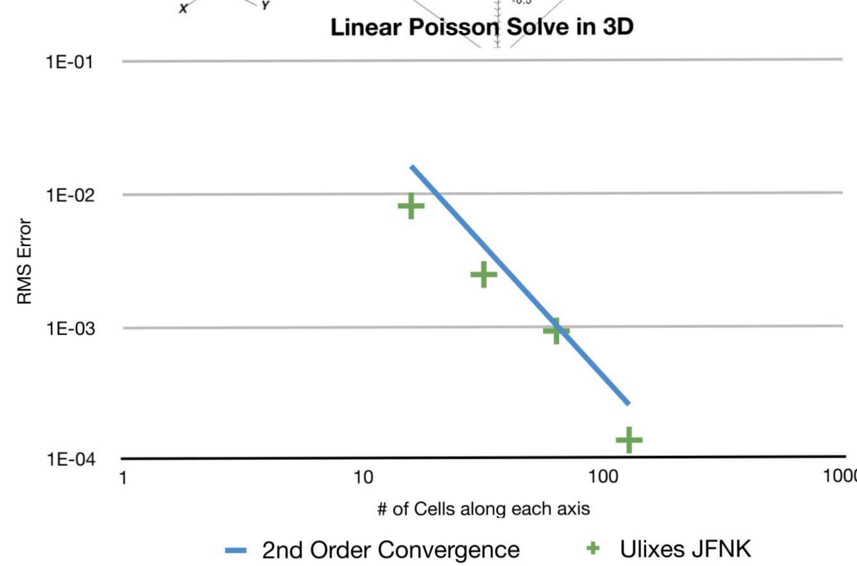

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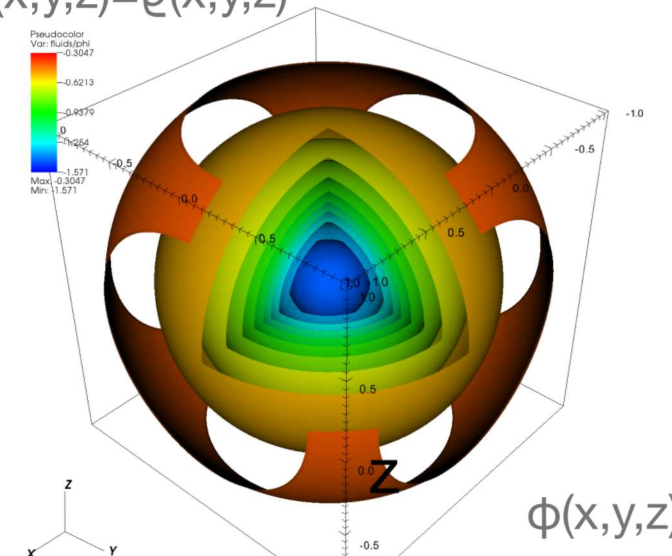

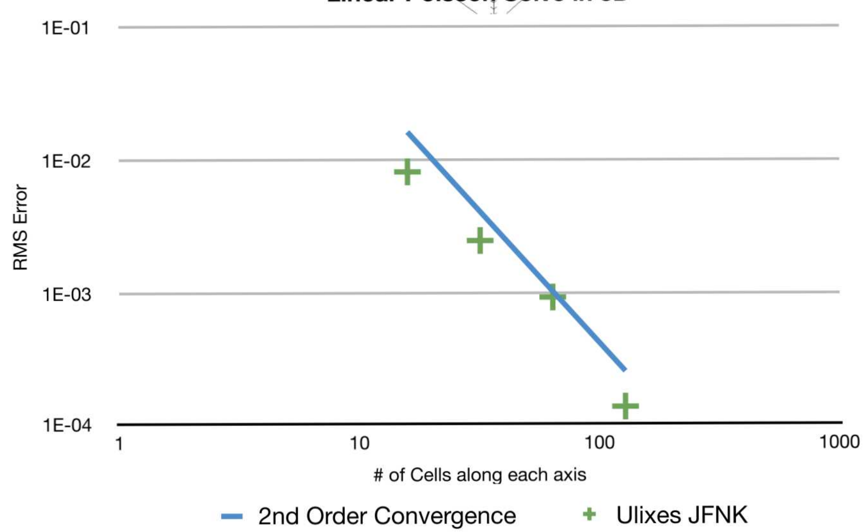

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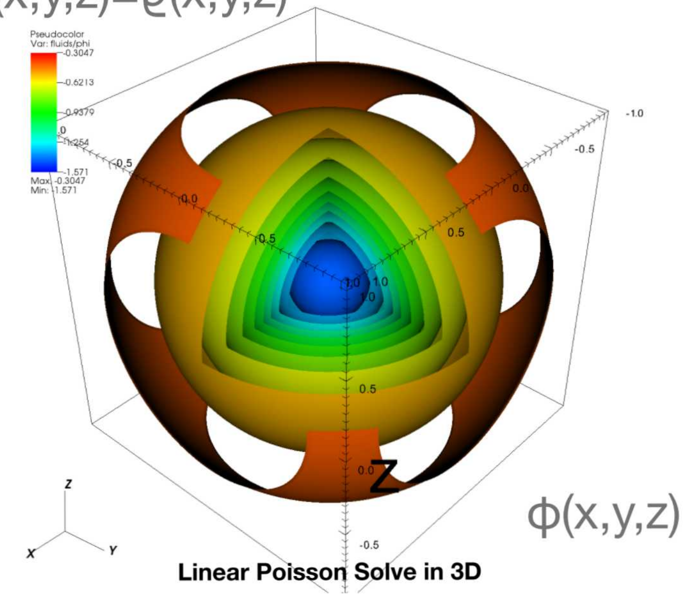
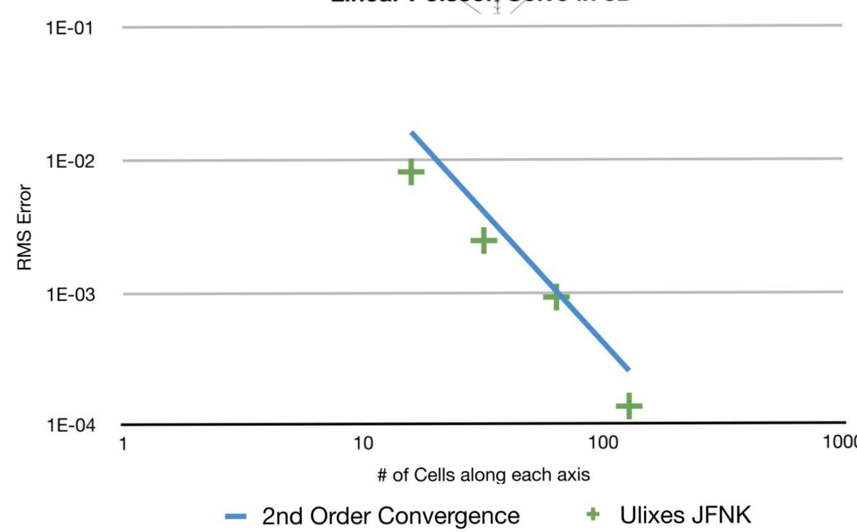


$\phi(x,y,z)$

Linear Poisson Solve in 3D



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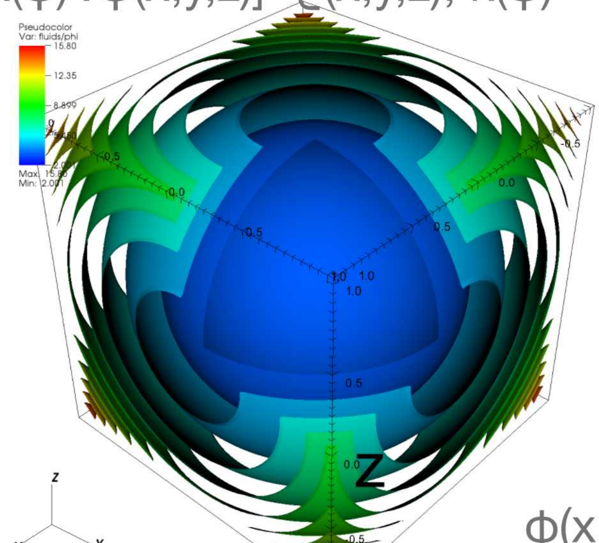

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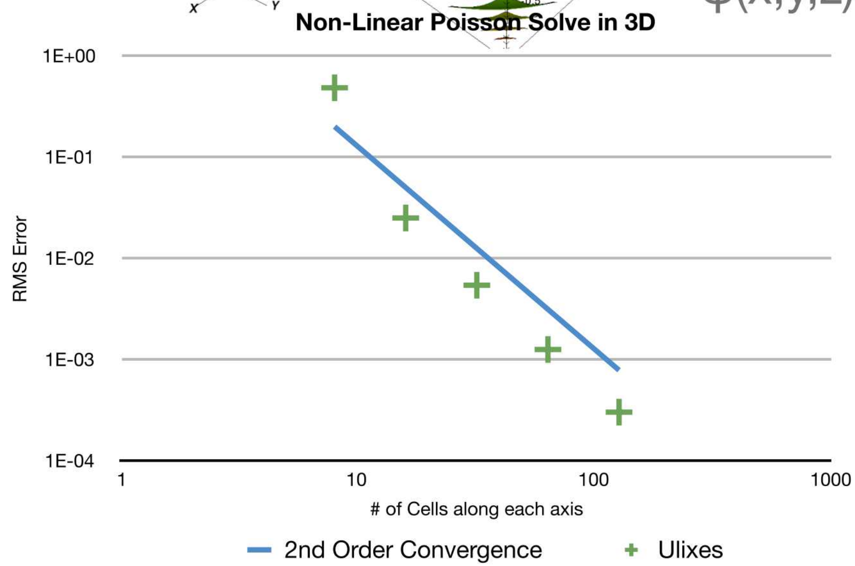

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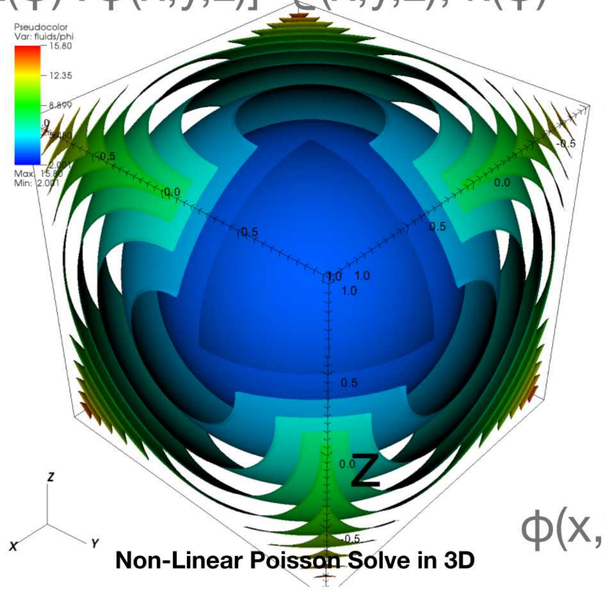

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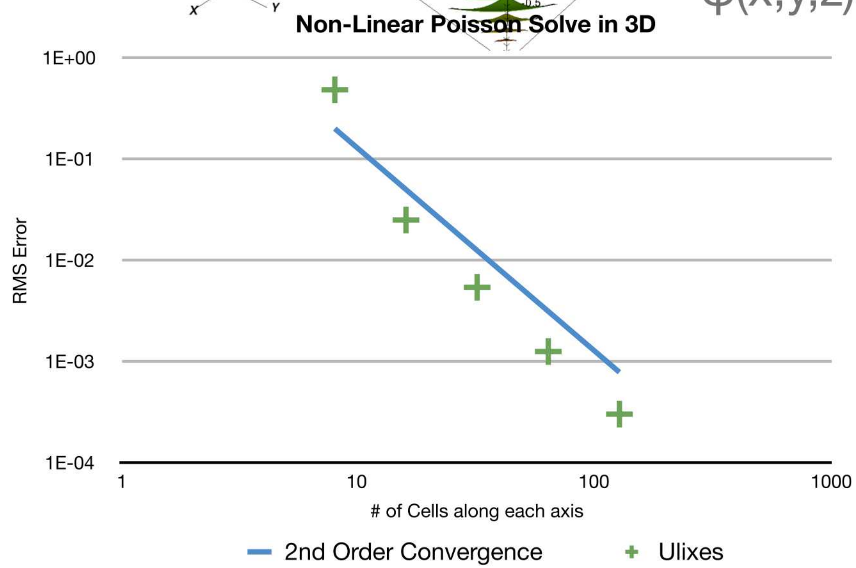

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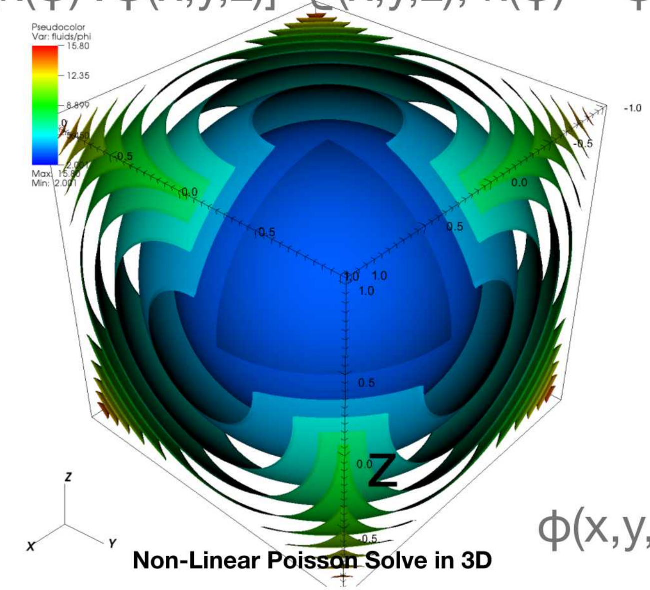

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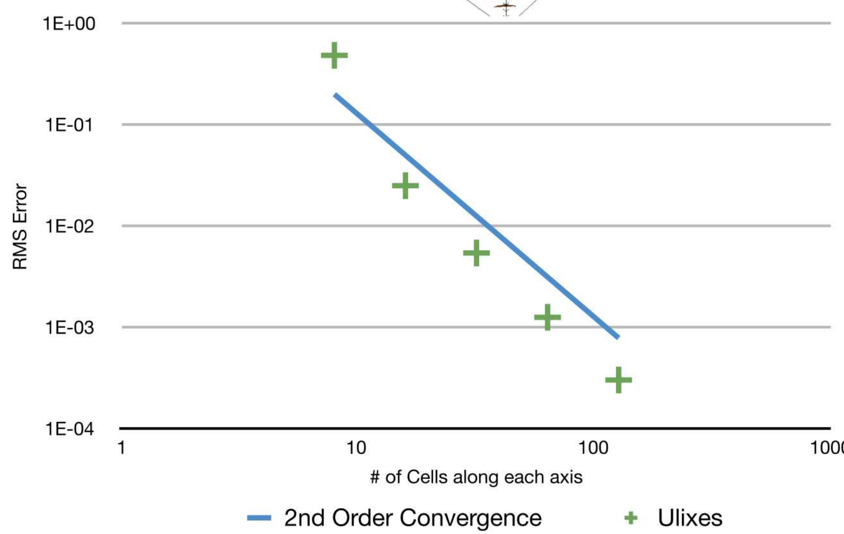


Algorithm Provides *Good* Scalability

Preconditioner is based on the matrix:

$$\frac{d^i q\,(x_a, y_a)}{dx^i} = \left[B_{\alpha,\beta} \frac{d^i p\,(x_a, y_a)_\alpha}{dx^i} \right] Q_\beta$$

Complications:

- Stencil not known a-priori
- B must be well-conditioned

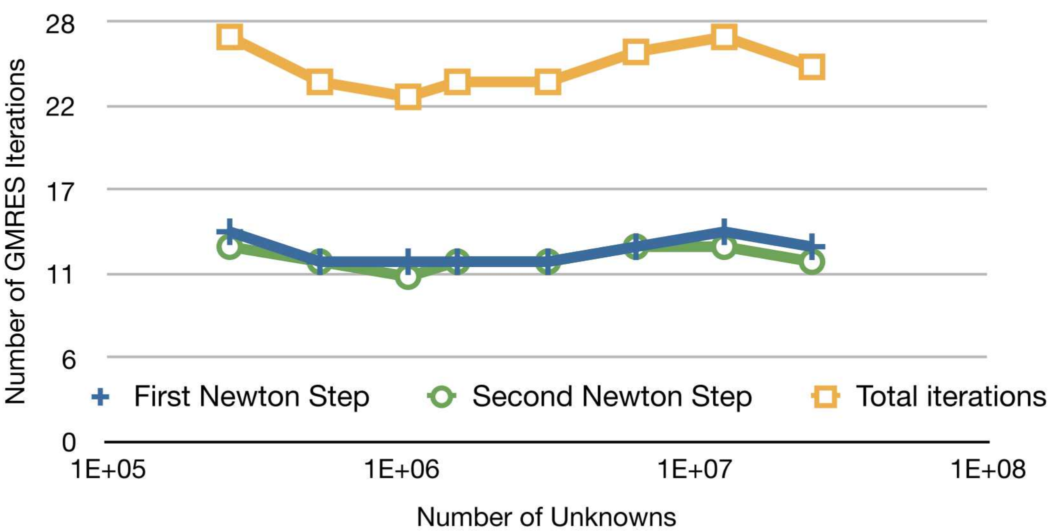
Methodology:

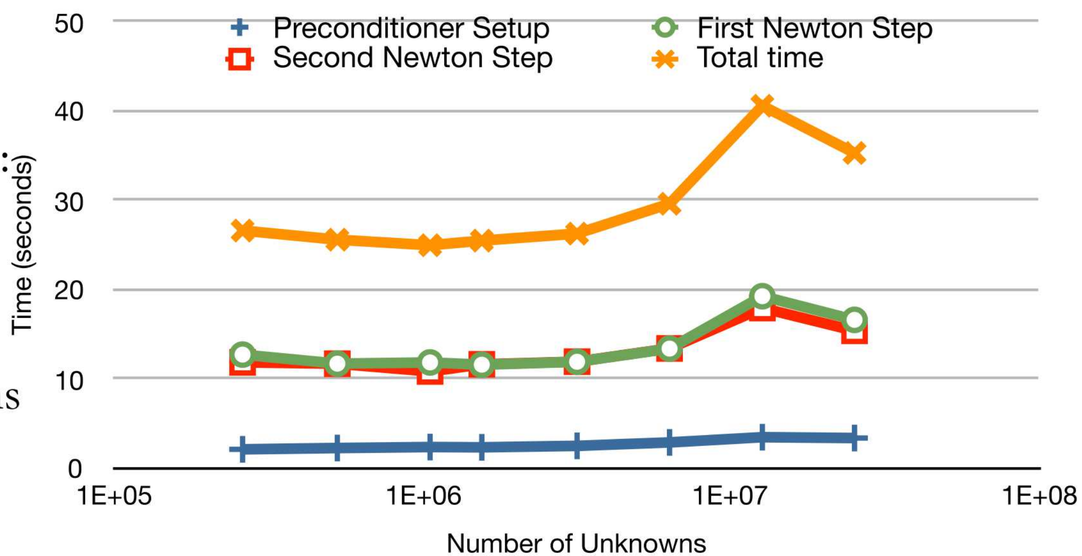
- Apply as a right preconditioner:

$$J_k P_k^{-1} P_k \delta \mathbf{x}_k = -\check{\mathbf{G}}_k$$

- Inverse computed using ML Uncoupled Smoothed Aggregation:
  - 5 Levels; Jacobi smoother on coarsest; Gauss-Seidel smoother on all others

Good weak scaling to 2x10[7] unknowns on NERSC Hopper





How to Precondition a Hyperbolic System?

Build on ideas proposed by Nejat & Olliver-Gooch (2008)

Non-linear system for hyperbolic problem (theta discretization):

$$\mathcal{F}(U^{n+1}) = U^{n+1} - U^n + (1-\theta)R(U^{n+1}) + \theta R(U^n)$$

Approximate the Jacobian as:

$$J(U^k)\delta U^k \approx \frac{\mathcal{F}(U^{n+1,k} + \sigma\delta U^k) - \mathcal{F}(U^{n+1,k})}{\sigma},$$

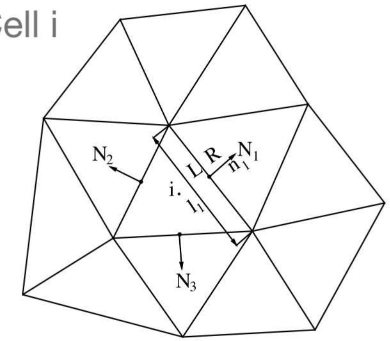
Linearize:

$$J(U^k)\delta U^k \approx \left[1 - \theta\delta t \frac{\partial R(U)}{\partial U}\right]\delta U$$

Inverting linearized Jacobian requires:

- Stencil for each cell
- Coupling between unknowns in matrix
- Utilize Roe solver to compute fluxes:
- Entropy fix renders flux differentiable

1st Order Stencil for Cell i



$$\frac{\partial R_i}{\partial U_{N_1}} = \frac{\partial F(U_i, U_{N_1})}{\partial U_{N_1}} \hat{n}_1 l_1,$$

$$\frac{\partial R_i}{\partial U_{N_2}} = \frac{\partial F(U_i, U_{N_2})}{\partial U_{N_2}} \hat{n}_2 l_2,$$

$$\frac{\partial R_i}{\partial U_{N_3}} = \frac{\partial F(U_i, U_{N_3})}{\partial U_{N_3}} \hat{n}_3 l_3,$$

$$\frac{\partial R_i}{\partial U_i} = \frac{\partial F(U_i, U_{N_1})}{\partial U_i} \hat{n}_1 l_1 + \frac{\partial F(U_i, U_{N_2})}{\partial U_i} \hat{n}_2 l_2 + \frac{\partial F(U_i, U_{N_3})}{U_i} \hat{n}_3 l_3.$$

For Roe Solver:

$$\frac{\partial F(U_i, U_{N_1})}{\partial U_{N_1}} = \frac{1}{2}\left[\frac{\partial F(U_{N_1})}{\partial U_{N_1}} - \left|\widetilde{A}\right|\right],$$

$$\frac{\partial F(U_i, U_{N_1})}{\partial U_i} = \frac{1}{2}\left[\frac{\partial F(U_i)}{\partial U_i} + |\widetilde{A}|\right].$$

$$|\widetilde{A}| = \widetilde{X}^{-1} \begin{vmatrix} f(\lambda_1) & & & \\ & f(\lambda_2) & & \\ & & f(\lambda_3) & \\ & & & f(\lambda_4) \end{vmatrix} \widetilde{X},$$

$$f(\lambda) = \begin{cases} |\lambda|, & |\lambda| \geqslant \delta, \\ \frac{\lambda^2 + \delta^2}{2\delta}, & |\lambda| < \delta. \end{cases}$$

Eigensystem Preconditioning for Hydrodynamics

Linearized Jacobian as Preconditioner:

$$J(U^k)\delta U^k \approx \left[1 - \theta\delta t \frac{\partial R(U)}{\partial U}\right]\delta U$$

Compute flux Jacobian from Roe Solver:

$$\frac{\partial R_i}{\partial U_{N_1}} = \frac{\partial F(U_i, U_{N_1})}{\partial U_{N_1}}\hat{n}_1 l_1, \quad \frac{\partial F(U_i, U_{N_1})}{\partial U_{N_1}} = \frac{1}{2}\left[\frac{\partial F(U_{N_1})}{\partial U_{N_1}} - \left|\widetilde{A}\right|\right]$$

$$|\widetilde{A}| = \widetilde{X}^{-1} \begin{vmatrix} f(\lambda_1) & & & \\ & f(\lambda_2) & & \\ & & f(\lambda_3) & \\ & & & f(\lambda_4) \end{vmatrix} \widetilde{X},$$

Coupling of unknowns is determined by structure of flux Jacobian

- Results in a set of linear, coupled PDE's

Conditioning of matrix is determined by the eigensystem

- Adjust eigensystem to improve conditioning: alter dispersion relation(s)

Start with Euler: required for multi-fluids

Adiabatic Hydro (Stone 2008)

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ -v_x^2 + \gamma' v^2/2 & -(\gamma-3)v_x & -\gamma' v_y & -\gamma' v_z & \gamma' \\ -v_x v_y & v_y & v_x & 0 & 0 \\ -v_x v_z & v_z & 0 & v_x & 0 \\ -v_x H + \gamma' v_x v^2/2 & -\gamma' v_x^2 + H & -\gamma' v_x v_y & -\gamma' v_x v_z & \gamma v_x \end{bmatrix}$$

$$\lambda = (v_x - a, v_x, v_x, v_x, v_x + a)$$

$$\mathbf{R} = \begin{bmatrix} 1 & 0 & 0 & 1 & 1 \\ v_x - a & 0 & 0 & v_x & v_x + a \\ v_y & 1 & 0 & v_y & v_y \\ v_z & 0 & 1 & v_z & v_z \\ H - v_x a & v_y & v_z & v^2/2 & H + v_x a \end{bmatrix}$$

$$\mathbf{L} = \begin{bmatrix} N_a(\gamma' v^2/2 + v_x a) & -N_a(\gamma' v_x + a) & -N_a\gamma' v_y & -N_a\gamma' v_z & N_a\gamma' \\ -v_y & 0 & 1 & 0 & 0 \\ -v_z & 0 & 0 & 1 & 0 \\ 1 - N_a\gamma' v^2 & \gamma' v_x/a^2 & \gamma' v_y/a^2 & \gamma' v_z/a^2 & -\gamma'/a^2 \\ N_a(\gamma' v^2/2 - v_x a) & -N_a(\gamma' v_x - a) & -N_a\gamma' v_y & -N_a\gamma' v_z & N_a\gamma' \end{bmatrix}$$

Eigensystem Preconditioner Provides *Good* Scalability for Compressible Flows

Apply using ML Domain-Decomposition Smoothed Aggregation with 5 levels:

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Timestep chosen so that highest resolution requires 2 Newton iterations

# of GMRES iterations:

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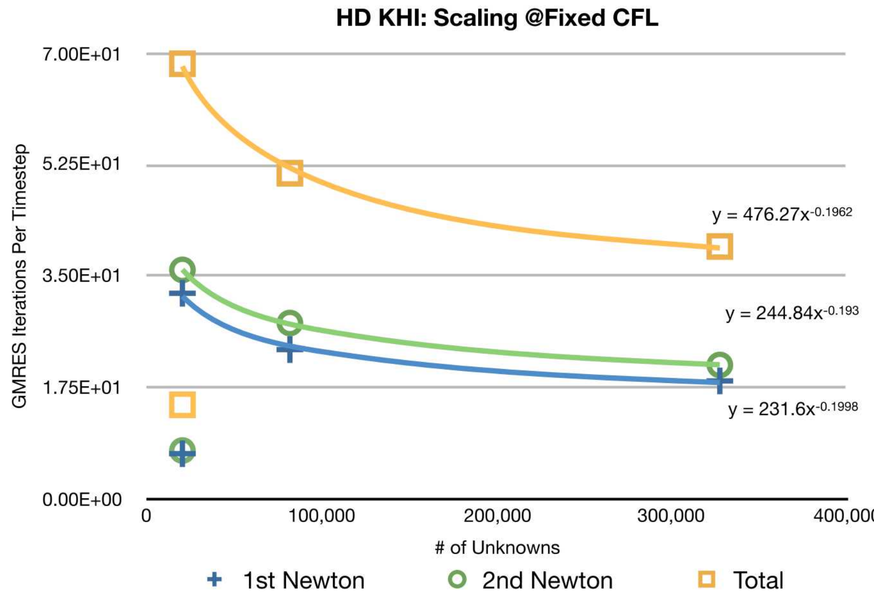
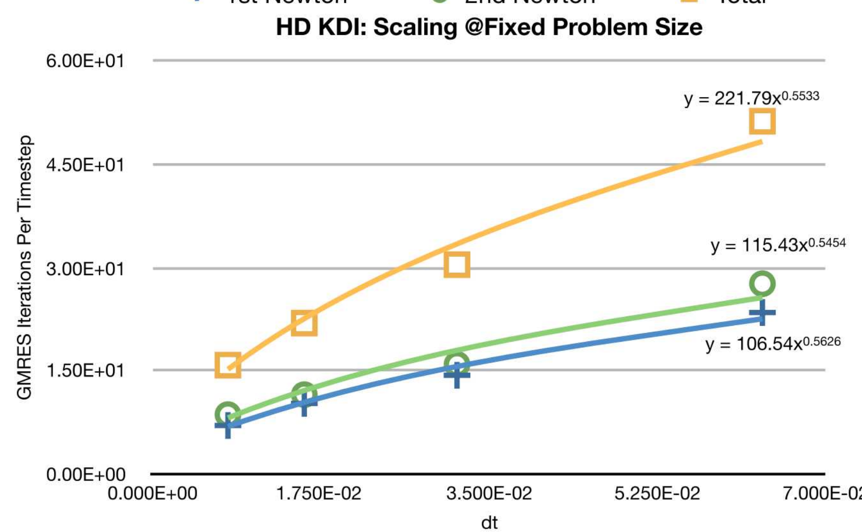
- $\sim dt^{1/2}$ @Fixed Problem size
- $\sim N^{0.2}$ with increasing N & CFL

Parallel Scaling:

- Time per GMRES iteration remains fixed
- Off node weak scaling is excellent





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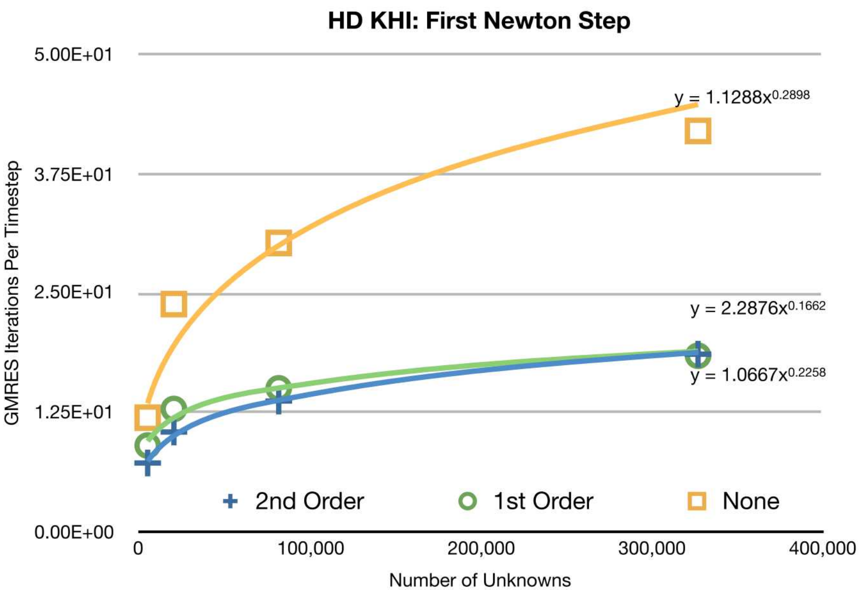

