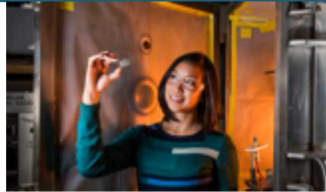
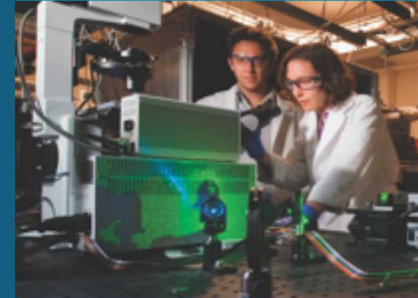




Sandia
National
Laboratories

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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



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2 Example Pulsed Power Application: Plasma Opening Switch



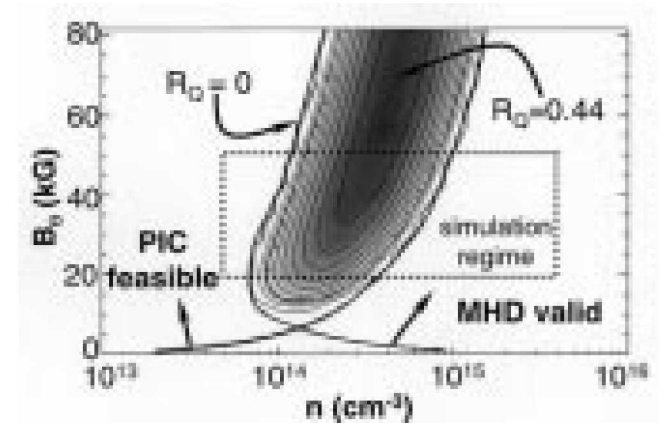
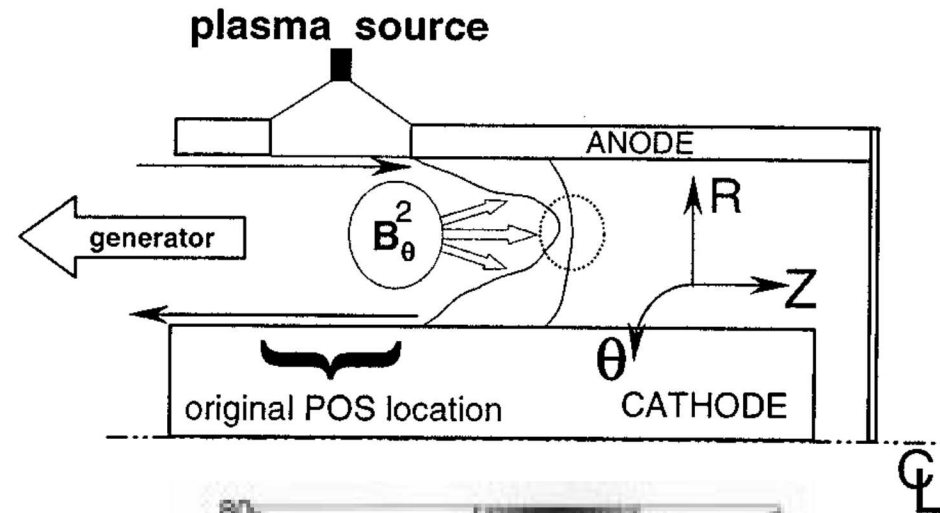
Plasma Opening Switch (**Schumer et al., 2001**):

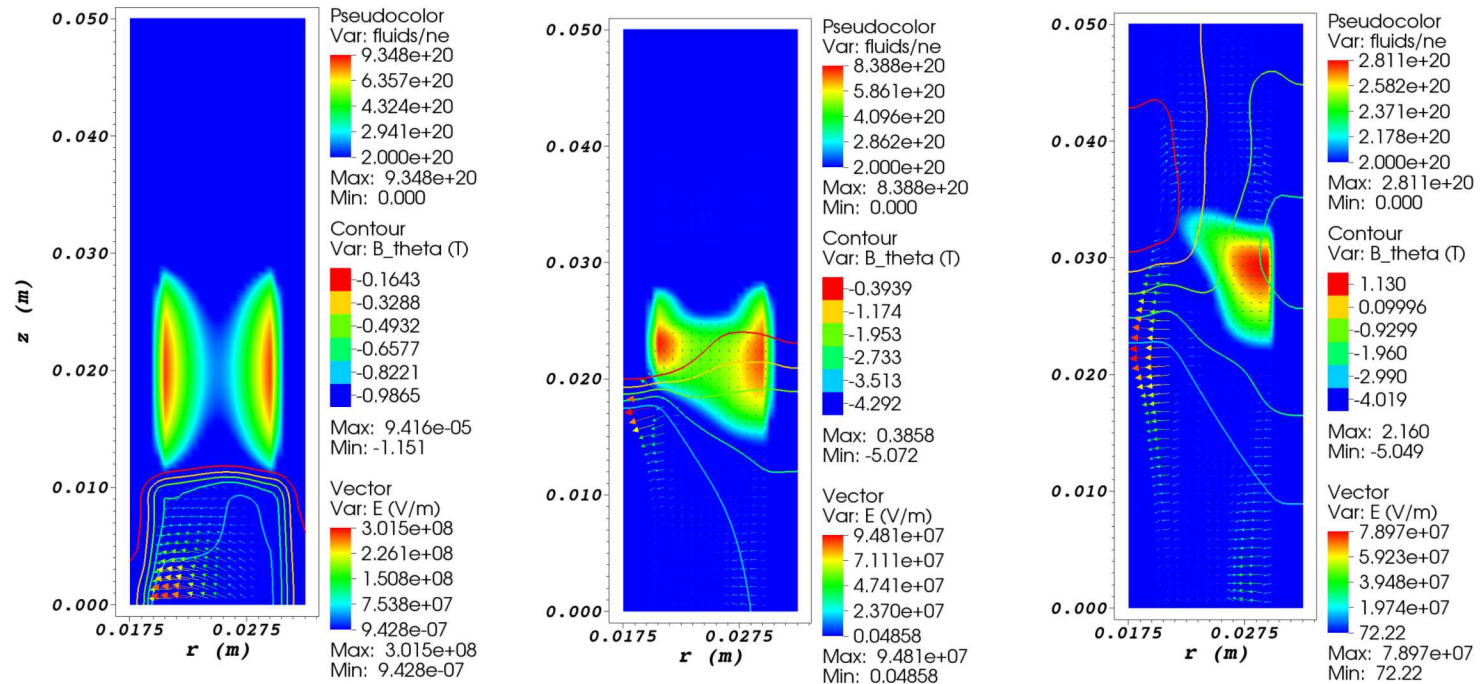
Largest scales, pulsed power requirements:

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

Smallest scales, plasma physics:

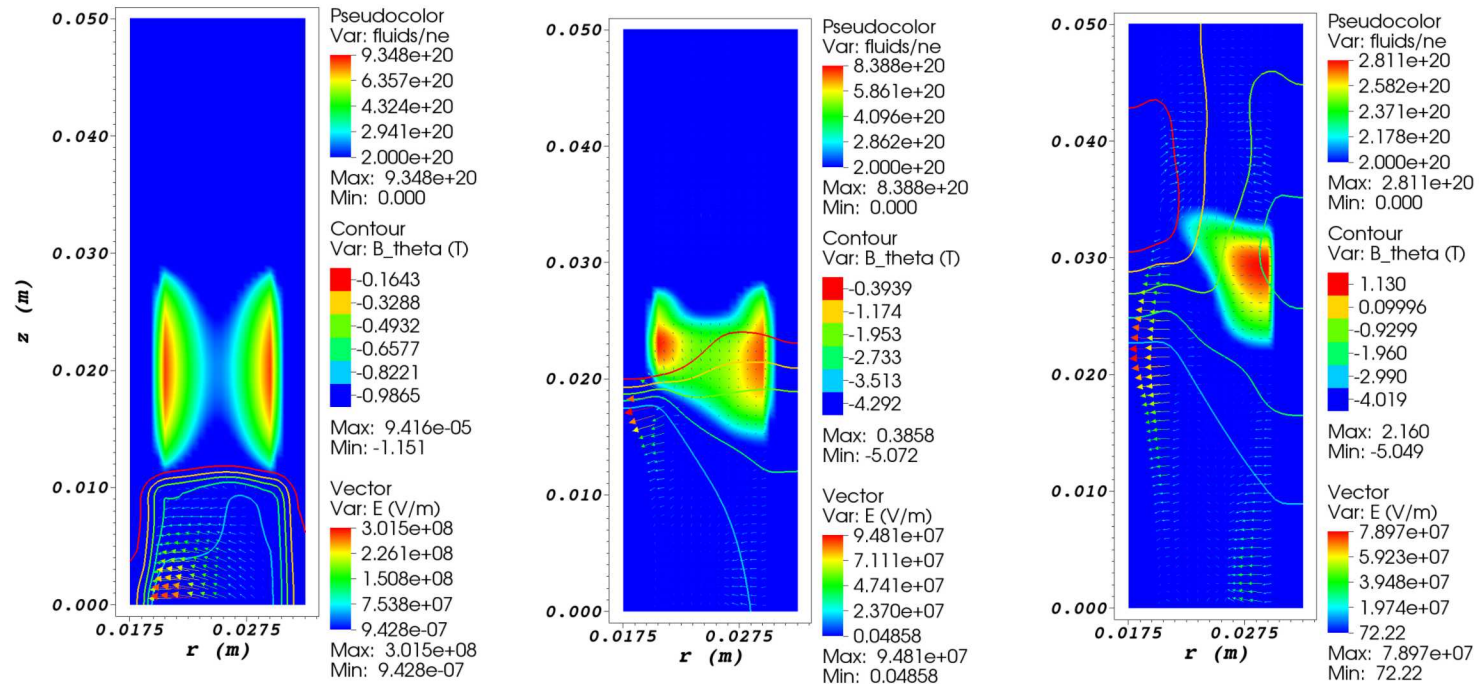
- Plasma density: $10^{12} - 10^{16} \text{ cm}^{-3}$
- Length scale: 10^{-5} cm (Debye)
- Timescale: 10^{-12} s (Plasma Freq.)





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



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



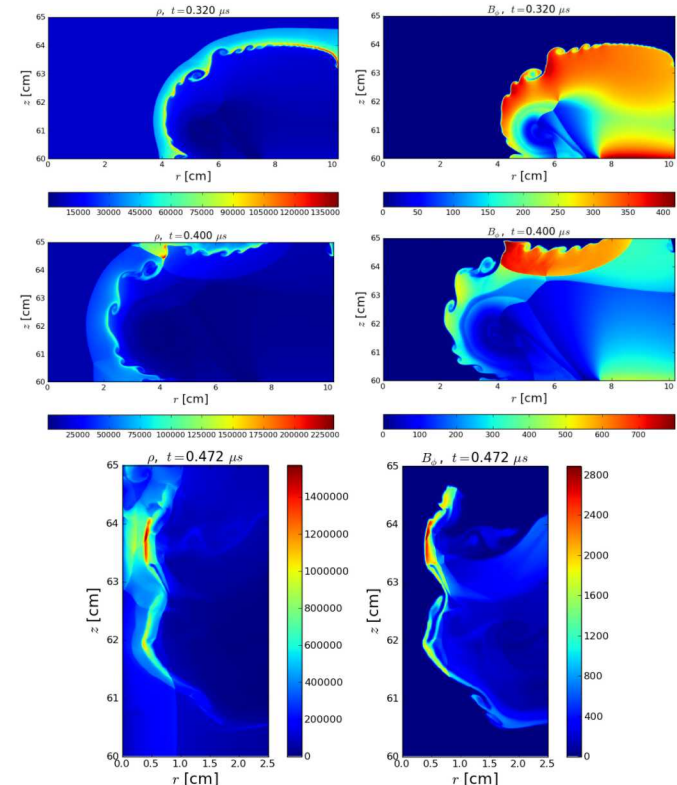
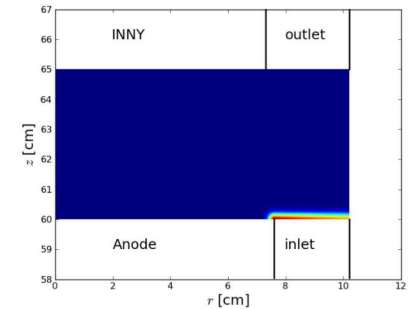
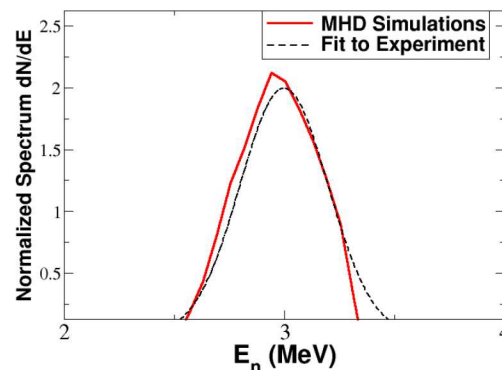
Mechanisms for pinch formation, ion acceleration and subsequent neutron production in Dense Plasma Focus are not well-understood

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...