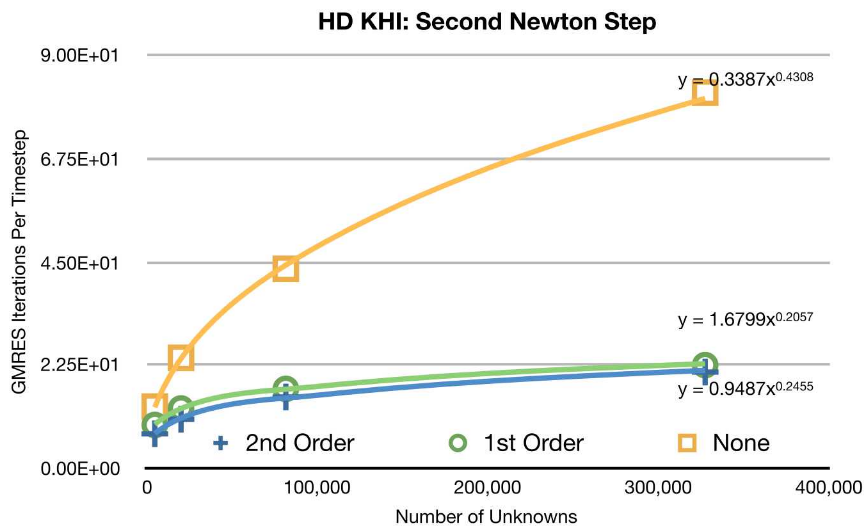

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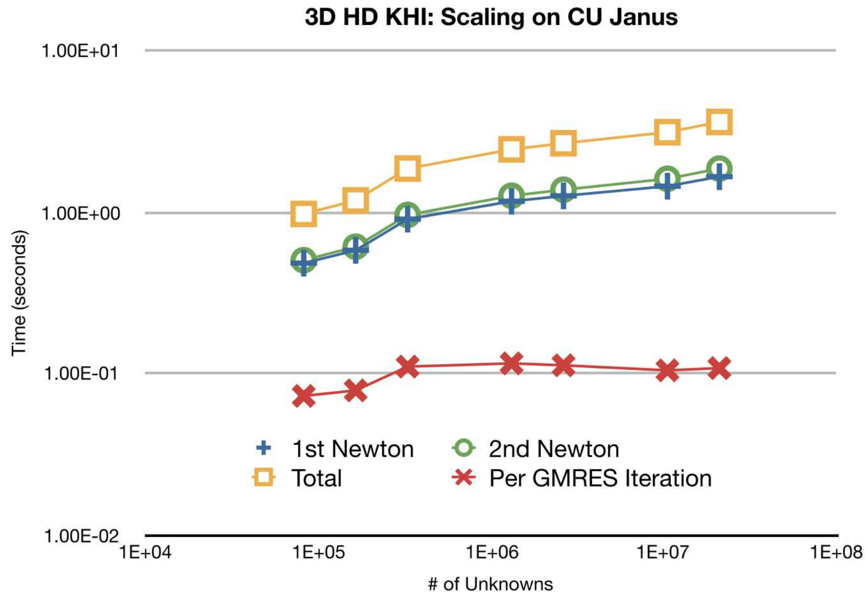
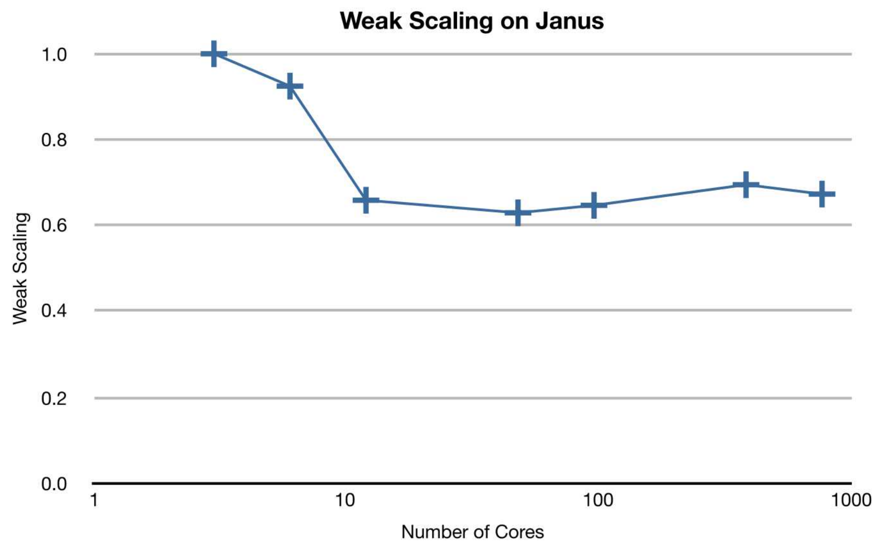
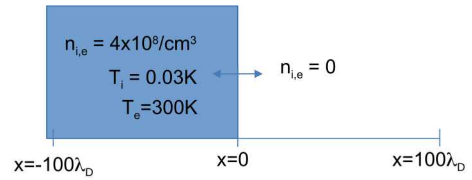




Plasma Expansion Benchmark

Mora (2003) provides an analytic model of the expansion of a plasma into a vacuum

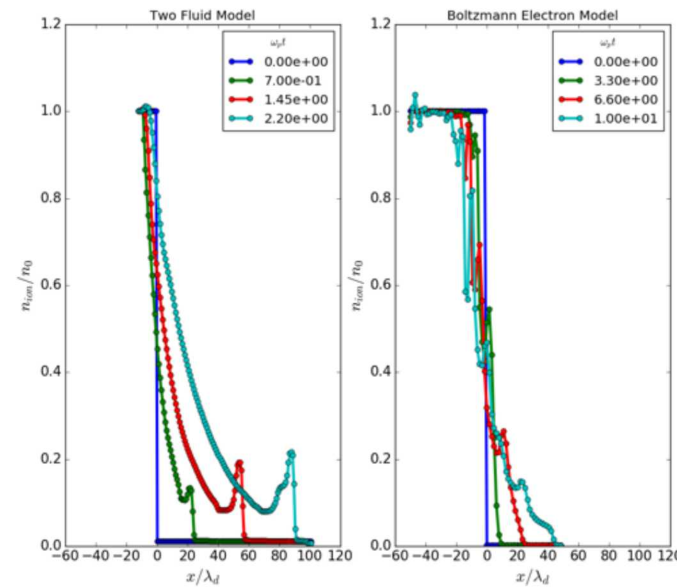


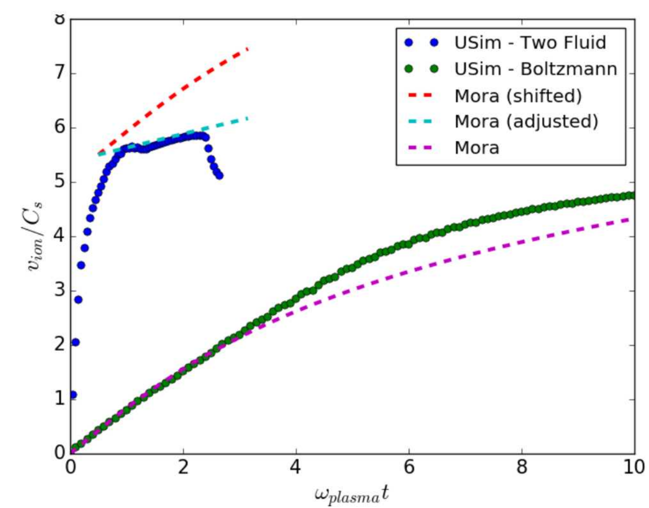
Model this process using either a two-fluid electrostatic model or using a Boltzmann electron model.

- In both cases, ions include compressibility effects
- In the two-fluid model, electrons are compressible
- Mora (2003) analytic theory assumes cold ions and Boltzmann electrons.

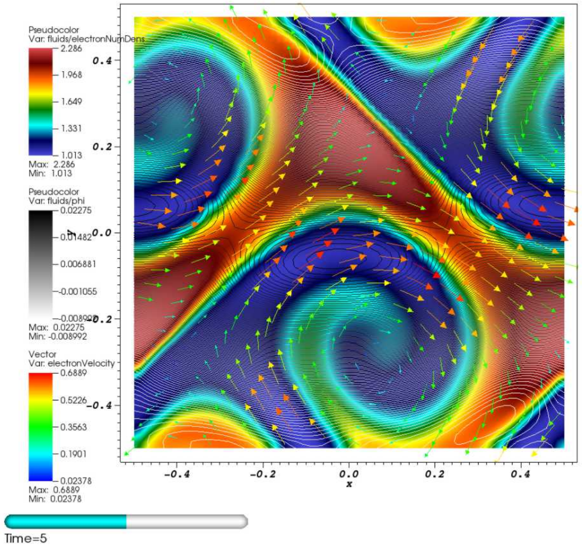
Compressibility causes transient behavior in the two-fluid model; at late times, expansion is well-described by Mora analytic theory once the ion density is accounted for.

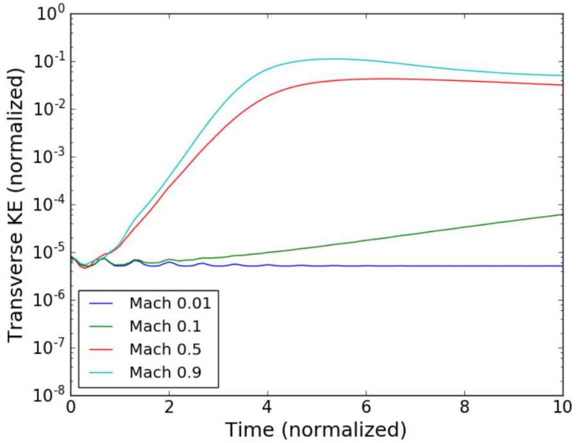
Boltzmann model provides good match to analytic theory at early times; at late times, compressibility again plays an important role and acts to accelerate the plasma beyond the analytic expectation.

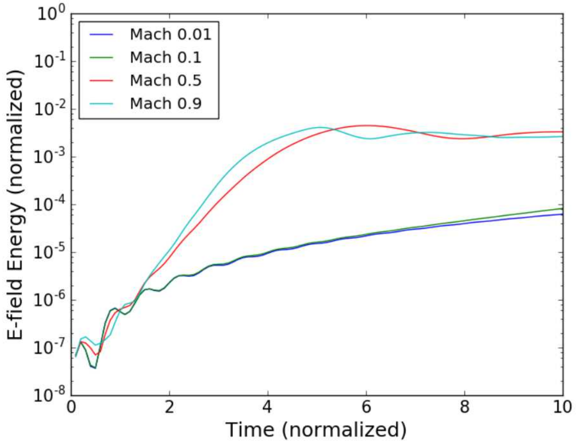




Electron Shear Instabilities with Electrostatic Diagnostics







Electron shear instabilities:

- Stationary ions (provide charge neutrality)
- Electron shear flow: linearly unstable to Kelvin Helmholtz instability

Enables study of EM penetration into plasma (Plasma Opening Switch)

Parameters chosen so that electron inertial length scale is size of domain, e.g. shear layer scale << electron inertial length

Electric potential computed based on charge separation as diagnostic.

Results:

- Transonic EKH: E-field amplified to ~10% of transverse kinetic energy
- Subsonic EKH: E-field amplified to equipartition with transverse kinetic energy

Single Fluid Magnetohydrodynamic Models

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0\,, \\
\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot \left[\rho \mathbf{v}\mathbf{v}^T - \mathbf{B}\mathbf{B}^T + \mathsf{I} \left(p + \frac{\mathbf{B}^2}{2} \right) \right] &= 0\,, \\
\frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot \left(\mathbf{v}\mathbf{B}^T - \mathbf{B}\mathbf{v}^T \right) + \nabla \psi &= 0\,, \\
\frac{\partial E}{\partial t} + \nabla \cdot \left[\left(E + p + \frac{\mathbf{B}^2}{2} \right) \mathbf{v} - (\mathbf{v} \cdot \mathbf{B})\, \mathbf{B} \right] &= 0\,,
\end{aligned}
$$

Target:

- multi-species fluid-plasma problems

Fundamental model:

- **hydrodynamics:** Navier-Stokes
- **multiple species:** ions, electrons and neutrals
- **coupling:** chemistry, collisions, and EM

Different species have different timescales:

- Ions, neutrals: slow
- Electrons: fast
- Maxwell: really fast

Simplify physics:

- MHD: single fluid, no light waves
- Extended MHD: Ohmic, Hall, electron inertia physics

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Constraint Preservation for Ideal MHD

Essential to preserve solenoidal constraint on the magnetic field:

- Introduce an additional equation describing constraint
- Augmented system carries two additional modes
- Modes are decoupled into a 2x2 linear hyperbolic system

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0\,, \\
\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot \left[\rho \mathbf{v}\mathbf{v}^T - \mathbf{B}\mathbf{B}^T + \mathsf{I}\left(p + \frac{\mathbf{B}^2}{2}\right)\right] &= 0\,, \\
\frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot \left(\mathbf{v}\mathbf{B}^T - \mathbf{B}\mathbf{v}^T\right) + \nabla \psi &= 0\,, \\
\frac{\partial E}{\partial t} + \nabla \cdot \left[\left(E + p + \frac{\mathbf{B}^2}{2}\right)\mathbf{v} - (\mathbf{v}\cdot\mathbf{B})\,\mathbf{B}\right] &= 0\,, \\
\frac{\partial \psi}{\partial t} + c_h^2 \nabla \cdot \mathbf{B} &= -\frac{c_h^2}{c_p^2}\psi\,,
\end{aligned}$$

$$\begin{aligned}
\frac{\partial B_x}{\partial t} &= -\frac{\partial \psi}{\partial x} \\
\frac{\partial \psi}{\partial t} &= -c_h^2 \frac{\partial B_x}{\partial x}
\end{aligned}$$

Godunov flux of this system can be computed exactly by:

$$B_x^* = \frac{B_{x,L} + B_{x,R}}{2} - \frac{1}{2c_h}(\psi_R - \psi_L)\,, \quad \psi^* = \frac{\psi_L + \psi_R}{2} - \frac{c_h}{2}(B_{x,R} - B_{x,L})$$

Modified states are used to calculate solution to Riemann problem using standard solver

How to Precondition a Hyperbolic System?

Build on ideas proposed by Nejat & Olliver-Gooch (2008)

Non-linear system for hyperbolic problem (theta discretization):

$$\mathcal{F}(U^{n+1}) = U^{n+1} - U^n + (1-\theta)R(U^{n+1}) + \theta R(U^n)$$

Approximate the Jacobian as:

$$J(U^k)\delta U^k \approx \frac{\mathcal{F}(U^{n+1,k} + \sigma\delta U^k) - \mathcal{F}(U^{n+1,k})}{\sigma},$$

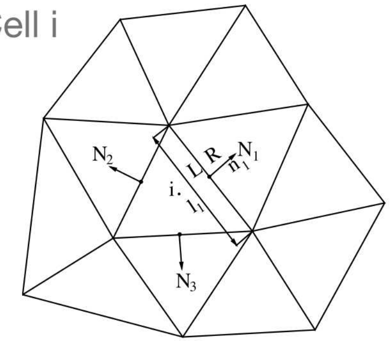
Linearize:

$$J(U^k)\delta U^k \approx \left[1 - \theta\delta t \frac{\partial R(U)}{\partial U}\right]\delta U$$

Inverting linearized Jacobian requires:

- Stencil for each cell
- Coupling between unknowns in matrix
- Utilize Roe solver to compute fluxes:
- Entropy fix renders flux differentiable

1st Order Stencil for Cell i



$$\frac{\partial R_i}{\partial U_{N_1}} = \frac{\partial F(U_i, U_{N_1})}{\partial U_{N_1}}\hat{n}_1 l_1,$$

$$\frac{\partial R_i}{\partial U_{N_2}} = \frac{\partial F(U_i, U_{N_2})}{\partial U_{N_2}}\hat{n}_2 l_2,$$

$$\frac{\partial R_i}{\partial U_{N_3}} = \frac{\partial F(U_i, U_{N_3})}{\partial U_{N_3}}\hat{n}_3 l_3,$$

$$\frac{\partial R_i}{\partial U_i} = \frac{\partial F(U_i, U_{N_1})}{\partial U_i}\hat{n}_1 l_1 + \frac{\partial F(U_i, U_{N_2})}{\partial U_i}\hat{n}_2 l_2 + \frac{\partial F(U_i, U_{N_3})}{U_i}\hat{n}_3 l_3.$$

For Roe Solver:

$$\frac{\partial F(U_i, U_{N_1})}{\partial U_{N_1}} = \frac{1}{2}\left[\frac{\partial F(U_{N_1})}{\partial U_{N_1}} - \left|\widetilde{A}\right|\right],$$

$$\frac{\partial F(U_i, U_{N_1})}{\partial U_i} = \frac{1}{2}\left[\frac{\partial F(U_i)}{\partial U_i} + |\widetilde{A}|\right].$$

$$|\widetilde{A}| = \widetilde{X}^{-1}\begin{vmatrix} f(\lambda_1) & & & \\ & f(\lambda_2) & & \\ & & f(\lambda_3) & \\ & & & f(\lambda_4) \end{vmatrix}\widetilde{X},$$

$$f(\lambda) = \begin{cases} |\lambda|, & |\lambda| \geqslant \delta, \\ \frac{\lambda^2+\delta^2}{2\delta}, & |\lambda| < \delta. \end{cases}$$

Eigensystem Preconditioning for MHD

Linearized Jacobian as Preconditioner:

$$J(U^k)\delta U^k \approx \left[1 - \theta\delta t \frac{\partial R(U)}{\partial U}\right]\delta U$$

Compute flux Jacobian from Roe Solver:

$$\frac{\partial R_i}{\partial U_{N_1}} = \frac{\partial F(U_i, U_{N_1})}{\partial U_{N_1}} \hat{n}_1 l_1, \quad \frac{\partial F(U_i, U_{N_1})}{\partial U_{N_1}} = \frac{1}{2}\left[\frac{\partial F(U_{N_1})}{\partial U_{N_1}} - \left|\widetilde{A}\right|\right]$$

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Coupling of unknowns is determined by structure of flux Jacobian

- Results in a set of linear, coupled PDE's

Conditioning of matrix is determined by the eigensystem

- Adjust eigensystem to improve conditioning: alter dispersion relation(s)

Adiabatic MHD (Mignone 2010)

$$A_x = \begin{pmatrix} v_x & \rho & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & v_x & 0 & 0 & 0 & B_y/\rho & B_z/\rho & 1/\rho & 0 \\ 0 & 0 & v_x & 0 & 0 & -B_x/\rho & 0 & 0 & 0 \\ 0 & 0 & 0 & v_x & 0 & 0 & -B_x/\rho & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & B_y & -B_x & 0 & 0 & v_x & 0 & 0 & 0 \\ 0 & B_z & 0 & -B_x & 0 & 0 & v_x & 0 & 0 \\ 0 & \Gamma p & 0 & 0 & 0 & 0 & 0 & v_x & 0 \\ 0 & 0 & 0 & 0 & c_h^2 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\lambda^{1,9} = \mp c_h\,, \quad \lambda^{2,8} = v_x \mp c_f\,, \quad \lambda^{3,7} = v_x \mp c_a\,, \quad \lambda^{4,6} = v_x \mp c_s\,, \quad \lambda^5 = v_x\,,$$

$$R = \begin{pmatrix} 0 & \rho\alpha_f & 0 & \rho\alpha_s & 1 & \rho\alpha_s & 0 & \rho\alpha_f & 0 \\ 0 & -c_f\alpha_f & 0 & -\alpha_s c_s & 0 & \alpha_s c_s & 0 & c_f\alpha_f & 0 \\ 0 & \alpha_s c_s \beta_y S & -\frac{\beta_z}{\sqrt{2}} & -\alpha_f c_f \beta_y S & 0 & \alpha_f c_f \beta_y S & -\frac{\beta_z}{\sqrt{2}} & -\alpha_s c_s \beta_y S & 0 \\ 0 & \alpha_s c_s \beta_z S & \frac{\beta_y}{\sqrt{2}} & -\alpha_f c_f \beta_z S & 0 & \alpha_f c_f \beta_z S & \frac{\beta_y}{\sqrt{2}} & -\alpha_s c_s \beta_z S & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & \alpha_s\sqrt{\rho}\alpha\beta_y & -\sqrt{\frac{\rho}{2}}\beta_z & -\alpha_f\sqrt{\rho}\alpha\beta_y & 0 & -\alpha_f\sqrt{\rho}\alpha\beta_y & \sqrt{\frac{\rho}{2}}\beta_z & \alpha_s\sqrt{\rho}\alpha\beta_y & 0 \\ 0 & \alpha_s\sqrt{\rho}\alpha\beta_z & \sqrt{\frac{\rho}{2}}\beta_y & -\alpha_f\sqrt{\rho}\alpha\beta_z & 0 & -\alpha_f\sqrt{\rho}\alpha\beta_z & -\sqrt{\frac{\rho}{2}}\beta_y & \alpha_s\sqrt{\rho}\alpha\beta_z & 0 \\ 0 & \alpha_f\Gamma p & 0 & \alpha_s\Gamma p & 0 & \alpha_s\Gamma p & 0 & \alpha_f\Gamma p & 0 \\ -c_h & 0 & 0 & 0 & 0 & 0 & 0 & 0 & c_h \end{pmatrix}$$

Decreased Scalability for Magnetized Compressible Flows

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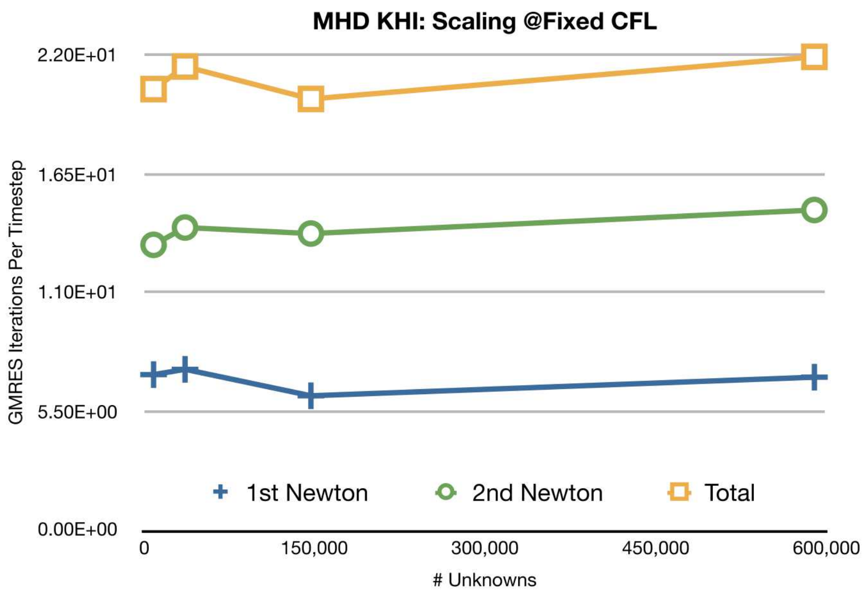

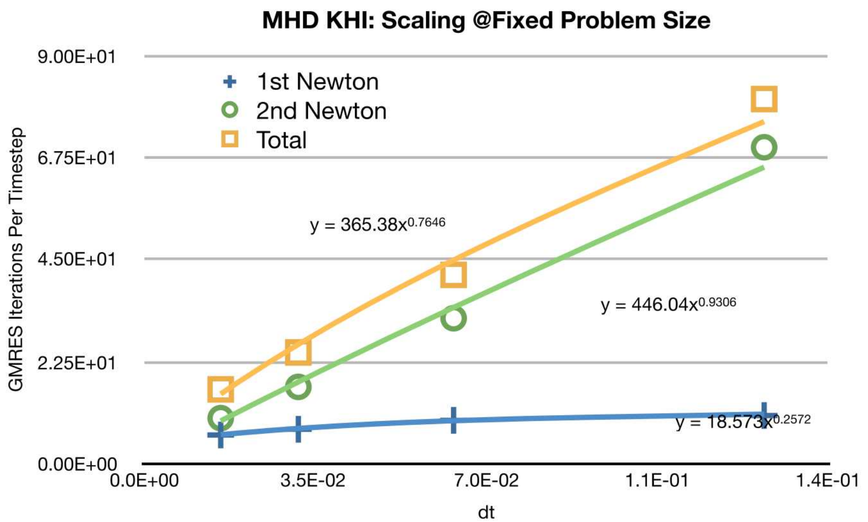

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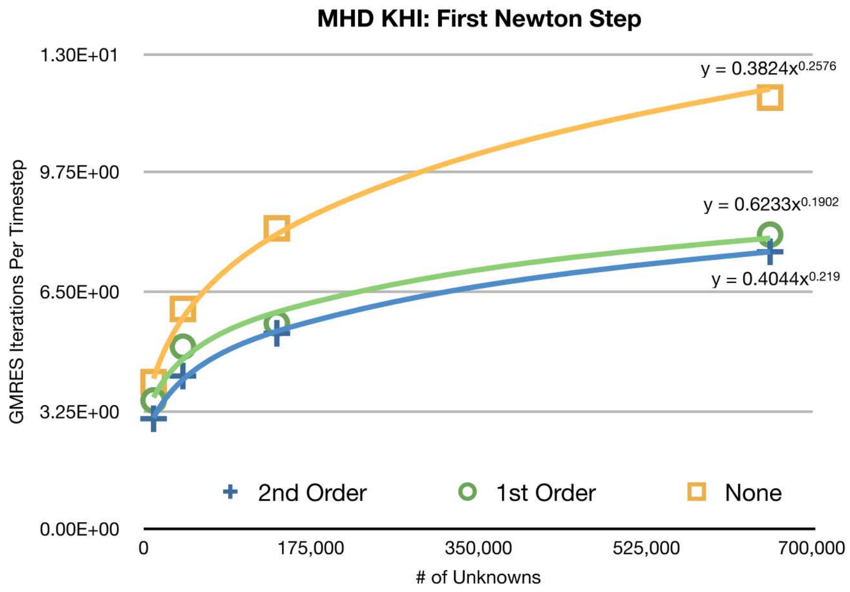

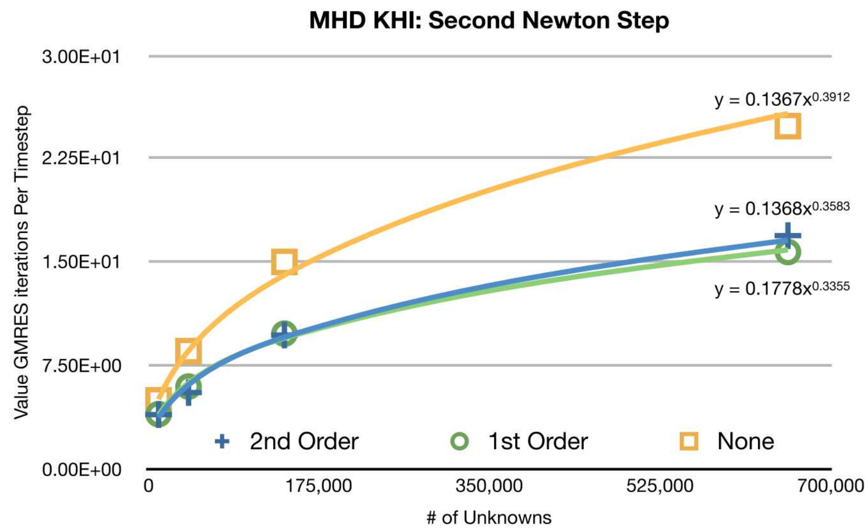

Decreased Scalability for Magnetized Compressible Flows. Why?

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Not all eigensystems are created equal!

- Even if eigenvectors are orthonormal and reproduce Jacobian
- Precise details of eigensystem (regularization) determines scalability.
- Replace highlighted elements of right-eigenvectors with those from Stone (2008)

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Eigensystem Preconditioning for MHD

Linearized Jacobian as Preconditioner:

$$J(U^k)\delta U^k \approx \left[1 - \theta\delta t \frac{\partial R(U)}{\partial U}\right] \delta U$$

Compute flux Jacobian from Roe Solver:

$$\frac{\partial R_i}{\partial U_{N_1}} = \frac{\partial F(U_i, U_{N_1})}{\partial U_{N_1}} \hat{n}_1 l_1, \quad \frac{\partial F(U_i, U_{N_1})}{\partial U_{N_1}} = \frac{1}{2}\left[\frac{\partial F(U_{N_1})}{\partial U_{N_1}} - \left|\widetilde{A}\right|\right]$$

$$|\widetilde{A}| = \widetilde{X}^{-1} \begin{vmatrix} f(\lambda_1) & & & \\ & f(\lambda_2) & & \\ & & f(\lambda_3) & \\ & & & f(\lambda_4) \end{vmatrix} \widetilde{X},$$

Not all eigensystems are created equal!

- Even if eigenvectors are orthonormal and reproduce Jacobian
- Precise details of eigensystem (regularization) determines scalability.
- Replace highlighted elements of right-eigenvectors with those from Stone (2008)

Adiabatic MHD (Mignone 2010)

$$\mathsf{A}_x = \begin{pmatrix} v_x & \rho & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & v_x & 0 & 0 & 0 & B_y/\rho & B_z/\rho & 1/\rho & 0 \\ 0 & 0 & v_x & 0 & 0 & -B_x/\rho & 0 & 0 & 0 \\ 0 & 0 & 0 & v_x & 0 & 0 & -B_x/\rho & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & B_y & -B_x & 0 & 0 & v_x & 0 & 0 & 0 \\ 0 & B_z & 0 & -B_x & 0 & 0 & v_x & 0 & 0 \\ 0 & \Gamma p & 0 & 0 & 0 & 0 & 0 & v_x & 0 \\ 0 & 0 & 0 & 0 & c_h^2 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\lambda^{1,9} = \mp c_h\,, \quad \lambda^{2,8} = v_x \mp c_f\,, \quad \lambda^{3,7} = v_x \mp c_a\,, \quad \lambda^{4,6} = v_x \mp c_s\,, \quad \lambda^5 = v_x\,,$$

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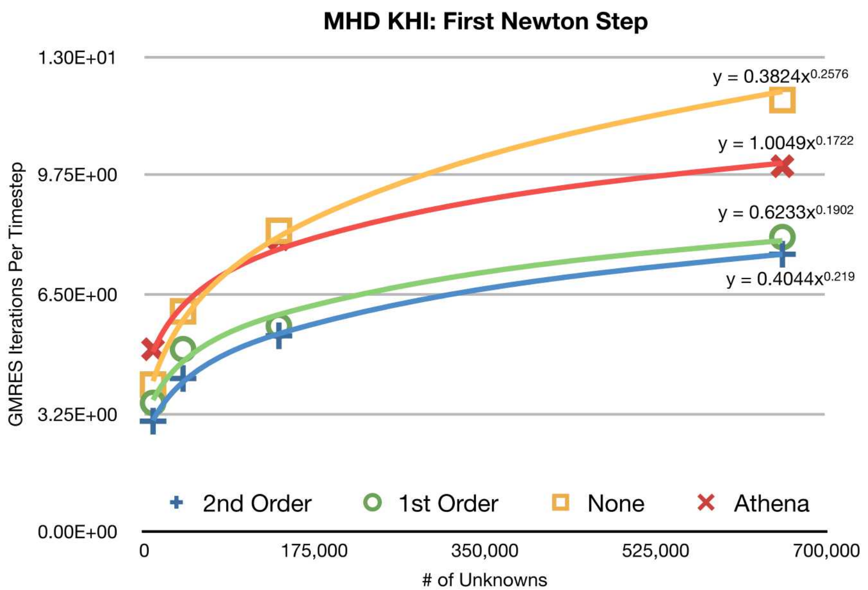
Decreased Scalability for Magnetized Compressible Flows

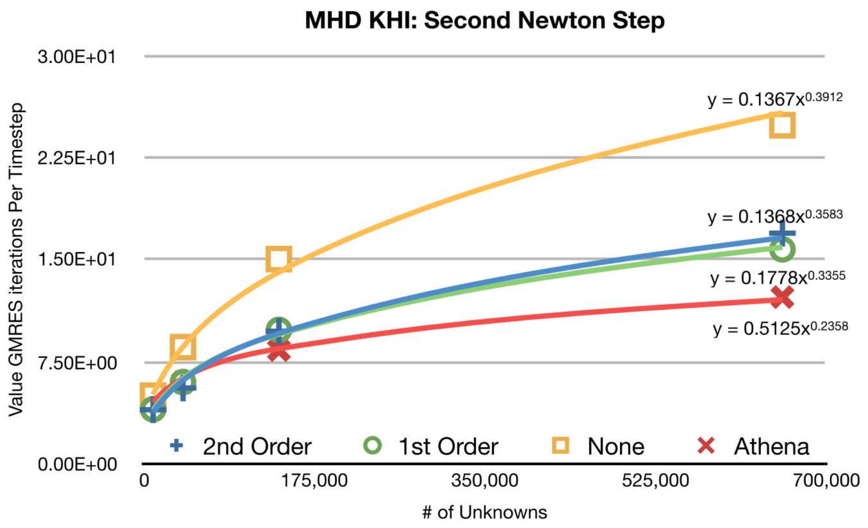
Apply using ML Domain-Decomposition Smoothed Aggregation with 5 levels:

- Block ILU smoothing with zero overlap and symmetric Gauss-Seidel relaxation on each level
- Block size chosen to be # of PDE's in system.