6 Prototype Pulsed-Power Problem: Plasma Shear Instabilities

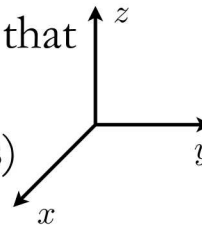


Understanding *how* the electromagnetic field penetrates into the plasma is a key aspect of understanding the operation of the plasma opening switch

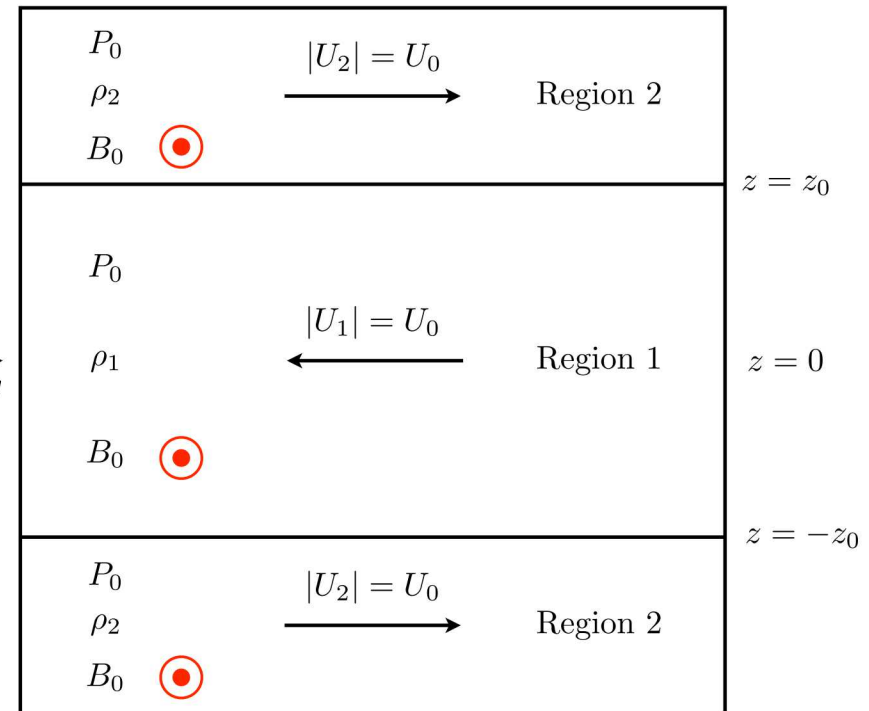
- By studying this as a prototype problem physics, we can remove the influence of boundary conditions

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)



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



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



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$$E = -\nabla \phi$$

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

Electrostatic case: still
need good
preconditioning for
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Implicit Solution Strategy: 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

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

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

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

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

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



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

$$E = -\nabla \phi$$

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

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
- Electrons: fast
- Maxwell: really fast

Simplify physics:

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



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

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

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Poisson's Equation needed for (e.g.)
electrostatics & constraints

- In 2d for data Q on points x, y with weights w , Vandermonde matrix:

$$\begin{bmatrix} w_0 1 & w_0 x_0 & w_0 y_0 & w_0 x_0 y_0 & w_0 x_0^2 & y_0^2 \\ w_1 1 & w_1 x_1 & y_1 & w_1 x_1 y_1 & w_1 x_1^2 & y_1^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ w_N 1 & w_N x_N & w_N y_N & w_N x_N y_N & w_N x_N^2 & w_N y_N^2 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix} = \begin{bmatrix} w_0 q_0 \\ w_1 q_1 \\ \vdots \\ w_N q_N \end{bmatrix}$$

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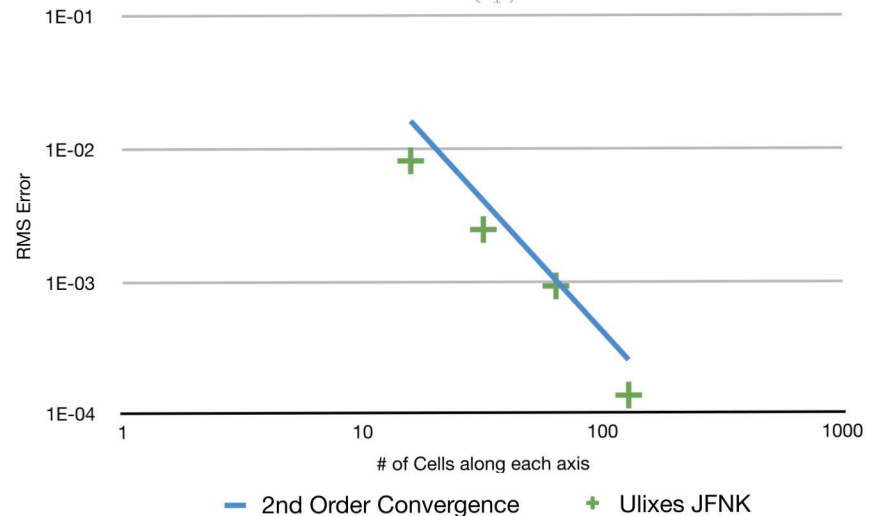
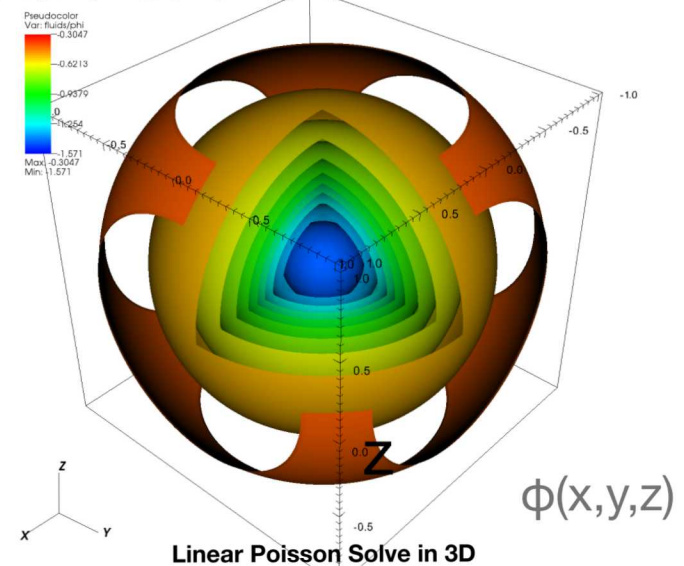
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Solving Poisson's Equation with Moving Least Squares Operators



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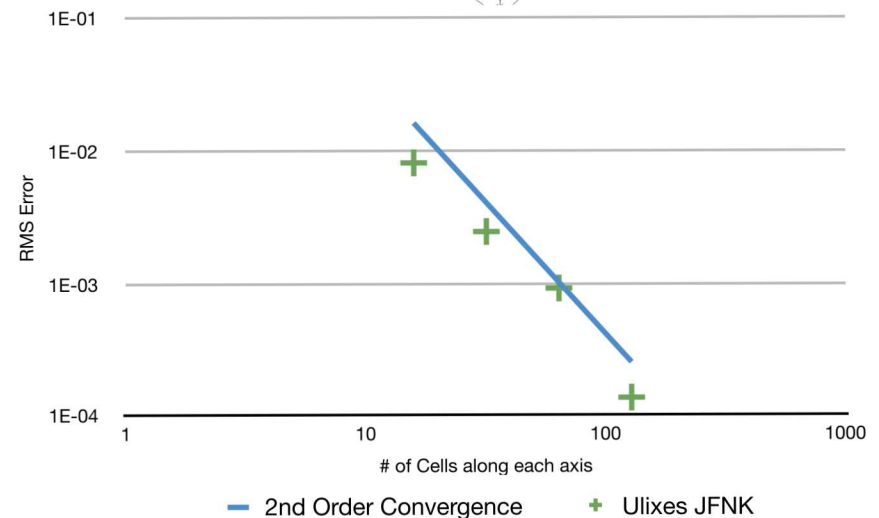
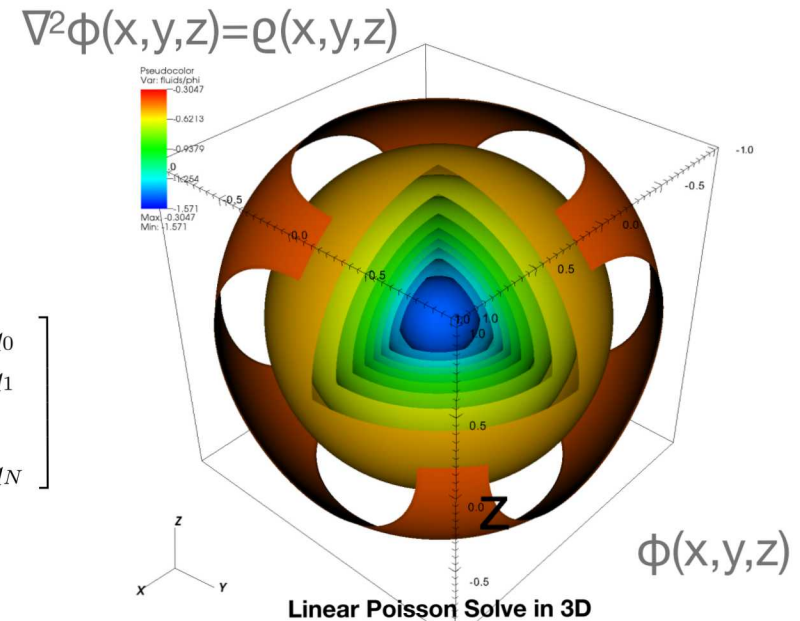
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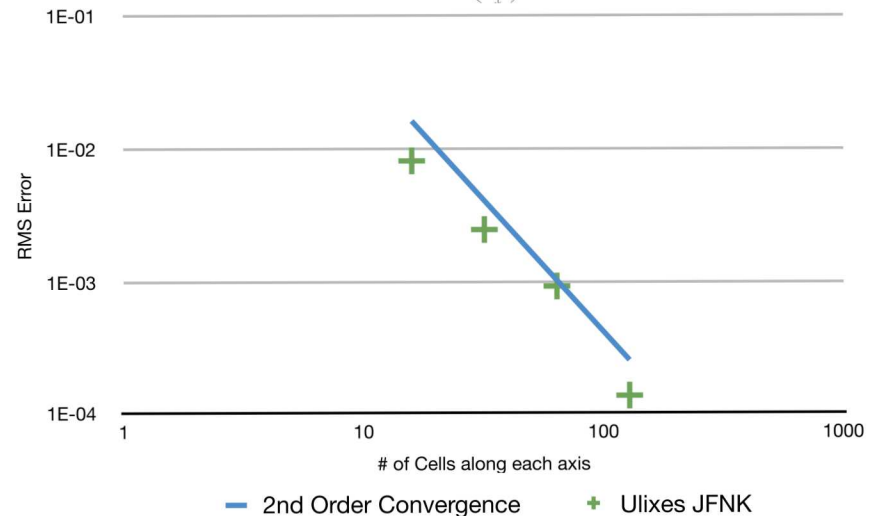
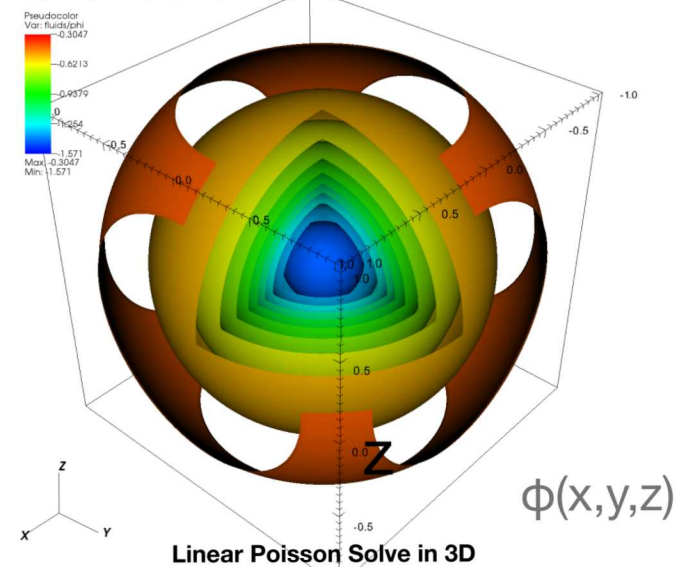
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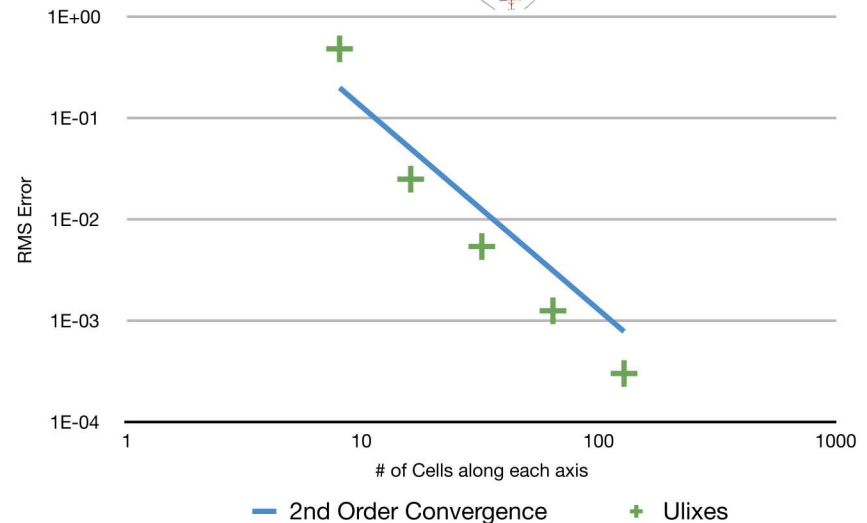
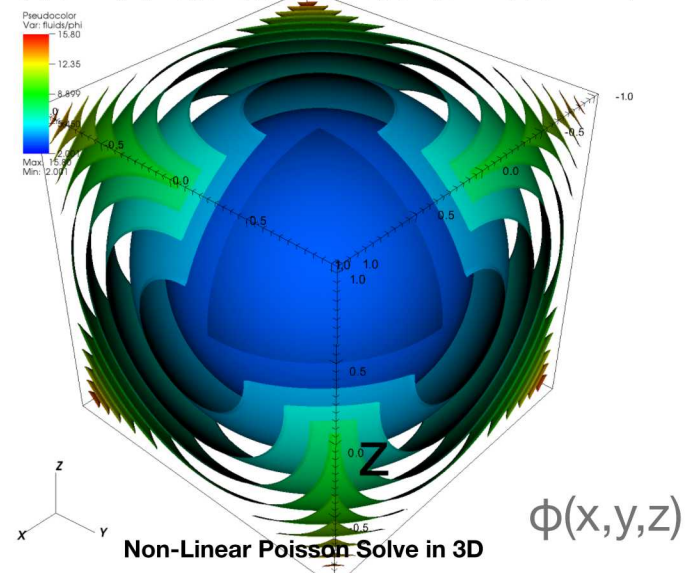
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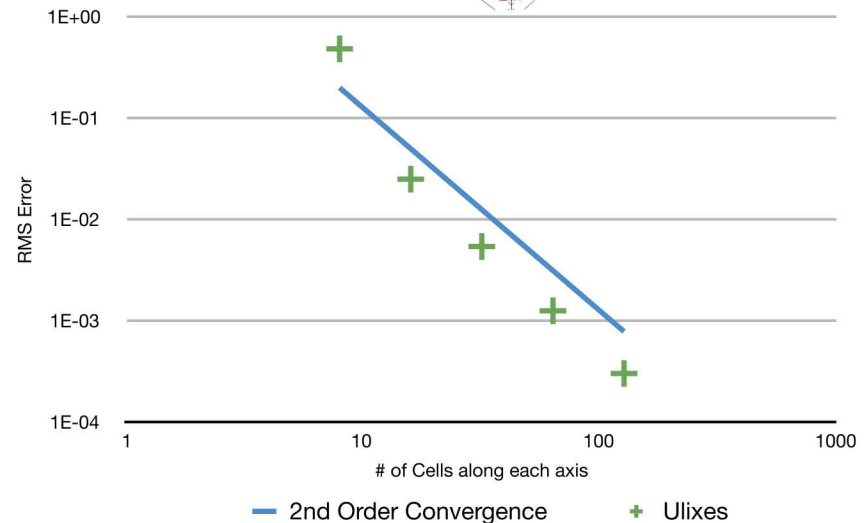
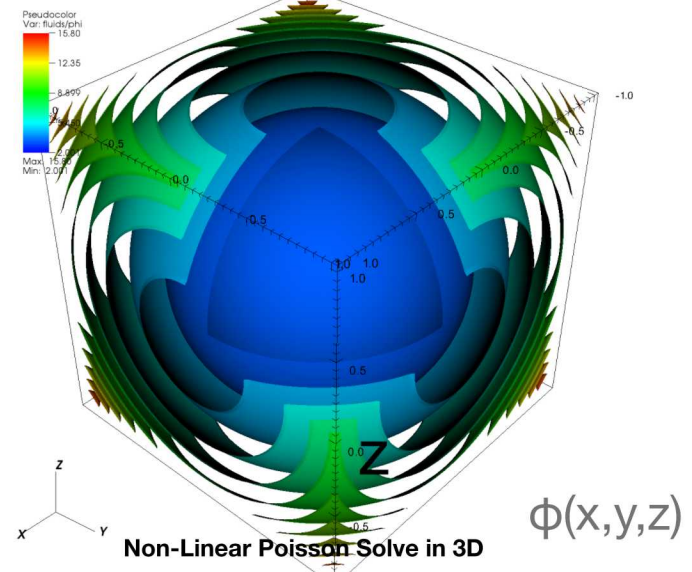
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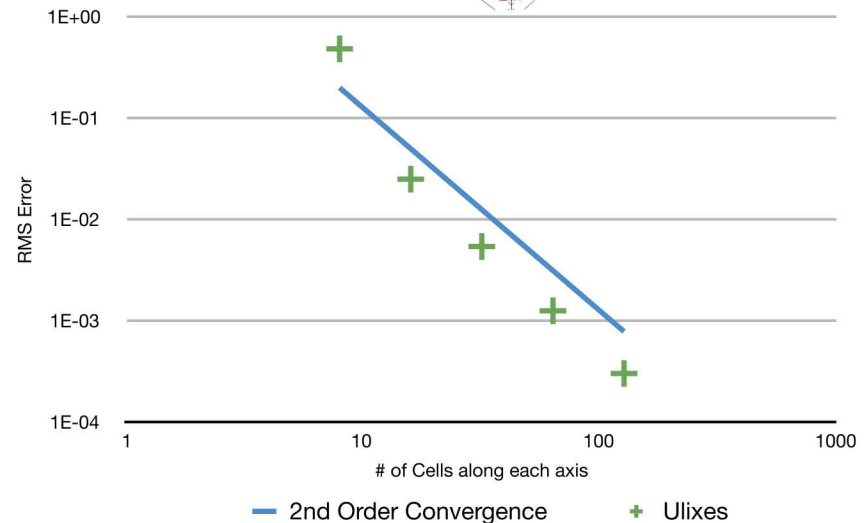
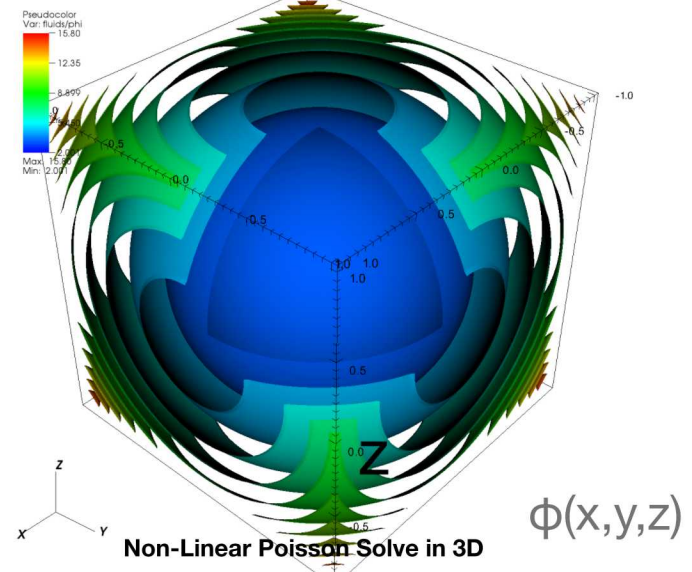
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Preconditioner is based on the matrix:

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

Complications:

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

Methodology:

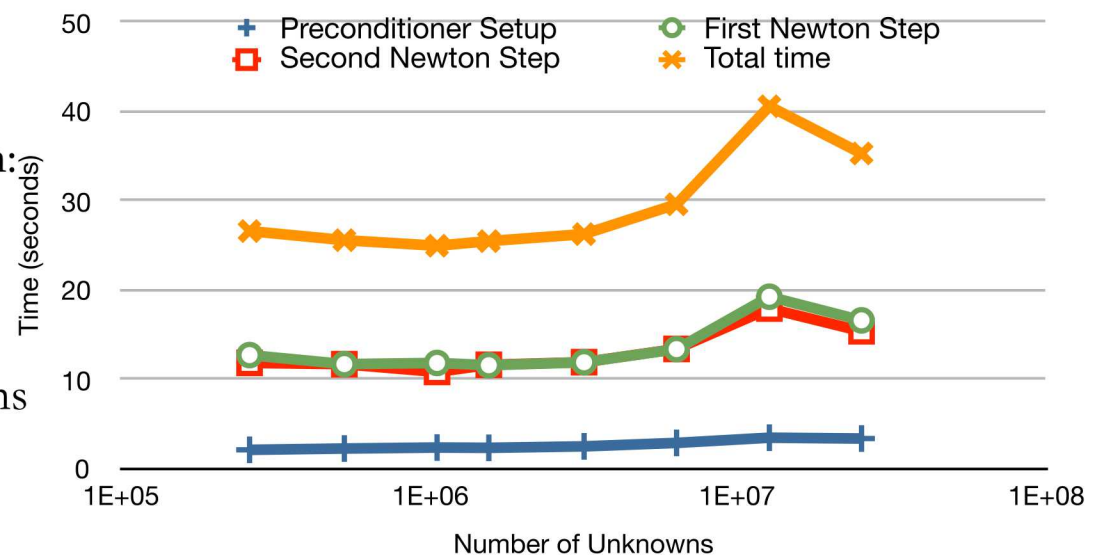
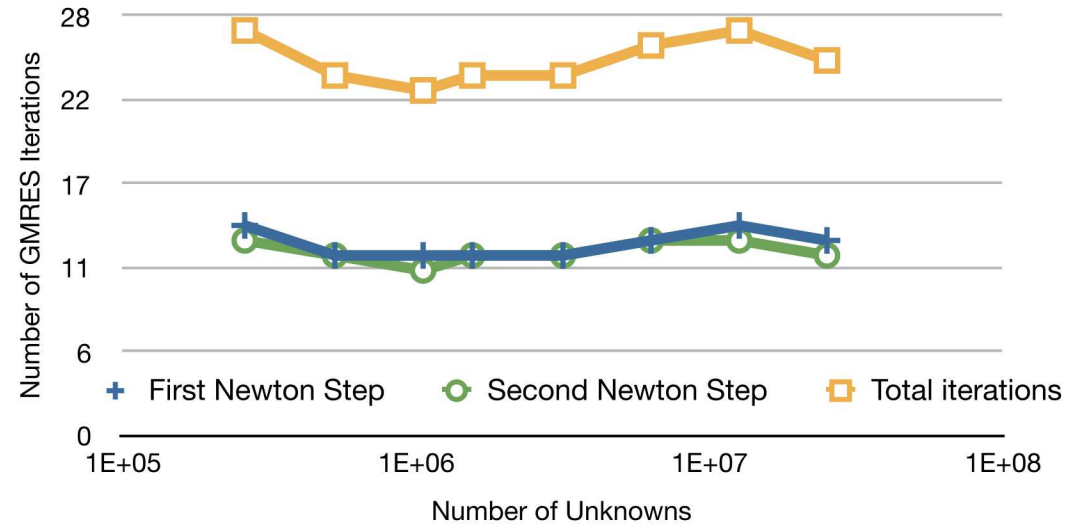
- Apply as a right preconditioner:

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

- Inverse computed using ML Uncoupled Smoothed Aggregation:

- 5 Levels; Jacobi smoother on coarsest; Gauss-Seidel smoother on all others

Good weak scaling to 2×10^7 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

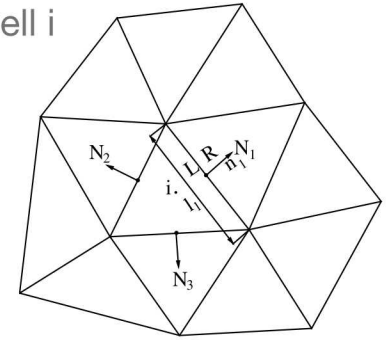
1st Order Stencil for Cell i

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

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

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

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



For Roe Solver:

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

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

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

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



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:

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

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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)

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:

- Block ILU smoothing with zero overlap and symmetric Gauss-Seidel relaxation on each level
- Block size chosen to be # of PDE's in system.
- ML cycle relaxes residual ~ 0

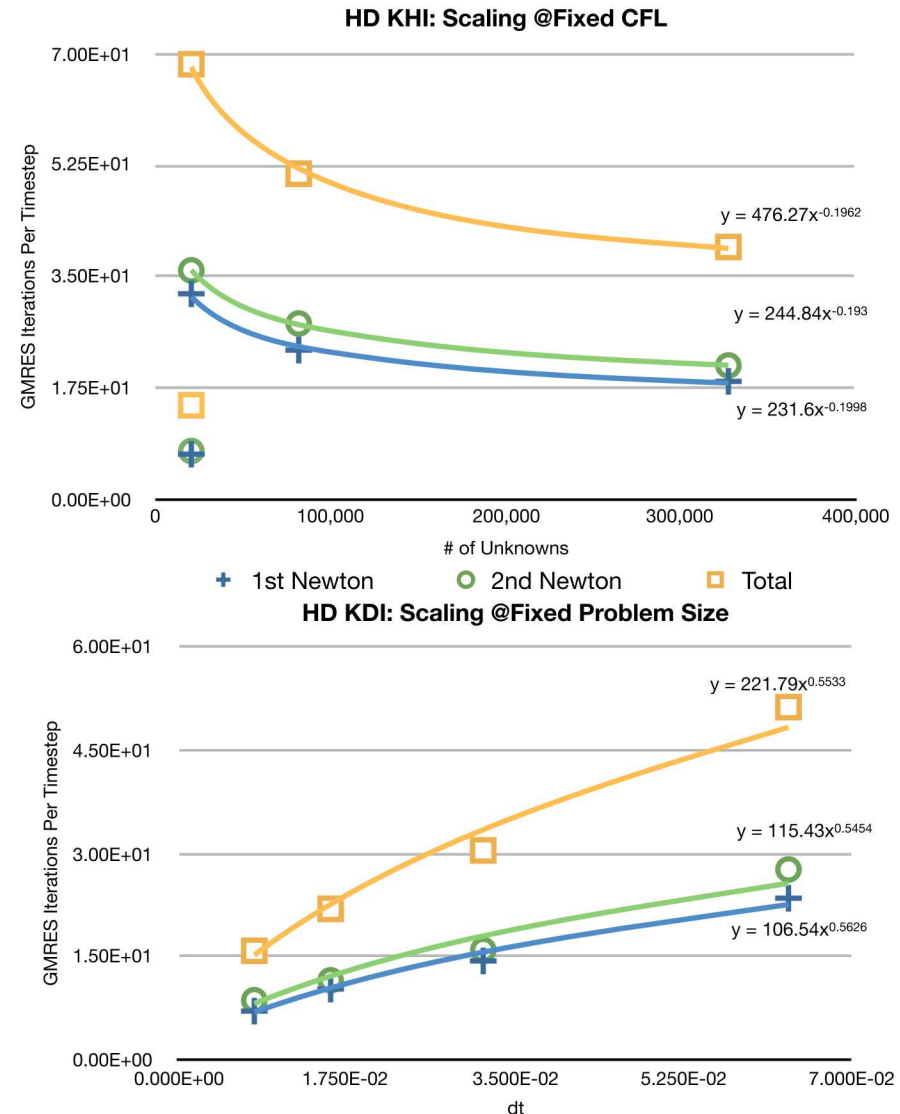
Timestep chosen so that highest resolution requires 2 Newton iterations

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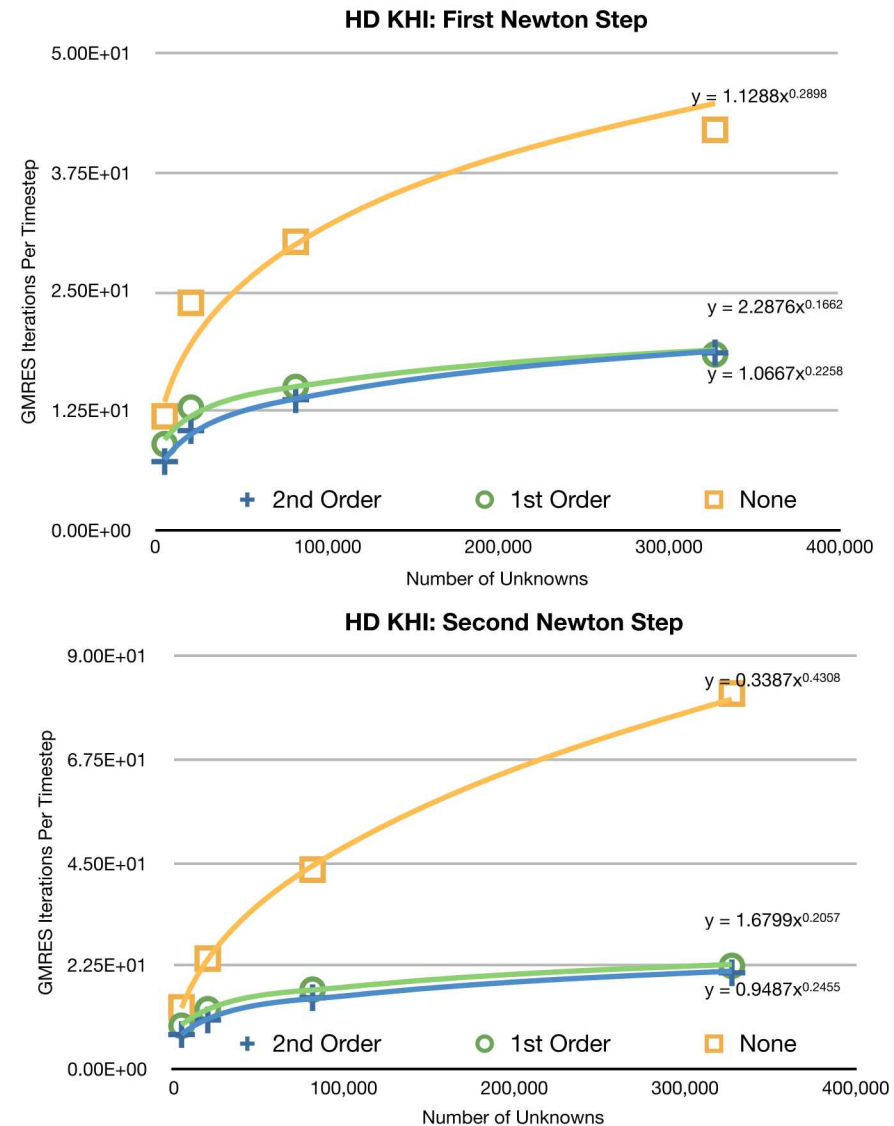
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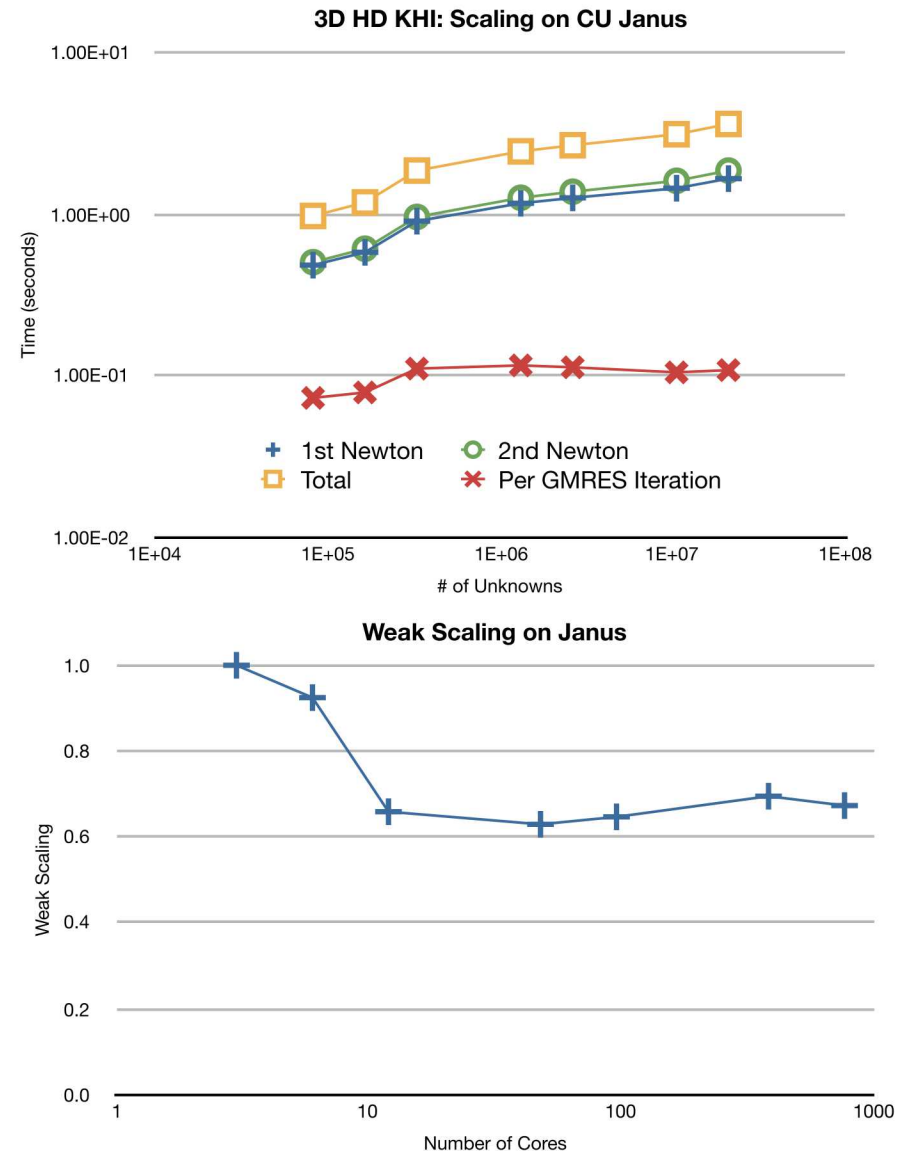
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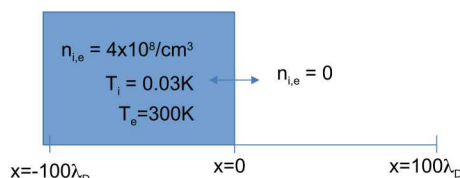
Parallel Scaling:

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





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

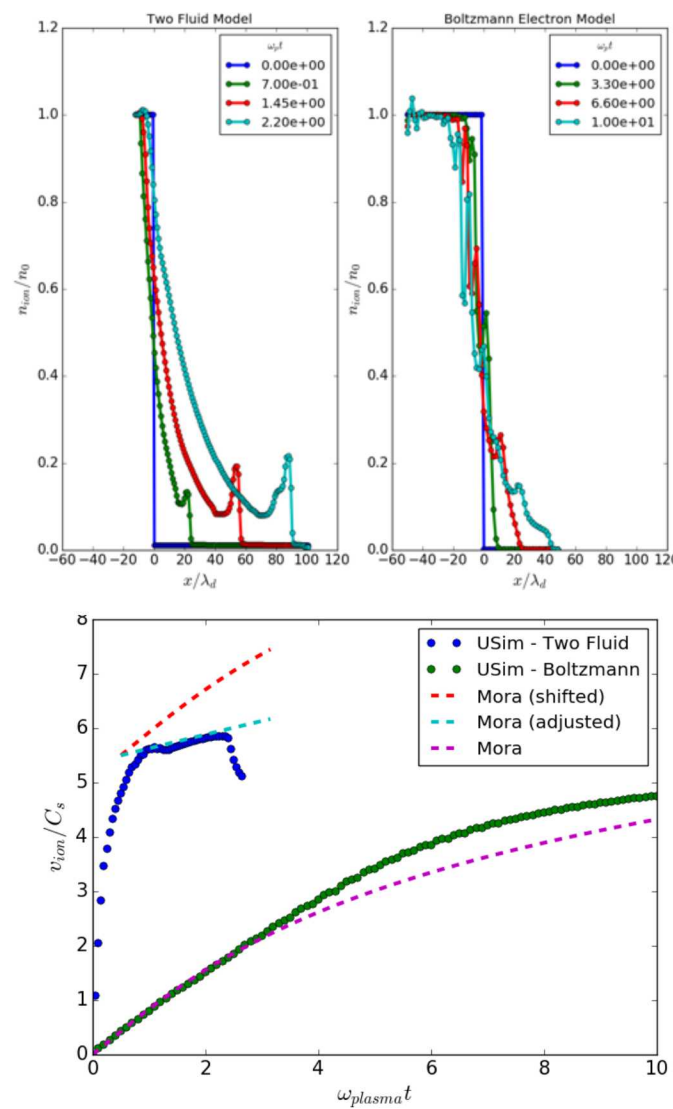


Model this process using either a two-fluid electrostatic model or using a Boltzmann electron model.

- 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.





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

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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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

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

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

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{v} \mathbf{B}^T - \mathbf{B} \mathbf{v}^T) + \nabla \psi = 0,$$

$$\frac{\partial E}{\partial t} + \nabla \cdot \left[\left(E + p + \frac{\mathbf{B}^2}{2} \right) \mathbf{v} - (\mathbf{v} \cdot \mathbf{B}) \mathbf{B} \right] = 0,$$

$$\frac{\partial \psi}{\partial t} + c_h^2 \nabla \cdot \mathbf{B} = -\frac{c_h^2}{c_p^2} \psi,$$

Godunov flux of this system can be computed exactly by:

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

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

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

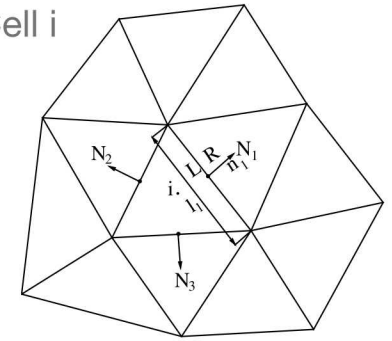
1st Order Stencil for Cell i

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

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

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

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



For Roe Solver:

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

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

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

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



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:

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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)

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

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

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

Decreased Scalability for Magnetized Compressible Flows



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

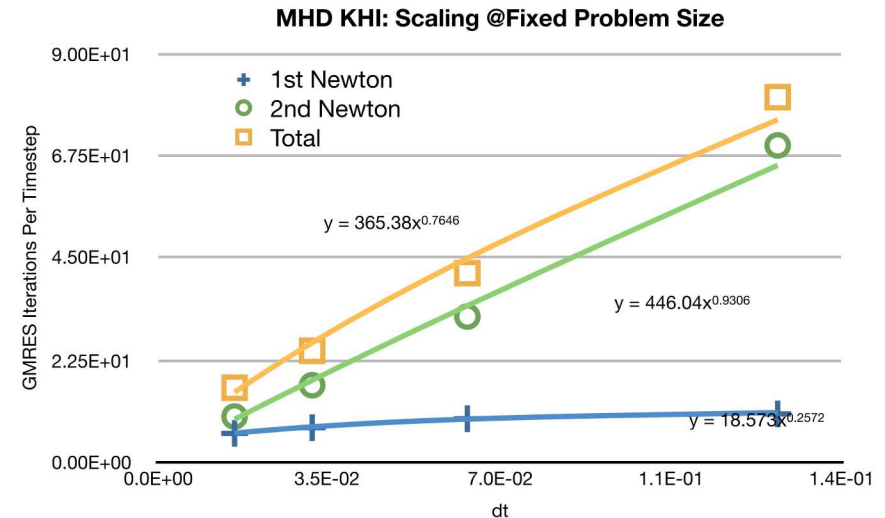
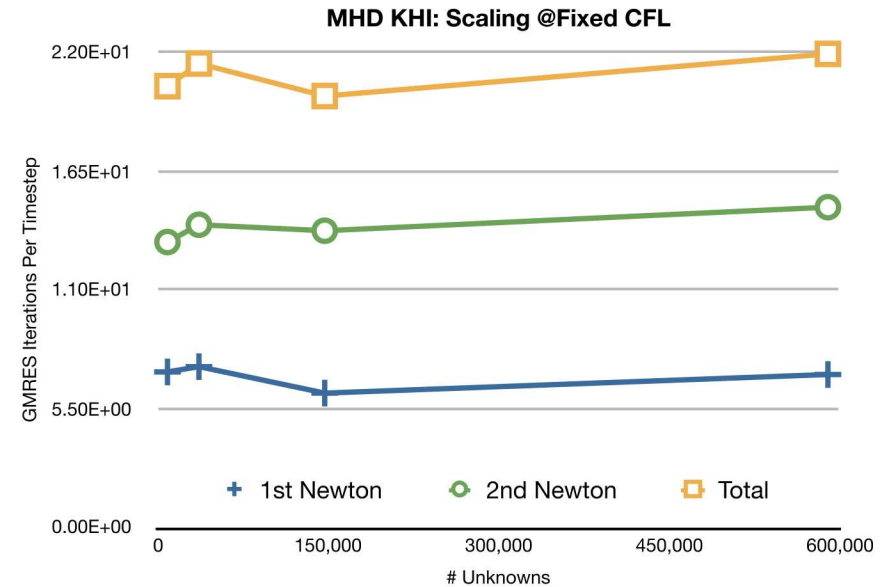
- Block ILU smoothing with zero overlap and symmetric Gauss-Seidel relaxation on each level
- Block size chosen to be # of PDE's in system.

Examine scaling of system:

- # of GMRES iterations for first Newton iteration shows good scalability with increasing N & CFL: $\sim N^{0.2}$
- # of GMRES iterations for second Newton iteration shows reduced scalability with increasing N & CFL: $\sim N^{0.3}$

of GMRES iterations:

- $\sim N^0$ @Fixed CFL
- $\sim dt^{0.9}$ @Fixed size for 2nd Newton



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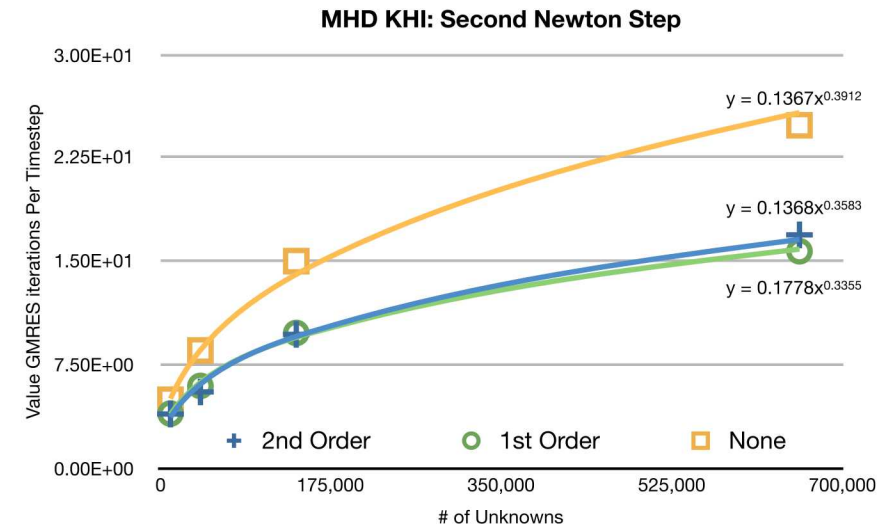
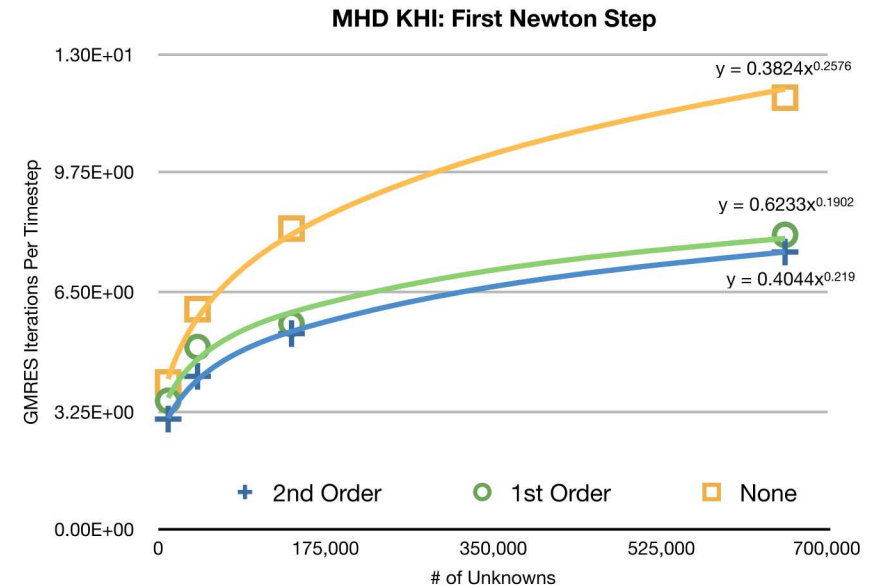
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$$= \begin{pmatrix} v_x & \rho & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & v_x & 0 & 0 & 0 & B_y/\rho & B_z/\rho & 1/\rho & 0 \\ 0 & 0 & v_x & 0 & 0 & -B_x/\rho & 0 & 0 & 0 \\ 0 & 0 & 0 & v_x & 0 & 0 & -B_x/\rho & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1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

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- Replace highlighted elements of right-eigenvectors with those from Stone (2008)

$$\mathbf{R} = \begin{bmatrix} \alpha_f & 0 & \alpha_s & 1 & \alpha_s & 0 & \alpha_f \\ V_{xf} - C_{ff} & 0 & V_{xs} - C_{ss} & v_x & V_{xs} + C_{ss} & 0 & V_{xf} + C_{ff} \\ V_{yf} + Q_s \beta_y^* & -\beta_z & V_{ys} - Q_f \beta_y^* & v_y & V_{ys} + Q_f \beta_y^* & \beta_z & V_{yf} - Q_s \beta_y^* \\ V_{zf} + Q_s \beta_z^* & \beta_y & V_{zs} - Q_f \beta_z^* & v_z & V_{zs} + Q_f \beta_z^* & -\beta_y & V_{zf} - Q_s \beta_z^* \\ R_{51} & R_{52} & R_{53} & R_{54} & R_{55} & R_{56} & R_{57} \\ A_s \beta_y^* / \rho & -\beta_z S / \sqrt{\rho} & -A_f \beta_y^* / \rho & 0 & -A_f \beta_y^* / \rho & -\beta_z S / \sqrt{\rho} & A_s \beta_y^* / \rho \\ A_s \beta_z^* / \rho & \beta_y S / \sqrt{\rho} & -A_f \beta_z^* / \rho & 0 & -A_f \beta_z^* / \rho & \beta_y S / \sqrt{\rho} & A_s \beta_z^* / \rho \end{bmatrix}$$