Examine scaling of system:

- Not all eigensystems are created equal!
- Precise details of eigensystem (regularization) determines scalability.
- Stone et al. (2008) eigensystem restores scalability observed in hydrodynamic system:
  - Decrease tolerance by *x100*
  - $\sim N^{0.22}$ with increasing N & CFL





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Route to an optimal solver:

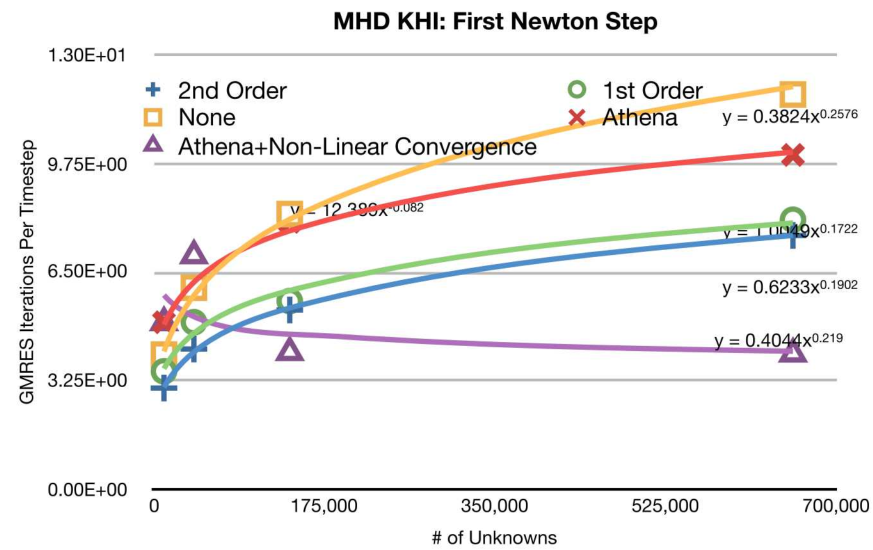
Non-linear convergence to this point determined by $||F(U)||_2 < tol$

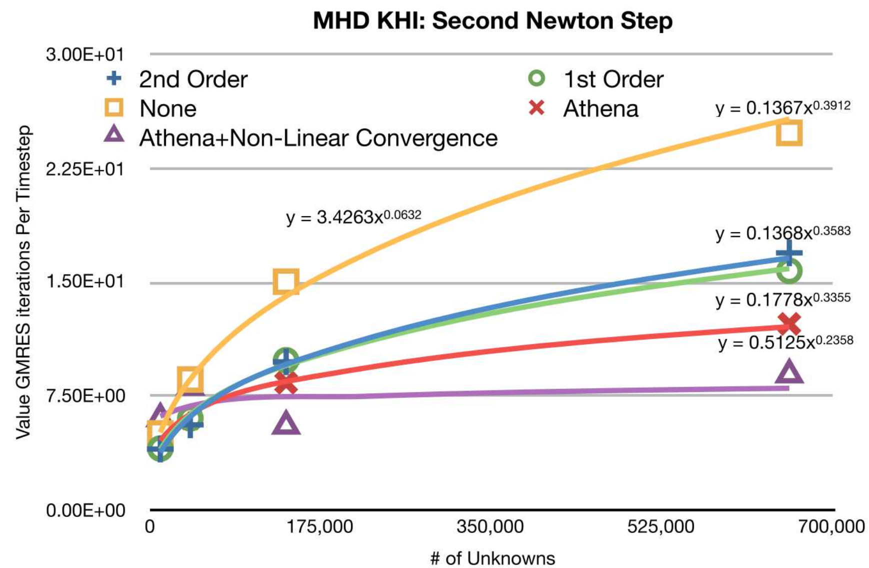
At each Newton iteration, we require that the linear solve converges to a fixed tolerance.

If we adjust the non-linear convergence criteria to: $\|\mathbf{G}(\mathbf{x}_k)\|_2 < \epsilon_a + \epsilon_r \|\mathbf{G}(\mathbf{x}_0)\|_2$

Linear solver: $\|J_k \delta \mathbf{x}_k + \mathbf{G}(\mathbf{x}_k)\|_2 < \zeta_k \|\mathbf{G}(\mathbf{x}_k)\|_2,$

Solver performance approaches optimal





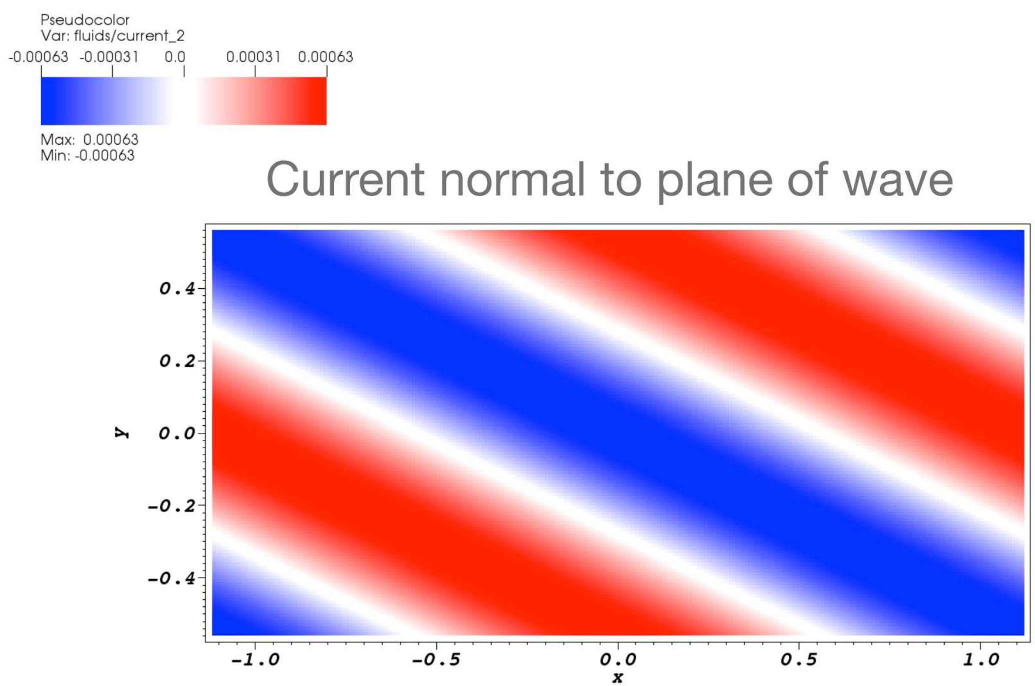
Obtain 2nd Order Convergence for **Non-Linear** Circular Polarized Alfven Waves in MHD

Circularly Polarized Alfven Wave:

- Exact, non-linear solution to ideal MHD equations

Extremely useful for:

- Diagnosing faults in numerical scheme (see e.g. Beckwith & Stone, 2011)
- Demonstrating overall 2nd order accuracy
- Divergence errors are included in RMS error



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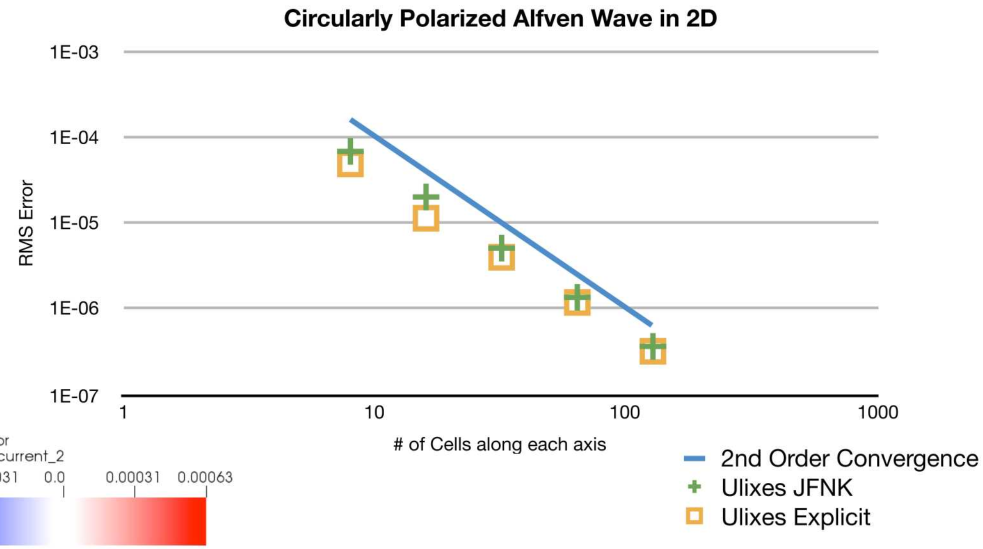
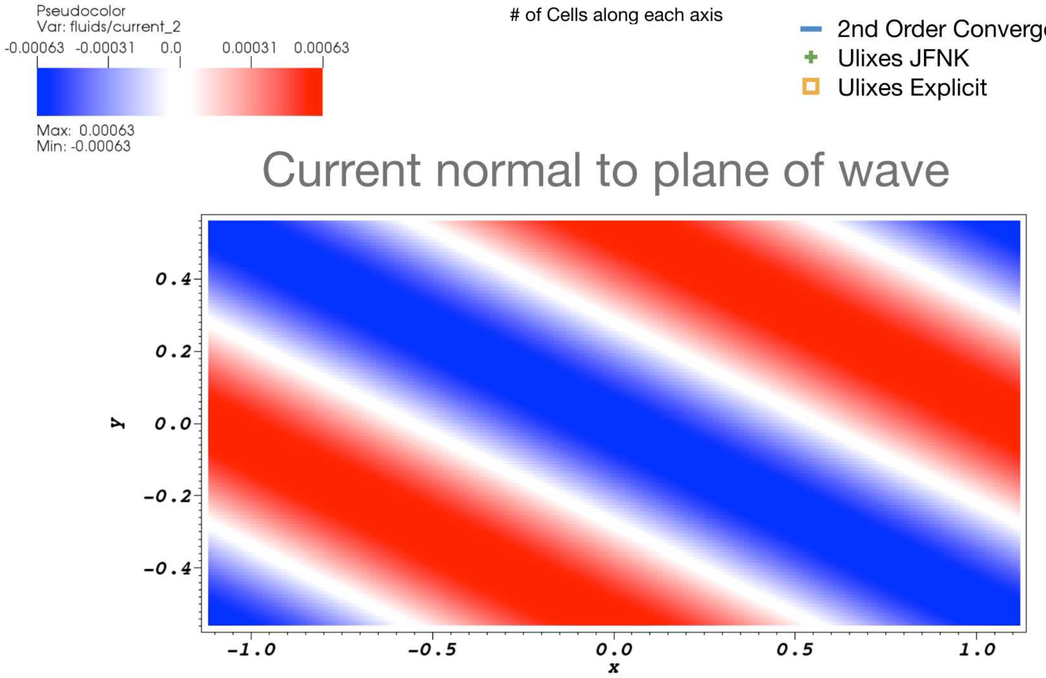


Current normal to plane of wave

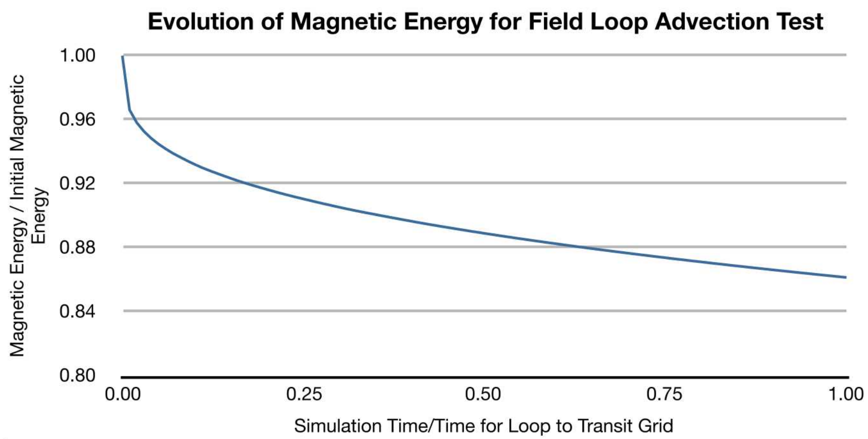


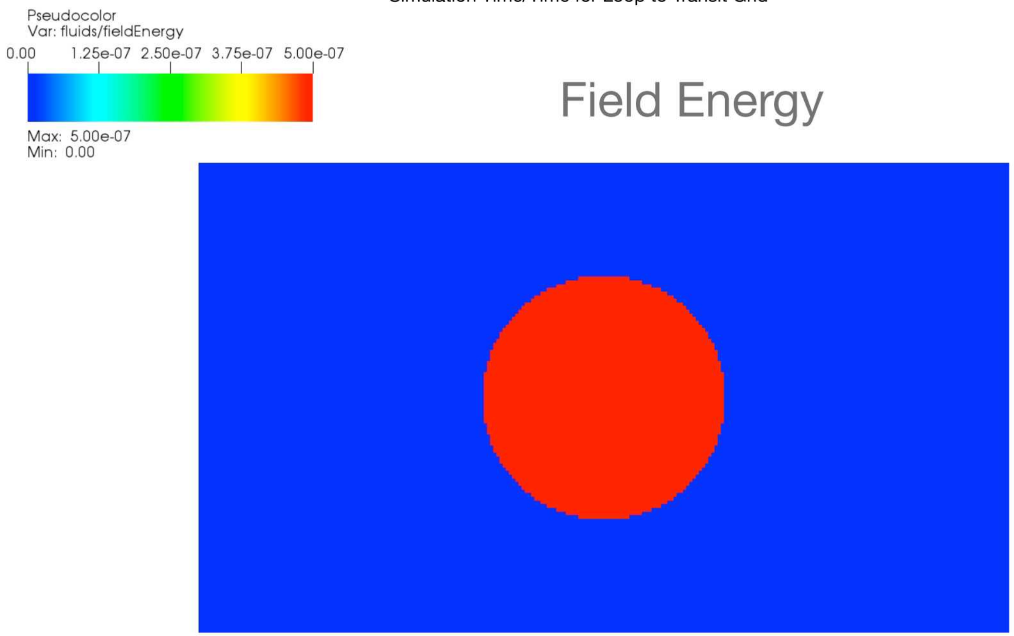
Preservation of Solenoidal Constraint: Field Loop Advection

Gardiner & Stone (2005, 2008): discriminating test of a schemes ability to preserve solenoidal constraint is advection of a weak magnetic field loop in multi-dimensions:

- Evolution of component of field normal to loop is governed by degree to which solenoidal constraint is preserved by scheme
- Violations of constraint typically lead to exponential growth of normal field

Solve using MUSCL with 2nd order accurate spatial reconstruction, 2nd order time-integration.