Decreased Scalability for Magnetized Compressible Flows

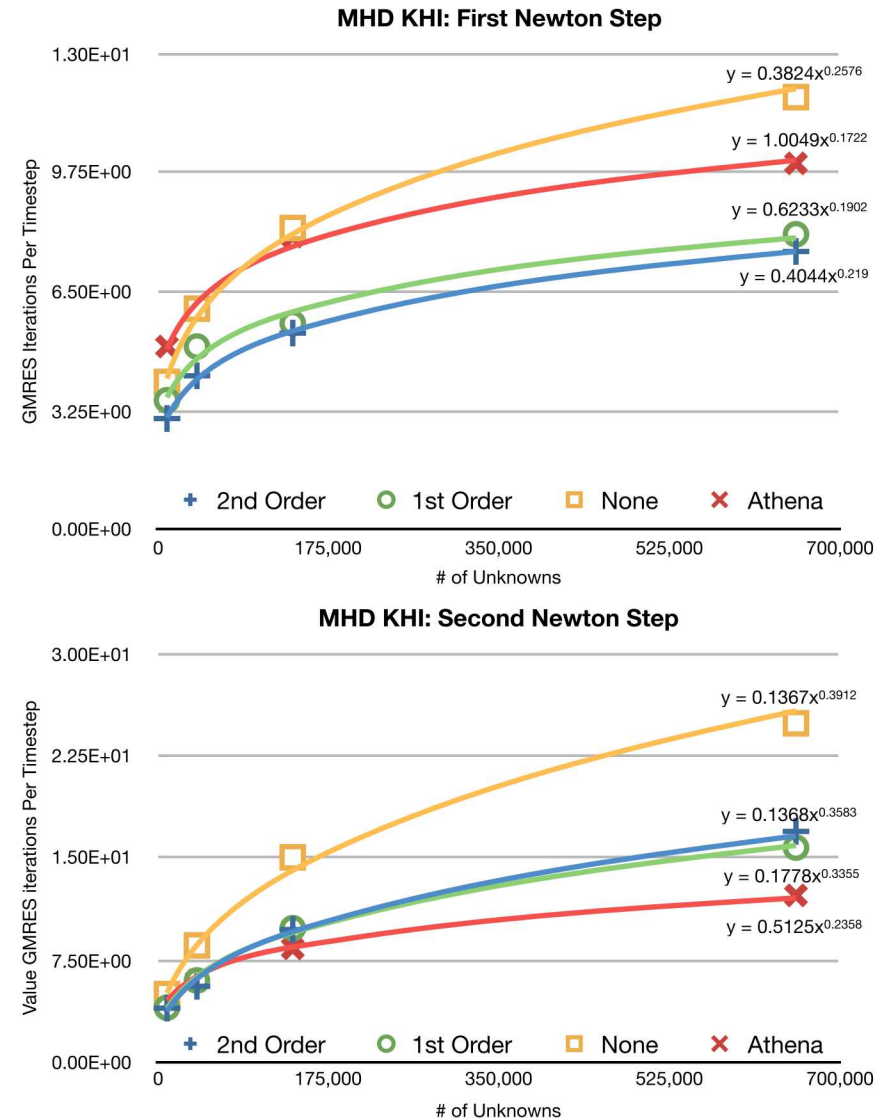


Apply using ML Domain-Decomposition
Smoothed Aggregation with 5 levels:

- 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 $\propto 100$
 - $\sim N^{0.22}$ with increasing N & CFL





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

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Route to an optimal solver:

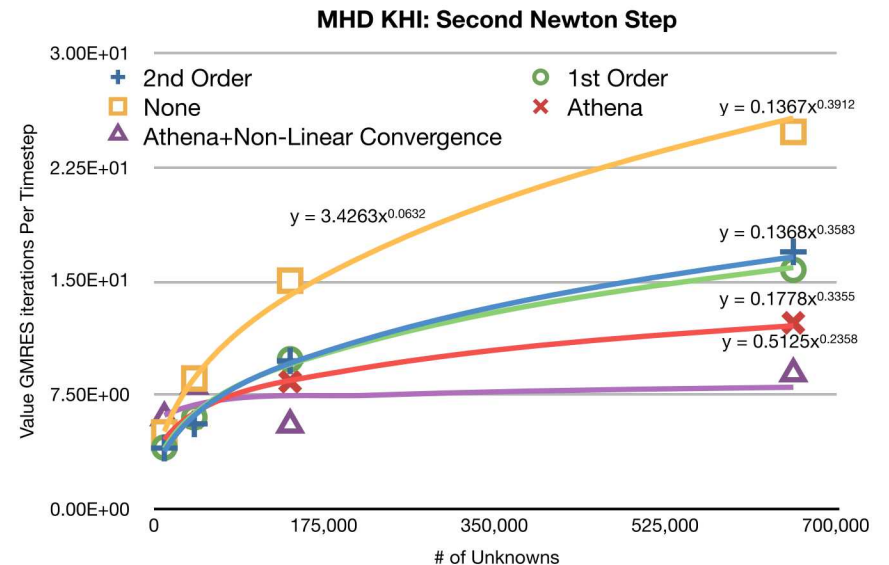
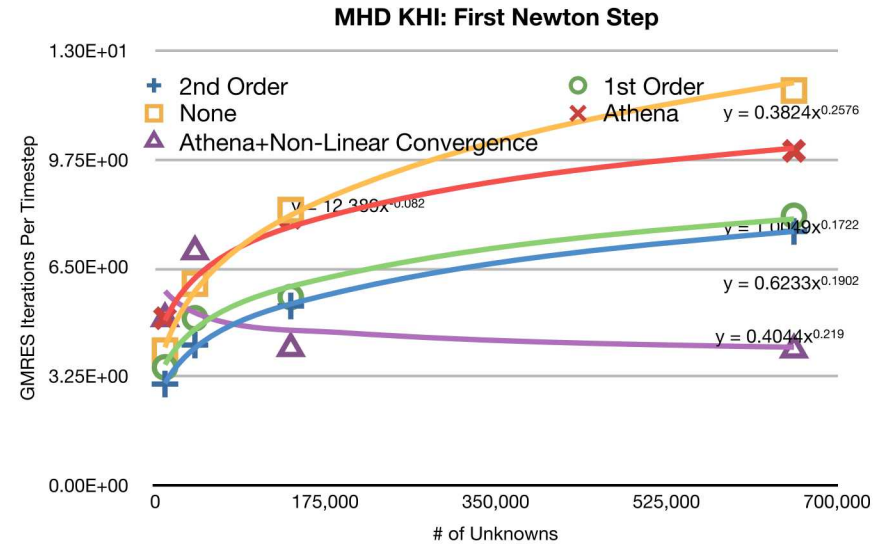
Non-linear convergence to this point determined by $\|F(U)\|_2 < tol$

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

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

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

Solver performance approaches optimal



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

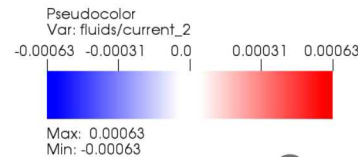


Circularly Polarized Alfven Wave:

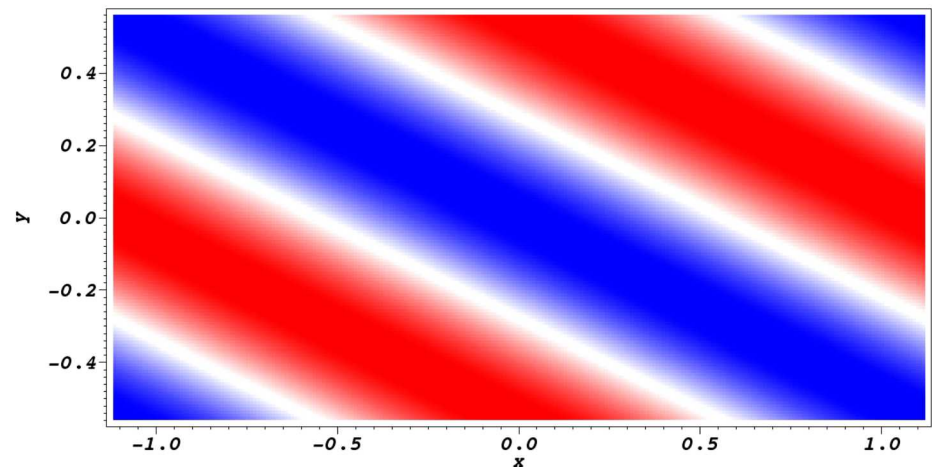
- Exact, non-linear solution to ideal MHD equations

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



Current normal to plane of wave



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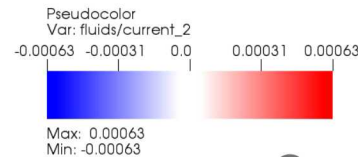
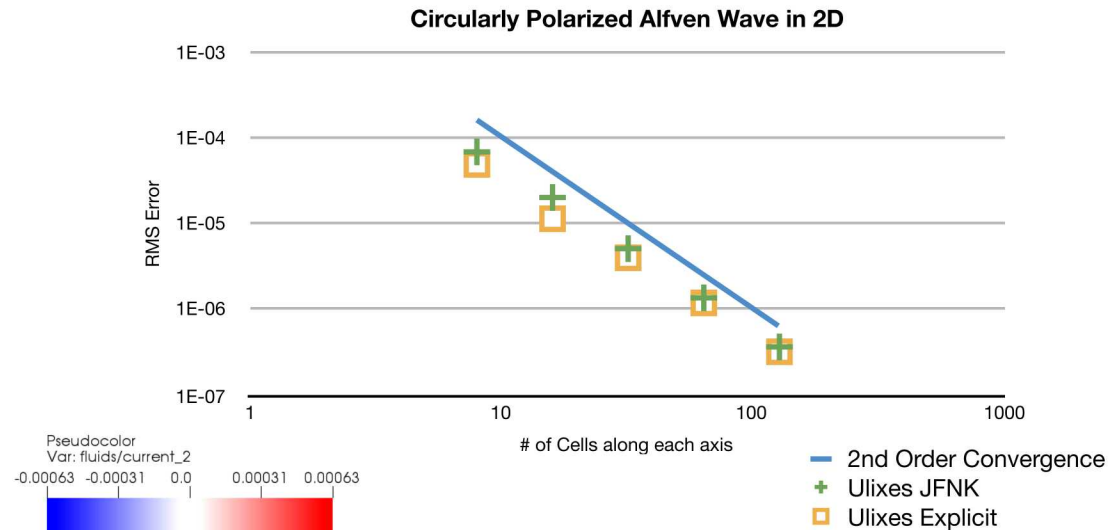


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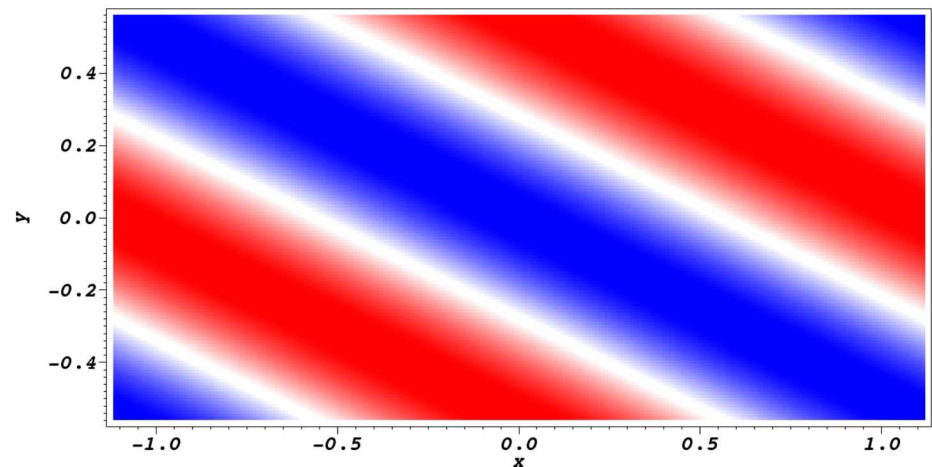
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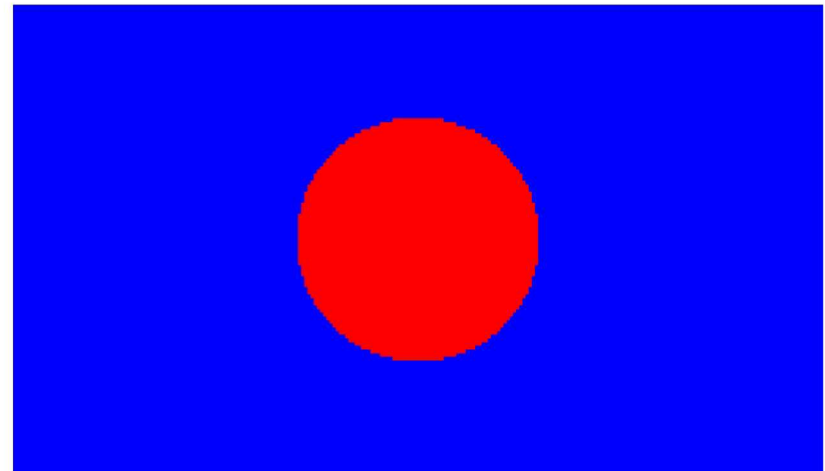
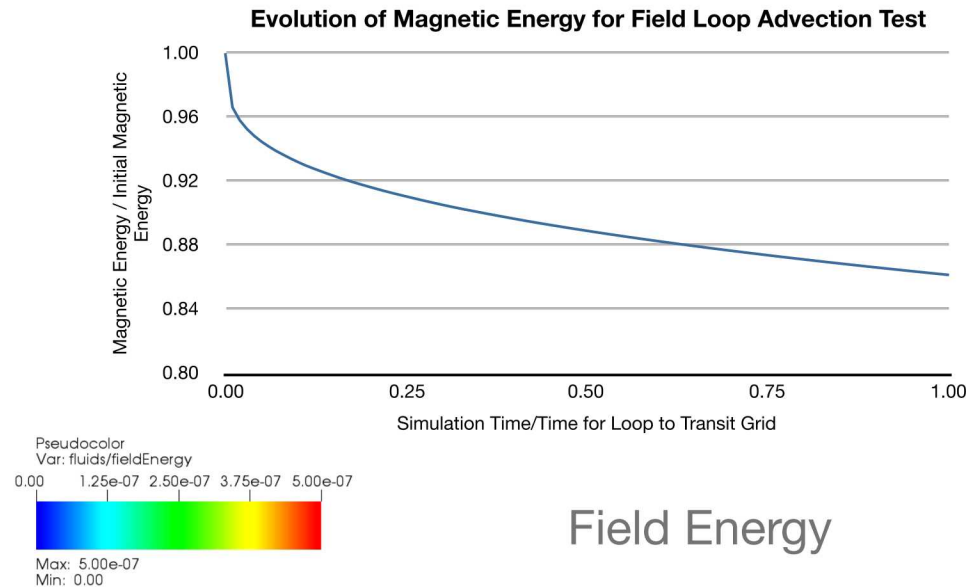




Gardiner & Stone (2005, 2008): discriminating test of a schemes ability to preserve solenoidal constraint is advection of a weak magnetic field loop in multi-dimensions:

- 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.

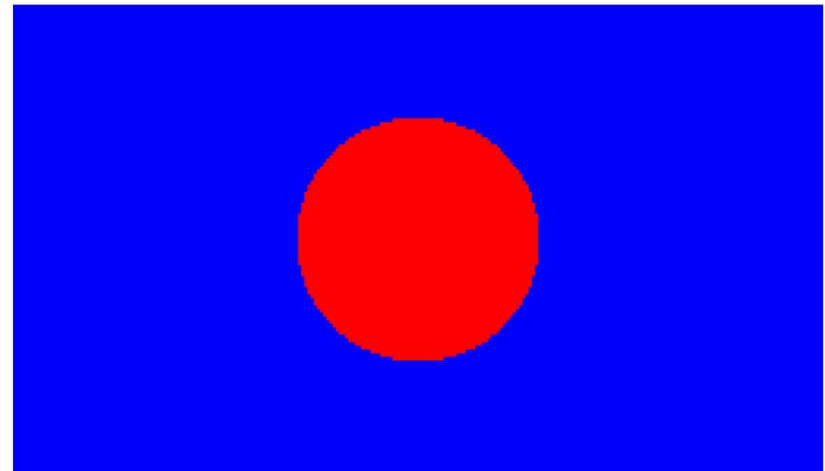
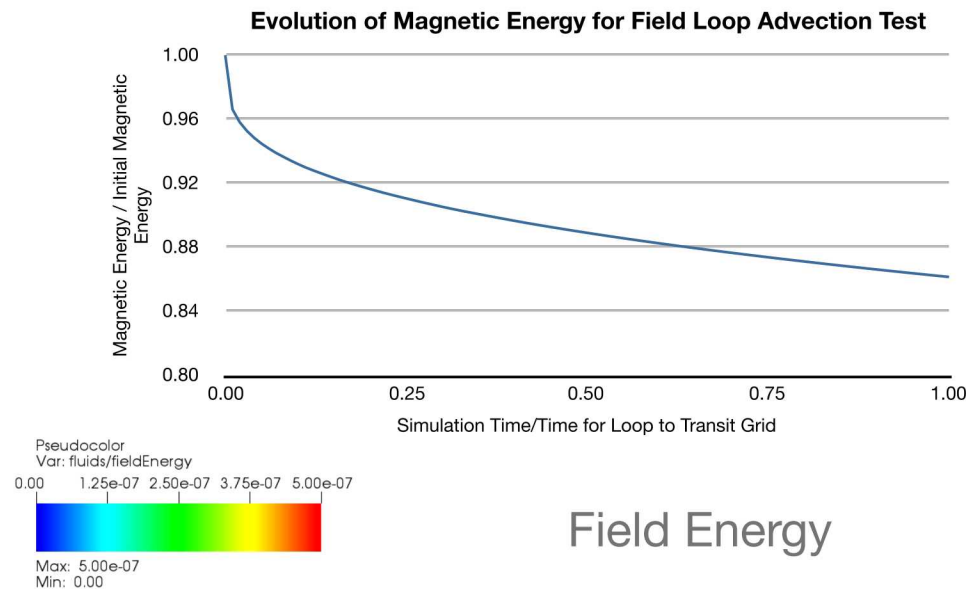




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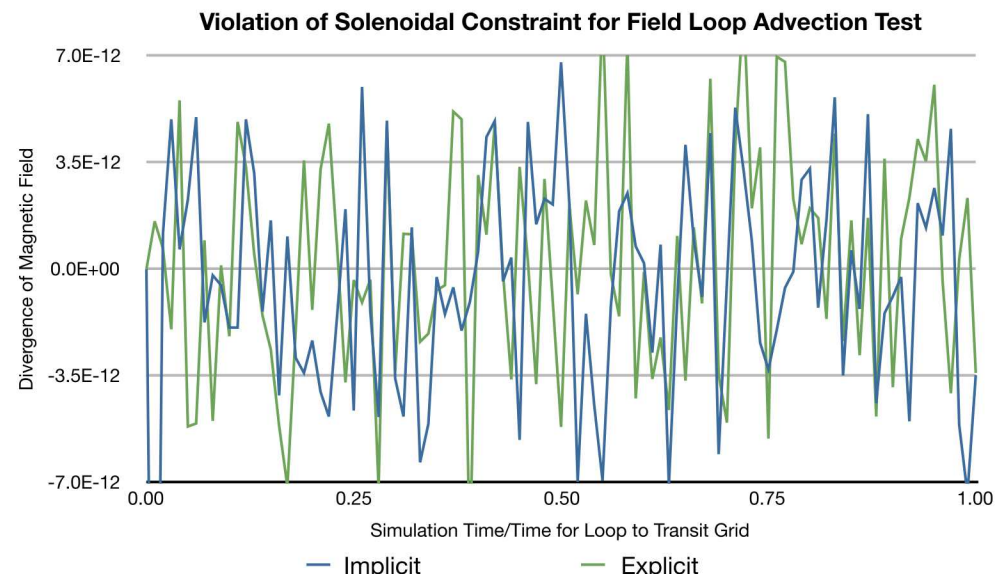
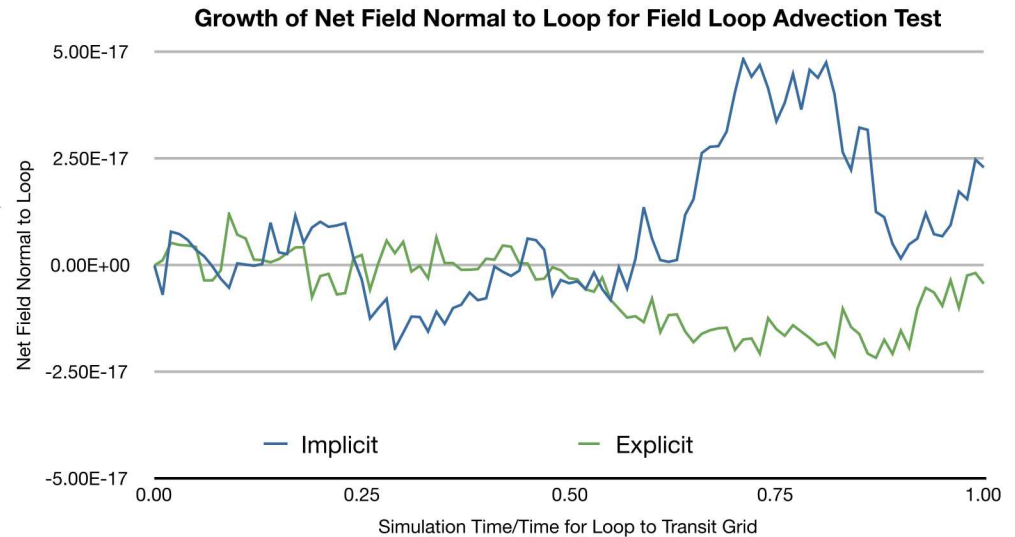




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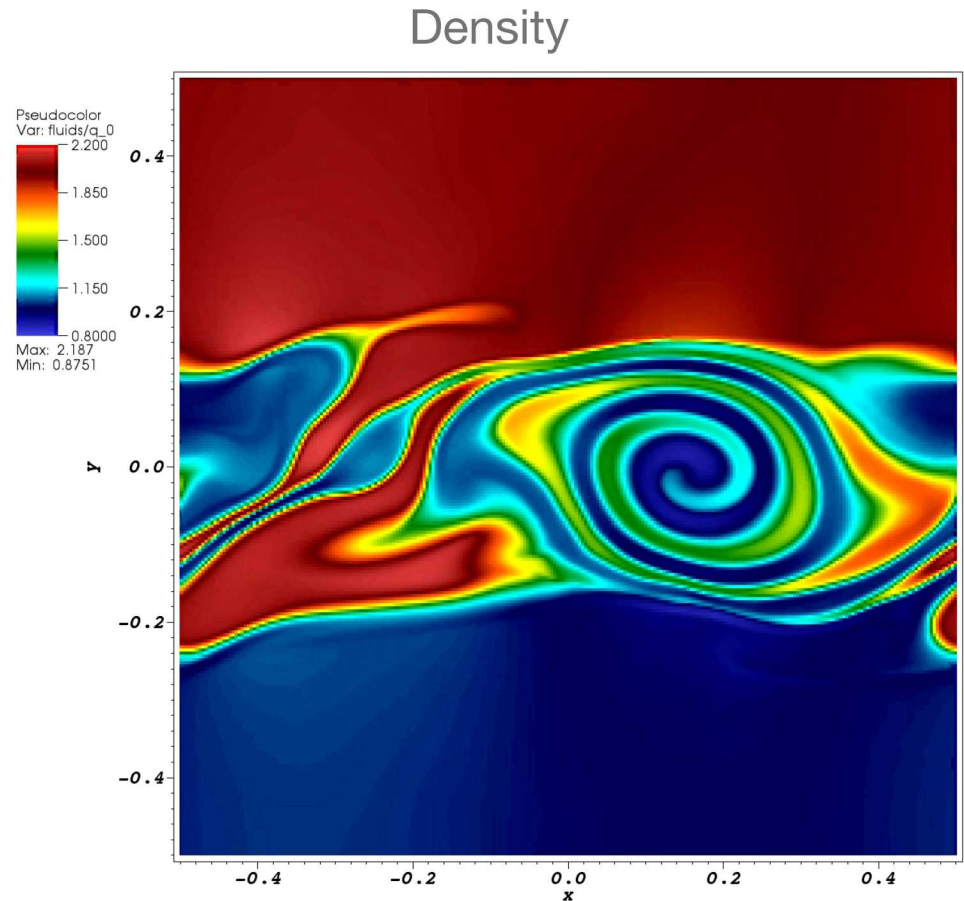
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Kelvin-Helmholtz instability provides a useful test of solver capability for non-linear compressible flows

- 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 .