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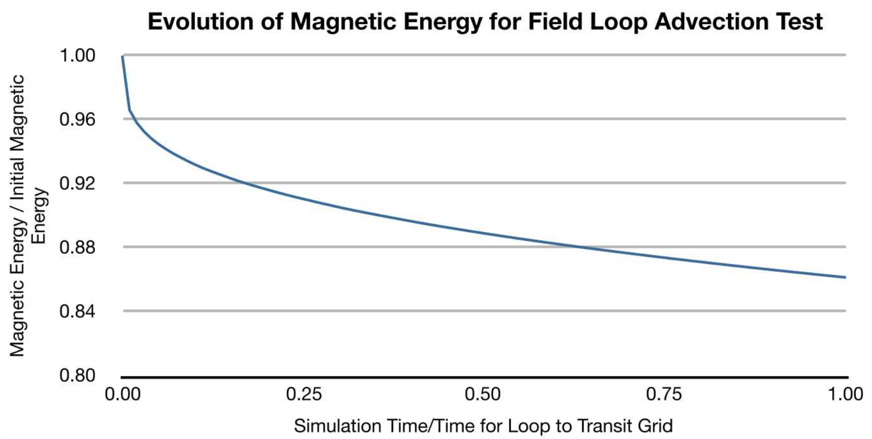

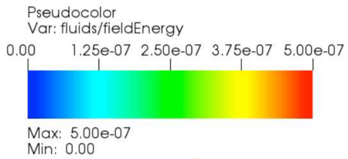

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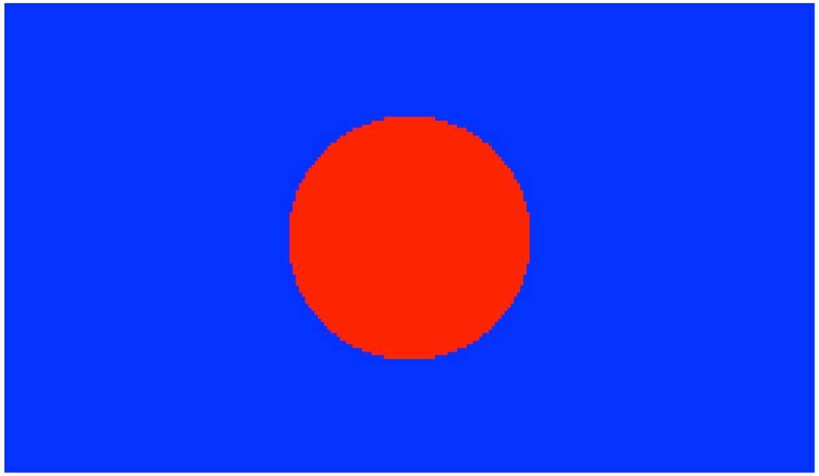

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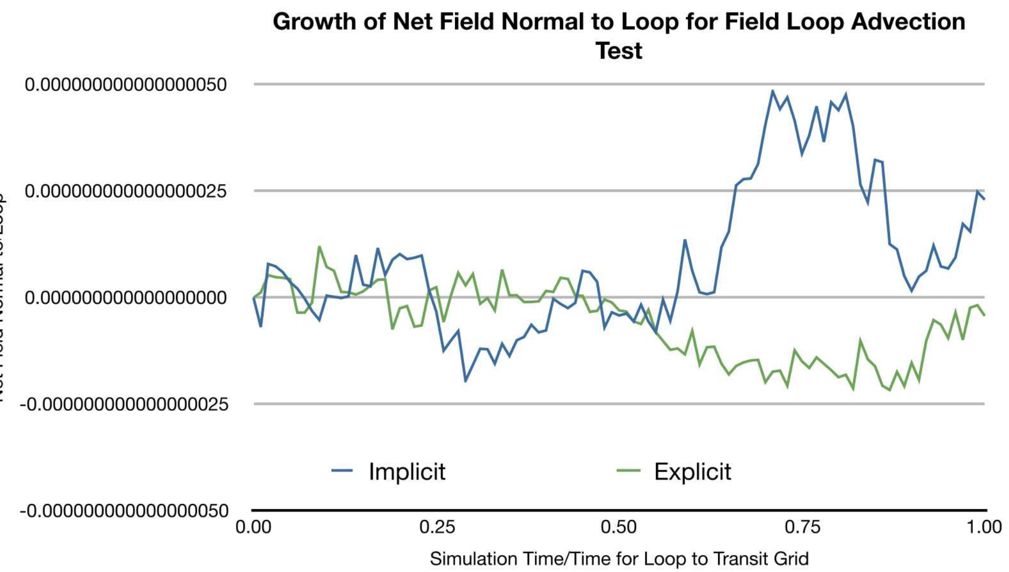
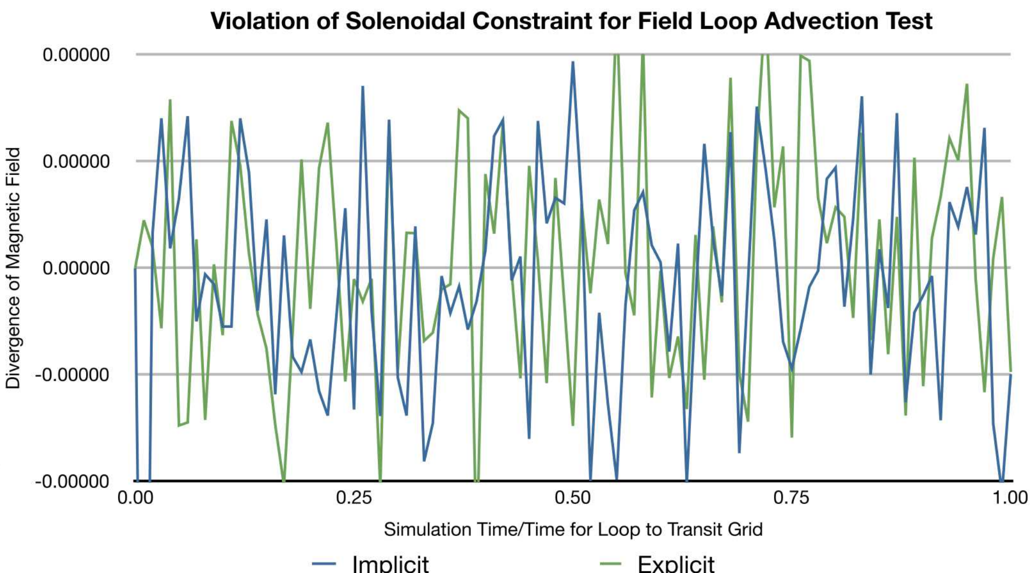
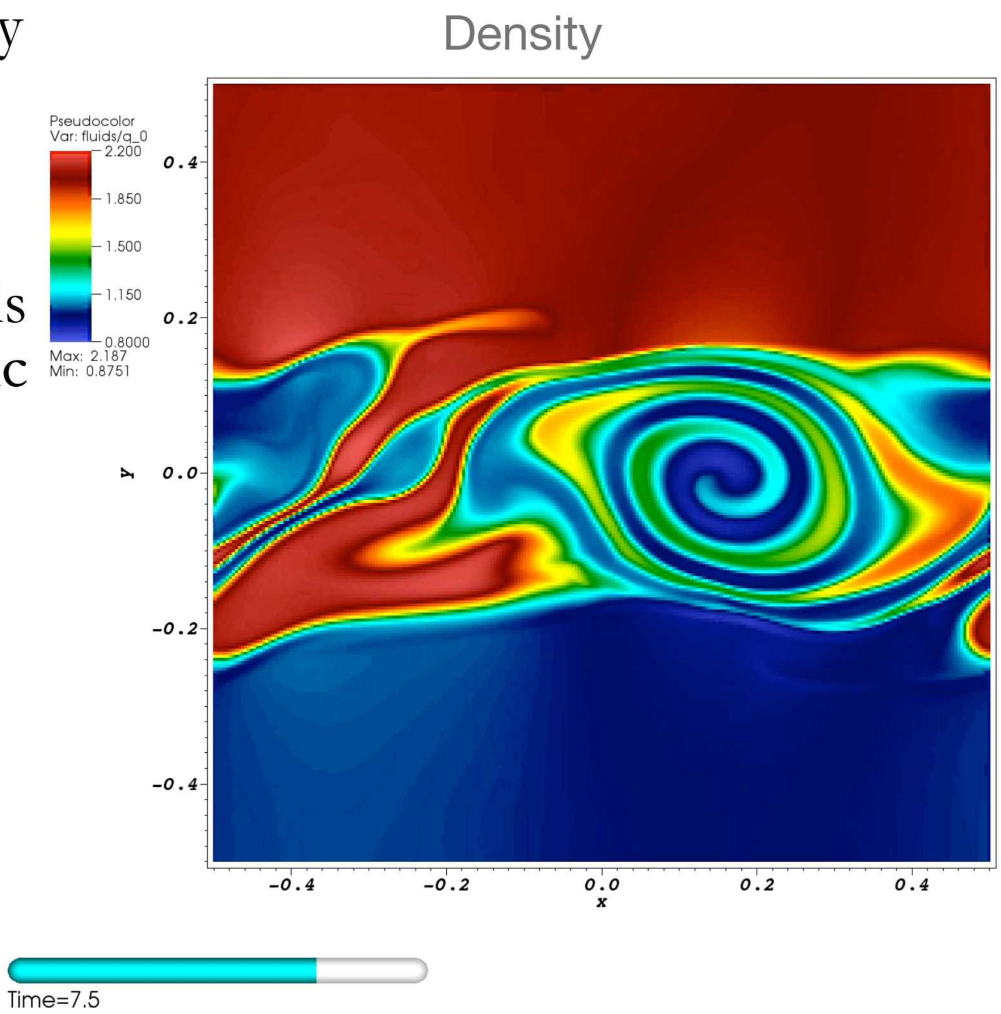




Scheme can Handle Transition from Linear to Non-Linear Regimes in Transonic Flows

Kelvin-Helmholtz instability provides a useful test of solver capability for non-linear compressible flows

- Magnetized version of this problem involves magnetic field amplification
- Solver is capable of evolving instability into non-linear regime
- Magnetic field amplification by factor ~10.



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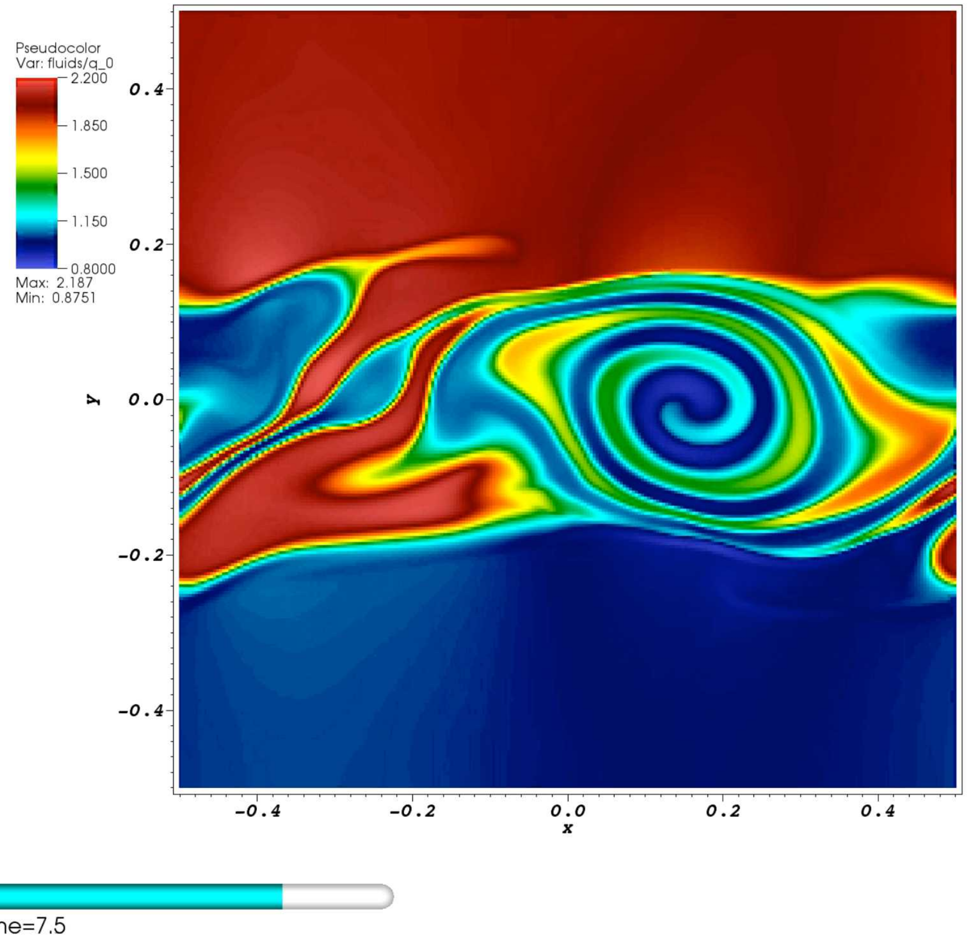

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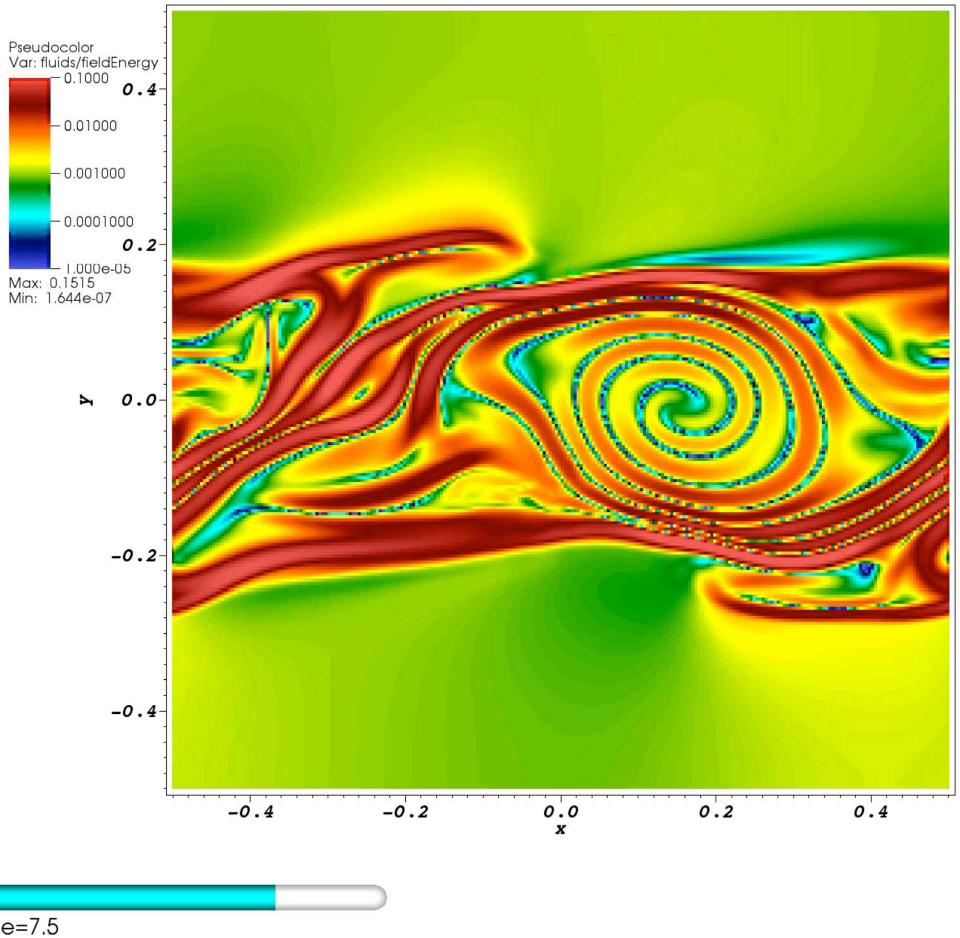

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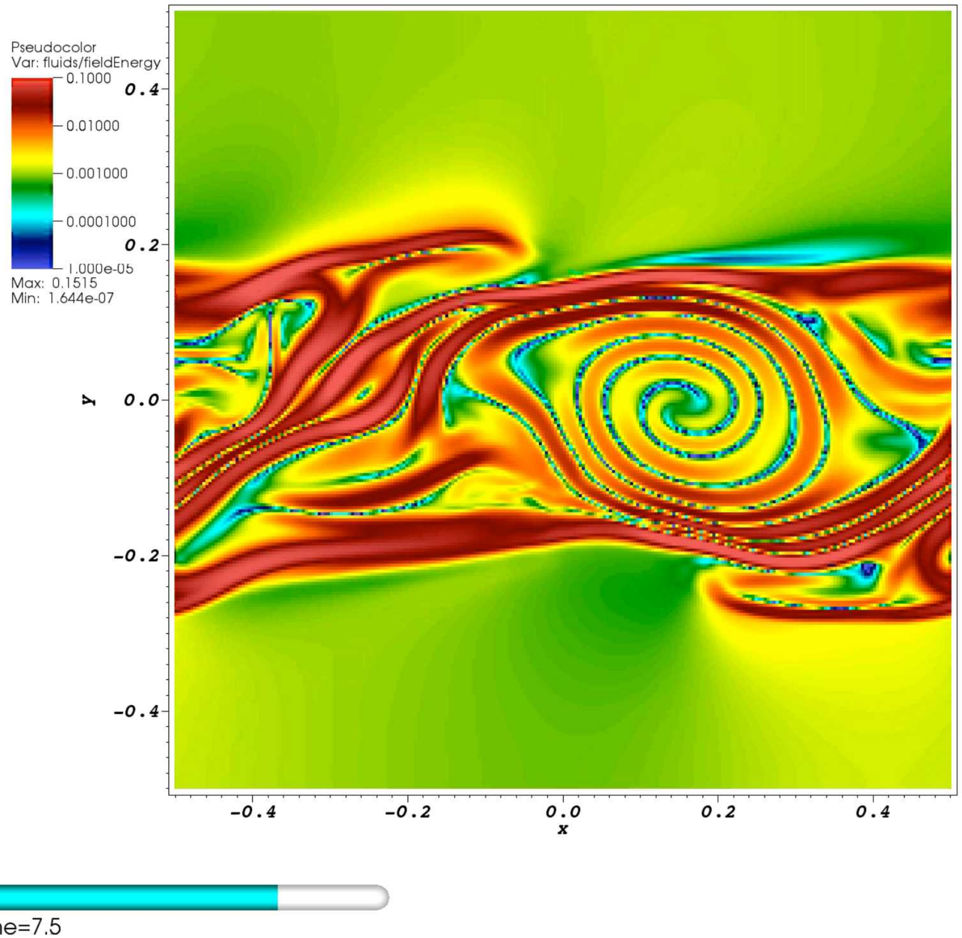

Two-Fluid Plasma-Electromagnetic Models

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot [\rho_i U_i] = 0;$$

$$\frac{\partial \rho_i U_i}{\partial t} + \nabla \cdot [\rho U_i U_i + P_i] = R_i + n_i q_i E + J_i \times B;$$

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$$\frac{\partial E}{\partial t} - c^2 \nabla \times B = -\frac{\sum_i J_i}{\epsilon_0}; \quad \frac{\partial B}{\partial t} + \nabla \times E = 0$$

Target:

- multi-species fluid-plasma problems

Fundamental model:

- **hydrodynamics:** Navier-Stokes
- **multiple species:** ions, electrons and neutrals
- **coupling:** chemistry, collisions, and EM

Different species have different timescales:

- Ions, neutrals: slow
- Electrons: fast
- Maxwell: really fast

Simplify physics:

- Two-Fluid: only ions, electrons
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$$\frac{\partial \rho_c}{\partial t} + \nabla \cdot \left[\sum_i \frac{q_i}{m_i} \rho_i U_i \right] = 0 \quad \frac{\partial \bar{J}}{\partial t} + \nabla \cdot \left[\sum_i \frac{q_i}{m_i} (\rho_i U_i U_i + P_i) \right] = \sum_i \frac{q_i}{m_i} \left(\frac{q_i}{m_i} \rho_i E + J_i \times B \right)$$

$$\frac{\partial e_i}{\partial t} + \nabla \cdot [U_i \cdot (e_i + P_i)] = V \cdot R_i + Q_i + J_i \cdot E$$

$$\frac{\partial E}{\partial t} - c^2 \nabla \times B = -\frac{\sum_i J_i}{\epsilon_0}; \quad \frac{\partial B}{\partial t} + \nabla \times E = 0$$

Target:

- multi-species fluid-plasma problems

Fundamental model:

- **hydrodynamics:** Navier-Stokes
- **multiple species:** ions, electrons and neutrals
- **coupling:** chemistry, collisions, and EM

Different species have different timescales:

- Ions, neutrals: slow
- Electrons: fast
- Maxwell: really fast

Simplify physics:

- Two-Fluid: only ions, electrons
- Two-fluid in MHD-like form: Ohmic, Hall, electron inertia

Reformulate Multi-Fluid Model: Take Advantage of MHD Eigensystem

$$\sum_\alpha \frac{q_\alpha}{m_\alpha}\rho_\alpha E + J_\alpha \times B = -\frac{1}{c^2}\frac{\partial S_{EM}}{\partial t} + \nabla \cdot T_{EM}$$

$$\sum_\alpha J_\alpha \cdot E = -\frac{\partial E_{EM}}{\partial t} - \nabla \cdot S_{EM}$$

$$S_{EM} = \frac{E \times B}{\mu_0}$$

$$T_{EM} = \frac{1}{\mu_0}\left(\frac{EE}{c^2} + BB + \mathbb{I}E_{\mathrm{EM}}\right)$$

$$E_{EM} = \frac{1}{2\mu_0}\left(\frac{|E|^2}{c^2} + |B|^2\right)$$

Use Maxwell's equations to rewrite:

- Lorentz force in terms of conservation of EM stress.
- Work-done in terms of conservation of EM energy

Allows reformulation of total momentum equation as a conservation law without source terms.

Rewrite two-fluid equations in MHD-like form:

- Reuse MHD preconditioner

- Incorporate:
  - u x B term
  - Resistive physics
  - Hall physics
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- Compute multi-fluid shocks in range of regimes using single solver framework:
  - Ideal MHD
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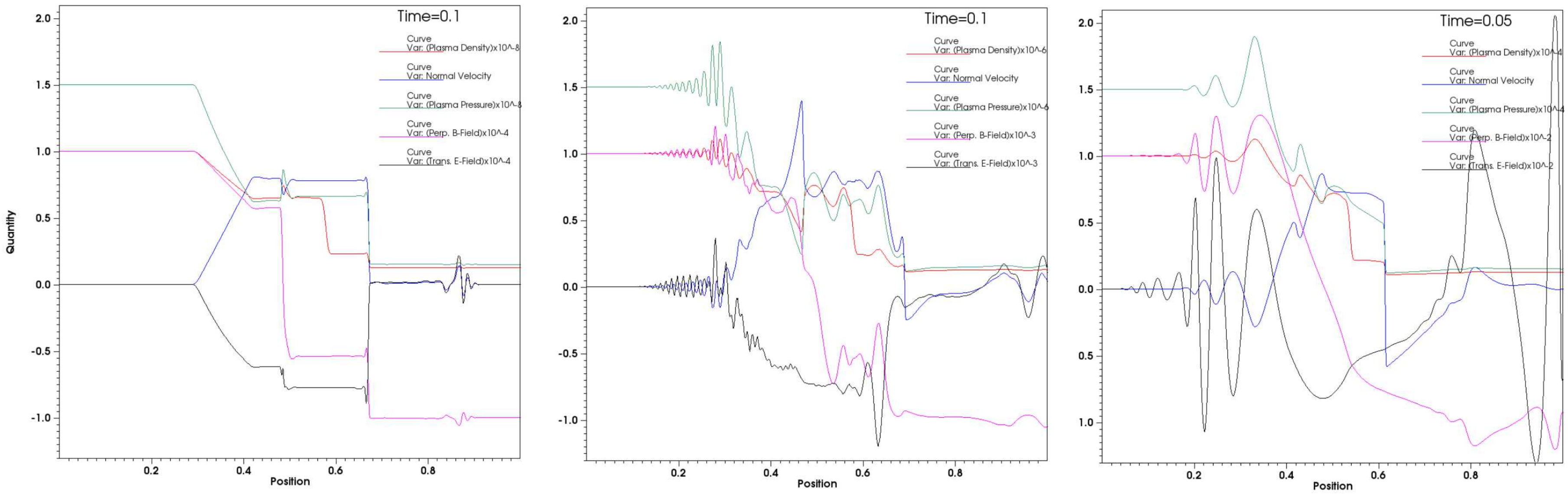
Benchmark Problems: Magnetized Shock Tube

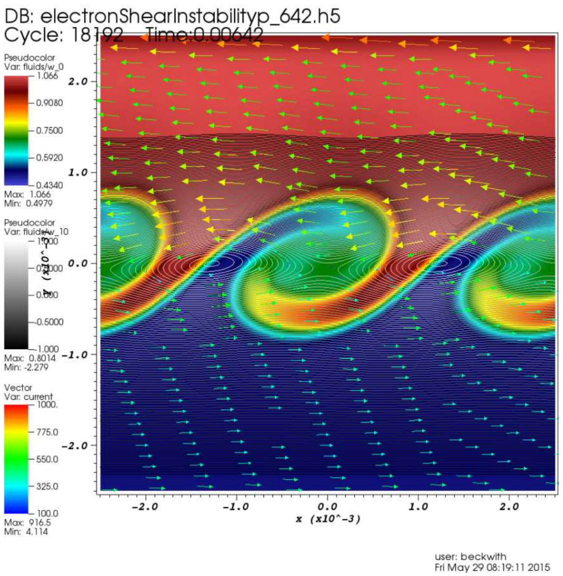


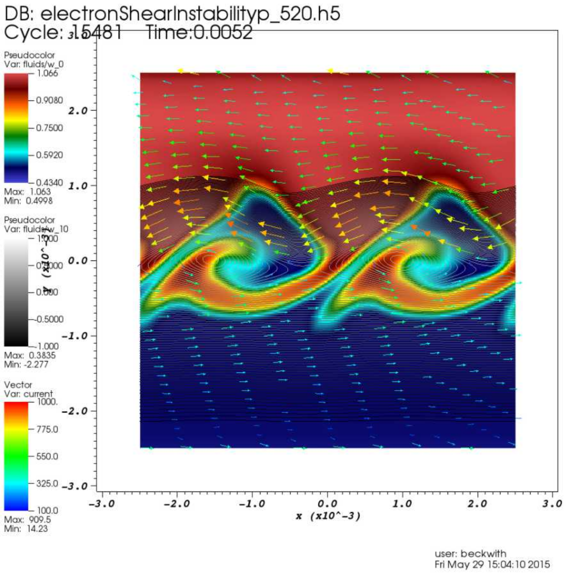
Example problems:

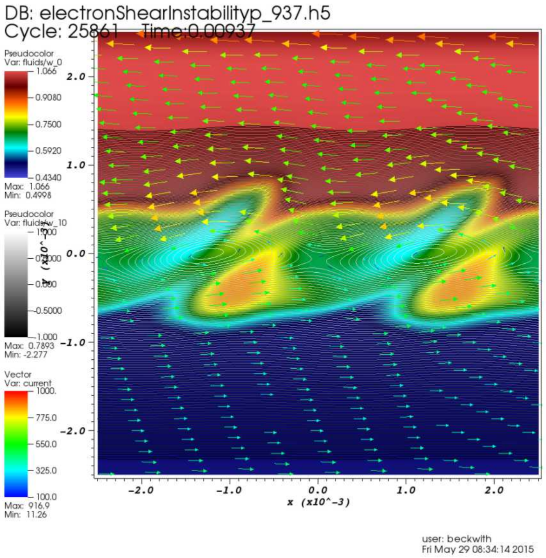
- Classic ‘Brio-Wu’ shock-tube:
  - MHD regime
  - Hall MHD regime
  - Multi-fluid regime
- Electron/Ion shear instabilities:
  - Ions linearly unstable to Kelvin-Helmholtz
  - Electrons non-linearly unstable.

- Example problems demonstrate:
  - MHD-like formulation reduces spurious divergence errors in electric field.
  - Pre-conditioner can handle CFL’s > 1000
  - Multi-fluid Reformulation can handle separate ion and electron dynamics
    - Classic KH modes in the mass density (ion motion)
    - Generation of magnetic islands (electron motion)

Benchmark Problems: Electron-Ion Shear Instability







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Electron Shear Instabilities with Electron-Ion Collisions and Full-Wave Electromagnetics

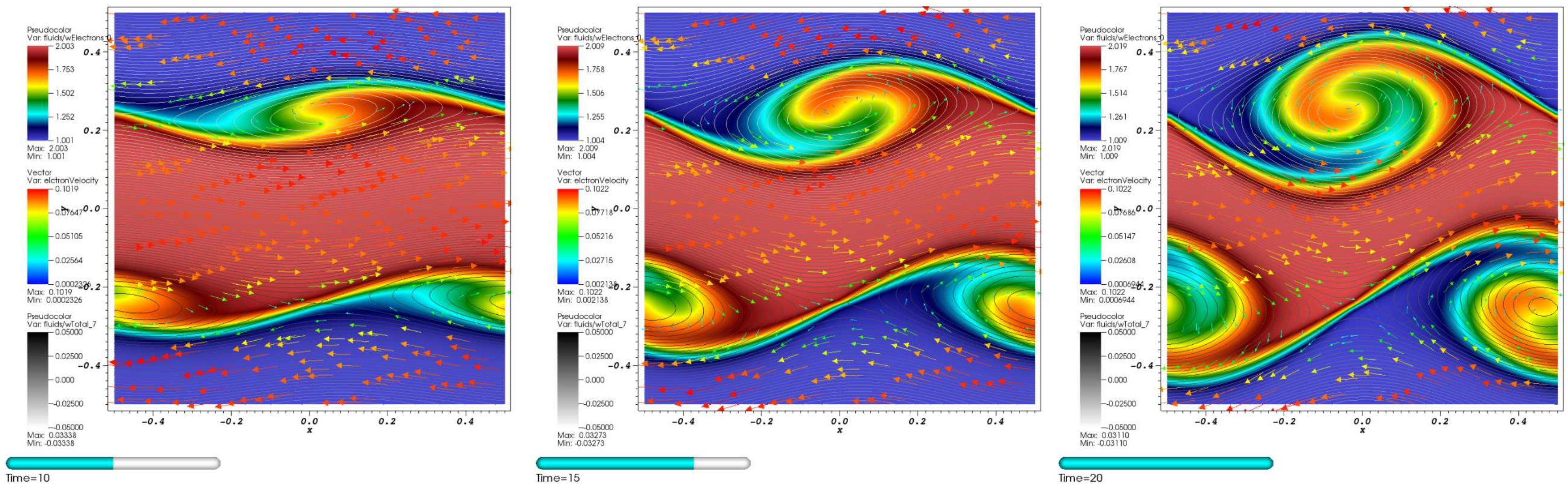
Subsonic EKH: electric field amplified to equipartition with transverse kinetic energy, implies that generated electric field can influence formation of shear flow

- If curl of electric field is non-zero, implies generation of magnetic field

We have re-run the Mach 0.1 calculation using a multi-fluid model in MHD-like form with a full-wave EM solver

Results: energy density in EM-fields exceeds that of the transverse kinetic energy:

- Characteristic vortices form within electron density and velocity
- EM dynamics exhibit high frequency Langmuir-like oscillations
- B-field spatial colocated with electron vortices



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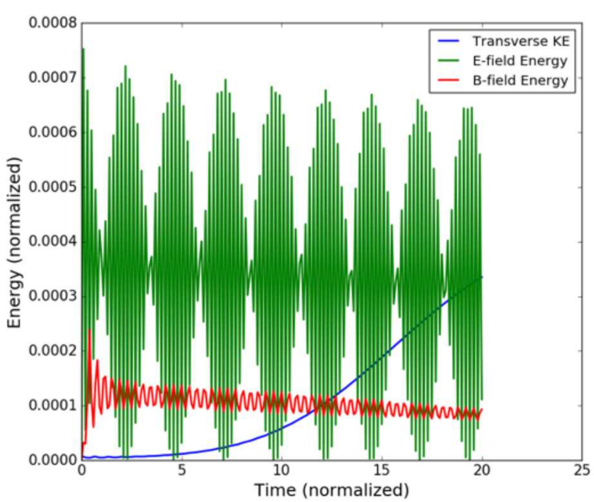
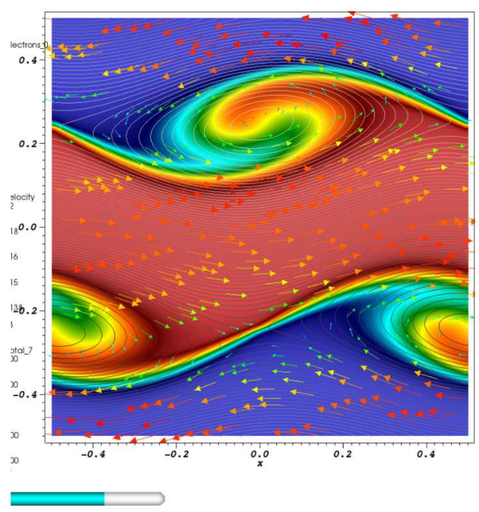
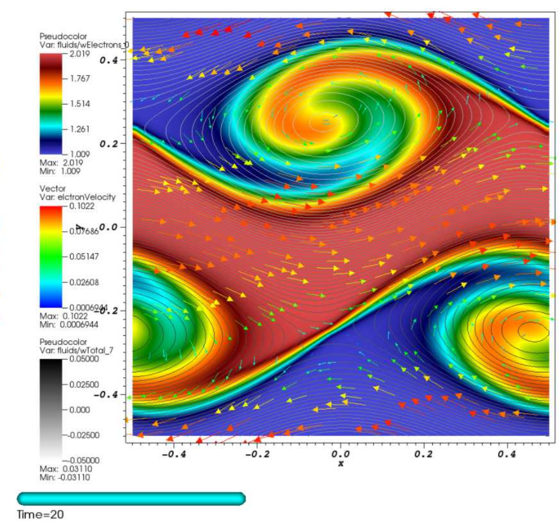






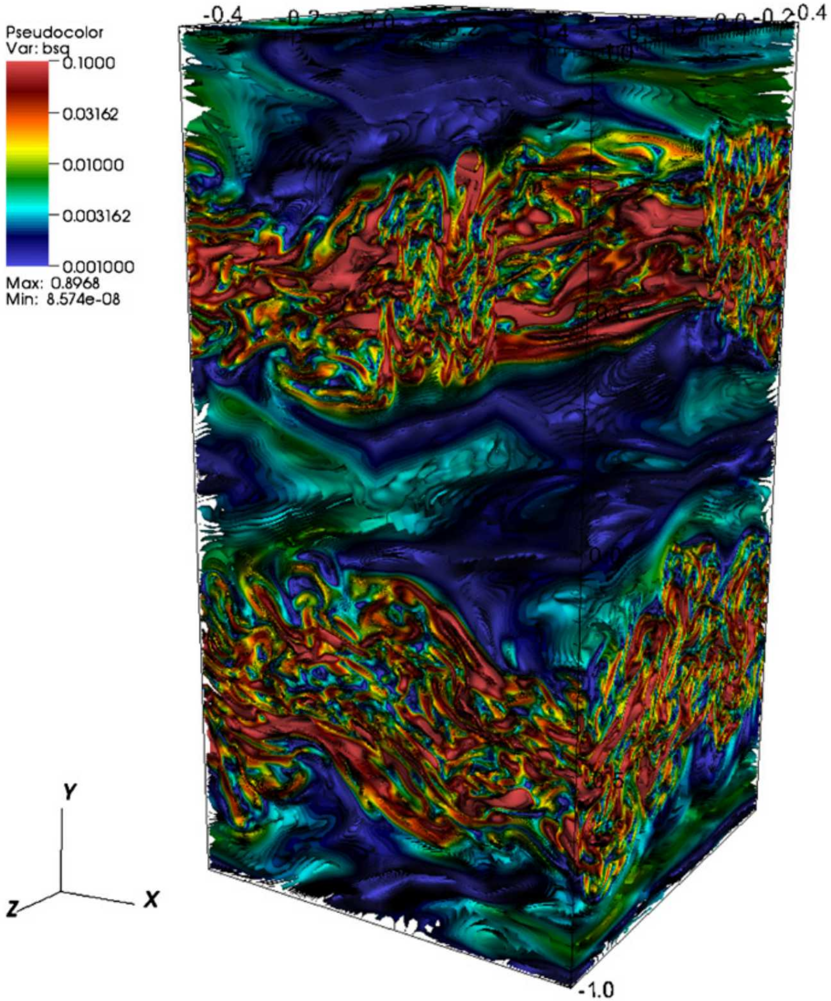
Can Simulations of Magnetized Turbulence Tell Us Anything?

Simulations of turbulence can rarely resolve the dissipation scale. How can we trust them?

- Verify simulations with unresolved dissipation against resolved case.

Test:

- Compare converged ILES simulations of decaying KHI using ILES with DNS simulations.
- Convergence for ILES: shape of power spectrum unchanged with 2x increase in resolution.



Salvesen, Beckwith et al. (2014)

Convergence Can Only Tell Us So Much

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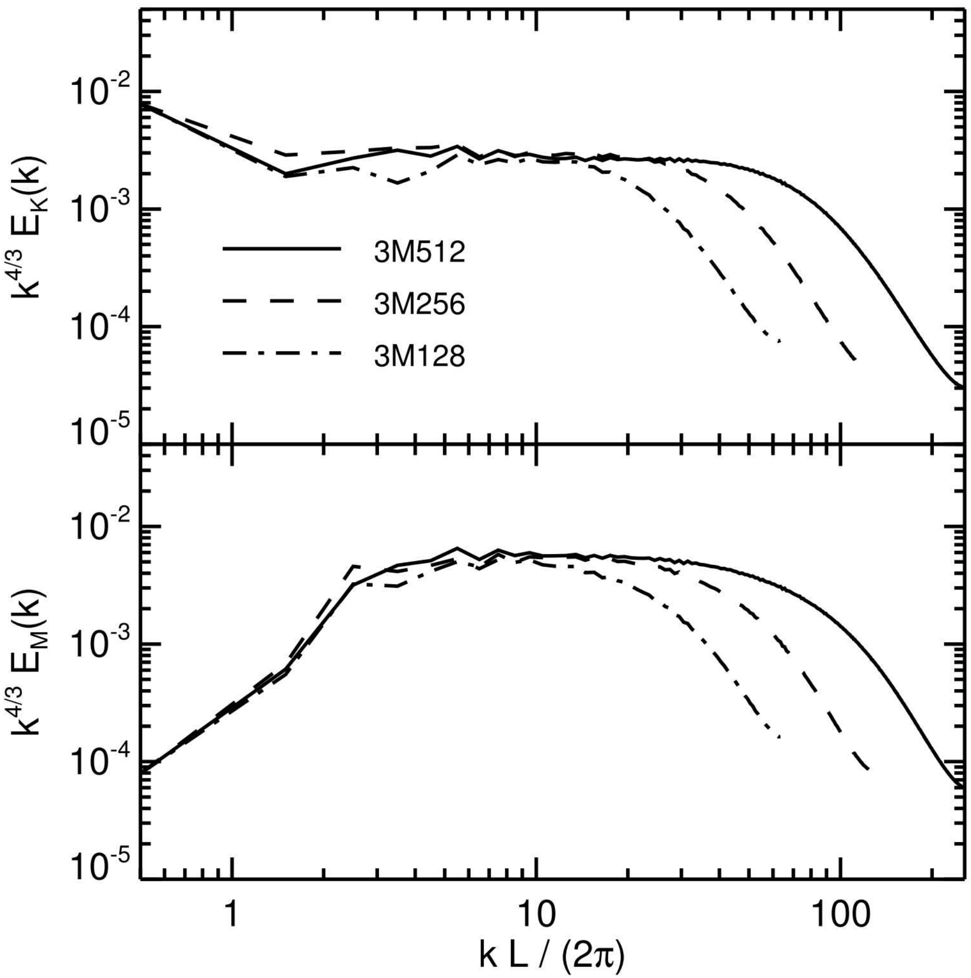


Salvesen, Beckwith et al. (2014)

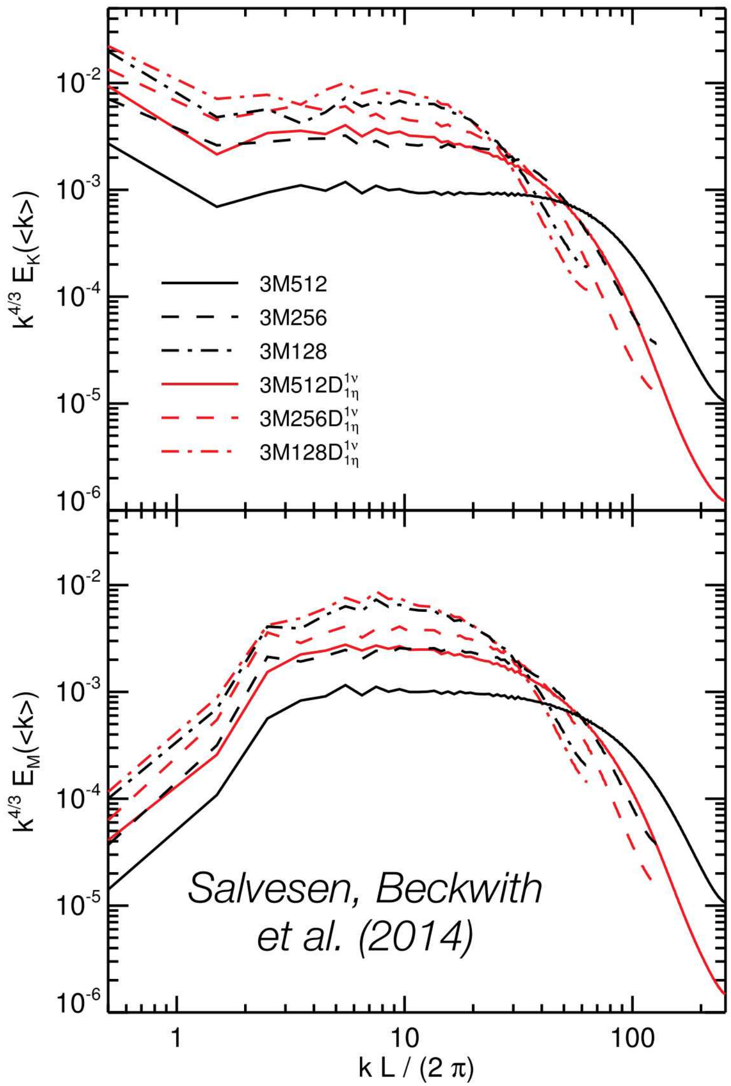
Verification of ILES Simulation Against DNS Simulation

Simulations of turbulence can rarely resolve the dissipation scale. How can we trust them?

- Verify simulations with unresolved dissipation against resolved case.

Add Navier-Stokes shear viscosity and Ohmic resistivity to decaying turbulence model.

Power spectrum obtained is a precise match, but with a 2x lower effective resolution.



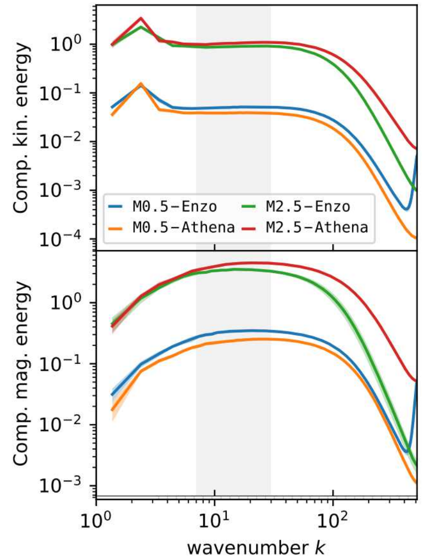
Non-Linear MHD Turbulence Cross-Code Benchmark

Simulations of turbulence can rarely resolve the dissipation scale. How can we trust them?

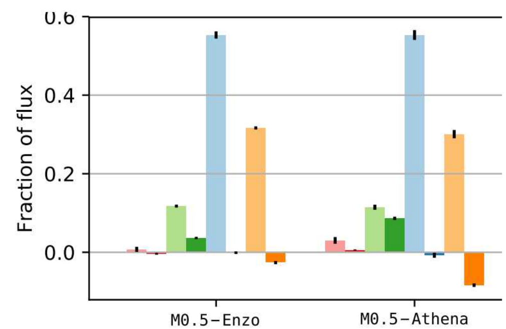
- Verify simulations with unresolved dissipation against resolved case.

Add Navier-Stokes shear viscosity and Ohmic resistivity to decaying turbulence model.

More recently, we have developed analysis tools for energy transfer in MHD turbulence that enable both cross-code comparison and comparison against analytic theory across a range of Mach numbers.



Left: Magnetic & Kinetic energy power spectra as a function of wavenumber for driven subsonic ideal MHD turbulence computed using two finite volume MHD schemes (Grete et al. 2017).
Below left: Cross-scale energy fluxes in the inertial range for driven subsonic ideal MHD turbulence computed using two finite volume MHD schemes (Grete et al. 2017).
Below right: Results for the same physical setup computed using spectral and analytic approaches (Debliquy et al. 2005).



π/r_A	0.75 (sim)	0.75 (th)
$\pi^{u<}_{u>}$	0.075	0.078
$\pi^{u<}_{b>}$	0.49	0.38
$\pi^{b<}_{u>}$	0.12	0.20
$\pi^{b<}_{b>}$	0.37	0.34
$\pi^{u<}_{b>}$	0.22	⋯
$\pi^{u>}_{b>}$	0.24	⋯
K^+	2.8	1.53
K^u	1.1	0.65
ν^*	⋯	1.3
η^*	⋯	0.63

Grete, O'Shea Beckwith & Christlieb (2017)

Summary

Key questions in pulsed power are plasma physics problems that benefit from multi-scale solvers.

Non-linear physics addressed by Jacobian-Free Newton-Krylov (JFNK) solvers adapted developed by DoE/NNSA efforts.

Performant JFNK solvers *require* preconditioning:

- Developed eigensystem-based preconditioning (linearize Jacobian): performant for compressible MHD
- Eigensystem-based scheme adaptable to resistive, Hall MHD and compressible multi-fluids

Developed a range of benchmark problems relevant to pulsed power applications

Investigated behavior of shear flows coupled to electromagnetic fields to understand the physics operating in plasma switches, dense plasma focus

Begun developing methods for validating simulations of magnetized turbulence that can be used to understand how energy is transferred between scales in the turbulence.