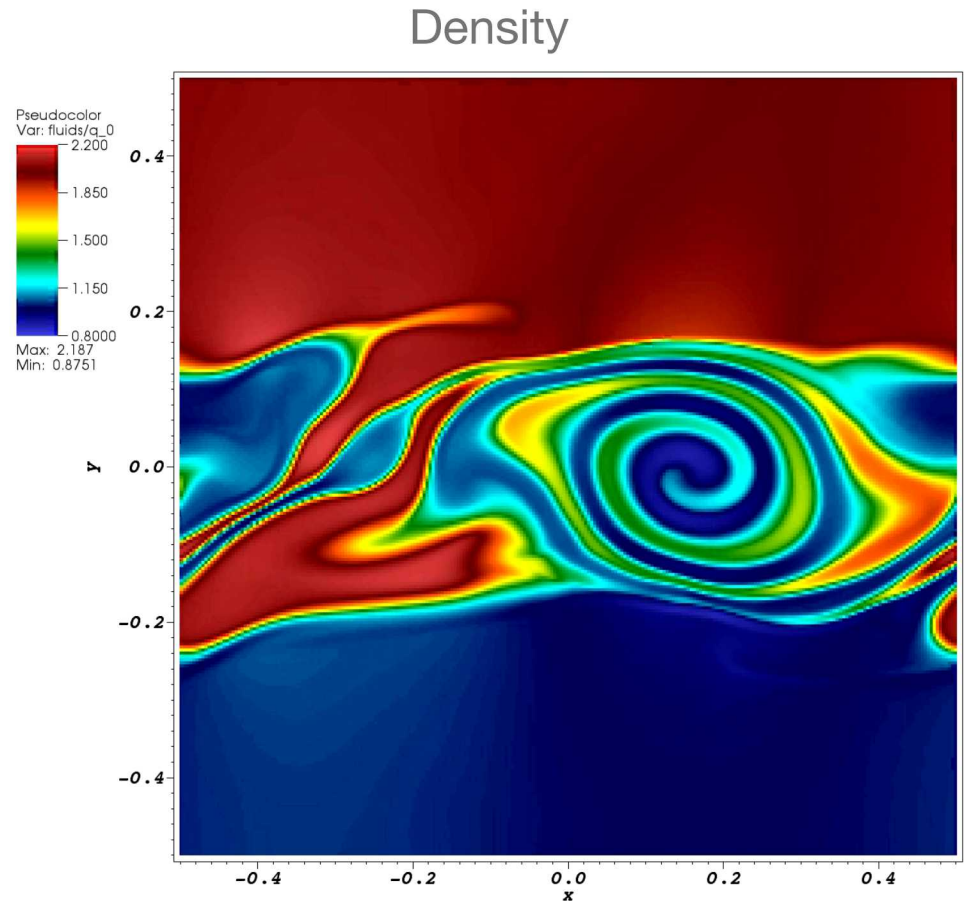


Time=7.5



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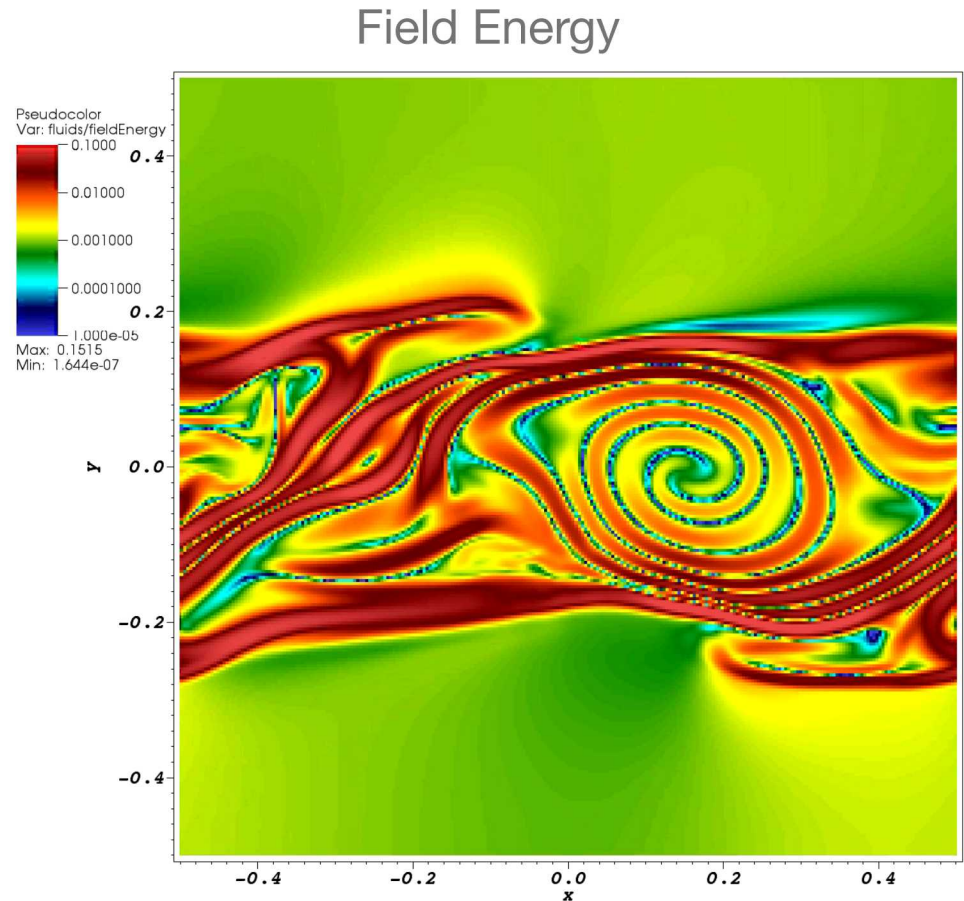


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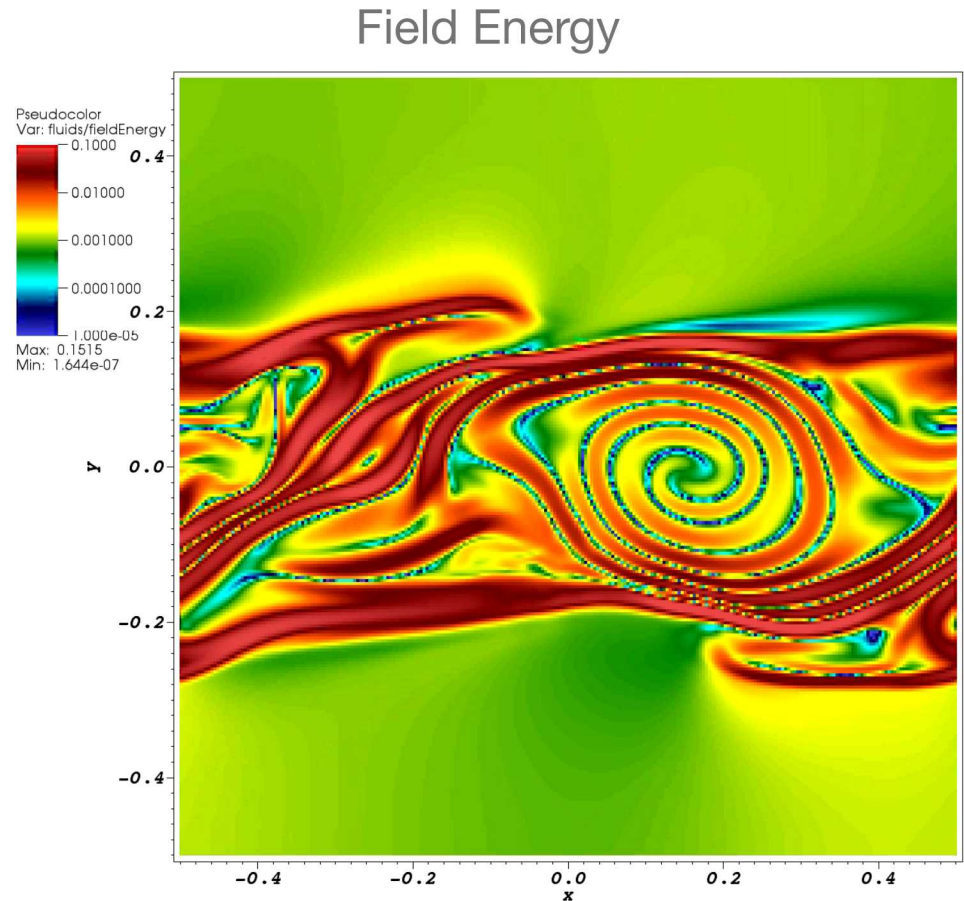


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- multi-species fluid-plasma problems

Fundamental model:

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

Different species have different timescales:

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Simplify physics:

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

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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:

- $u \times B$ term
- Resistive physics
- Hall physics
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- Compute multi-fluid shocks in range of regimes using single solver framework:
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Controlling Numerical Charge Separation

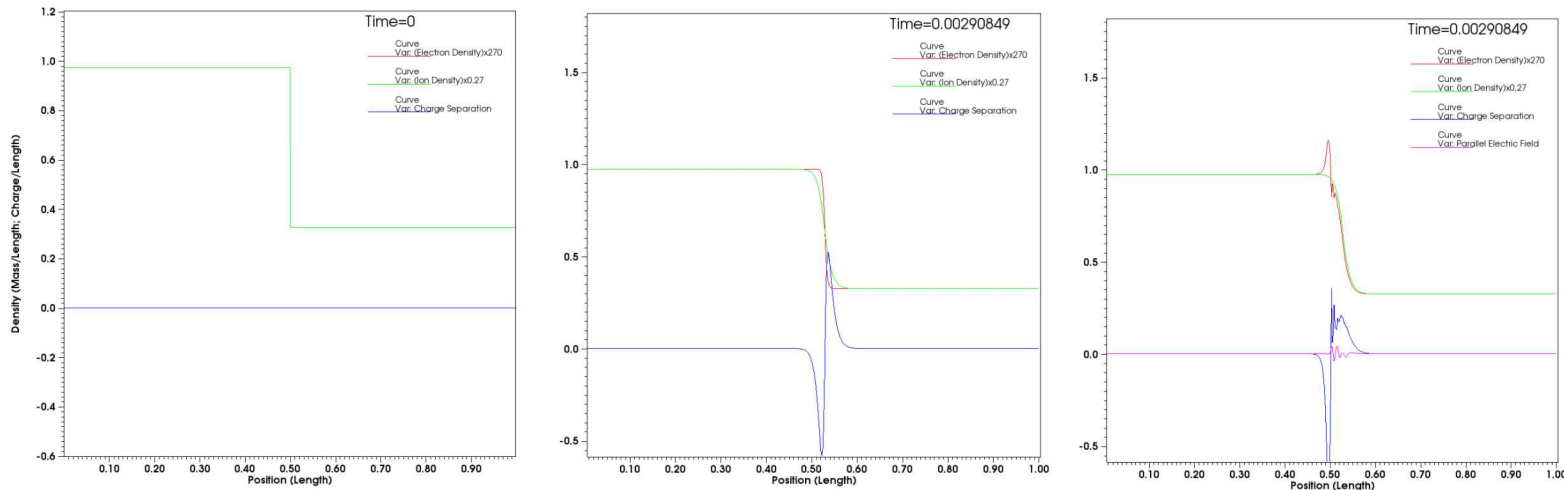
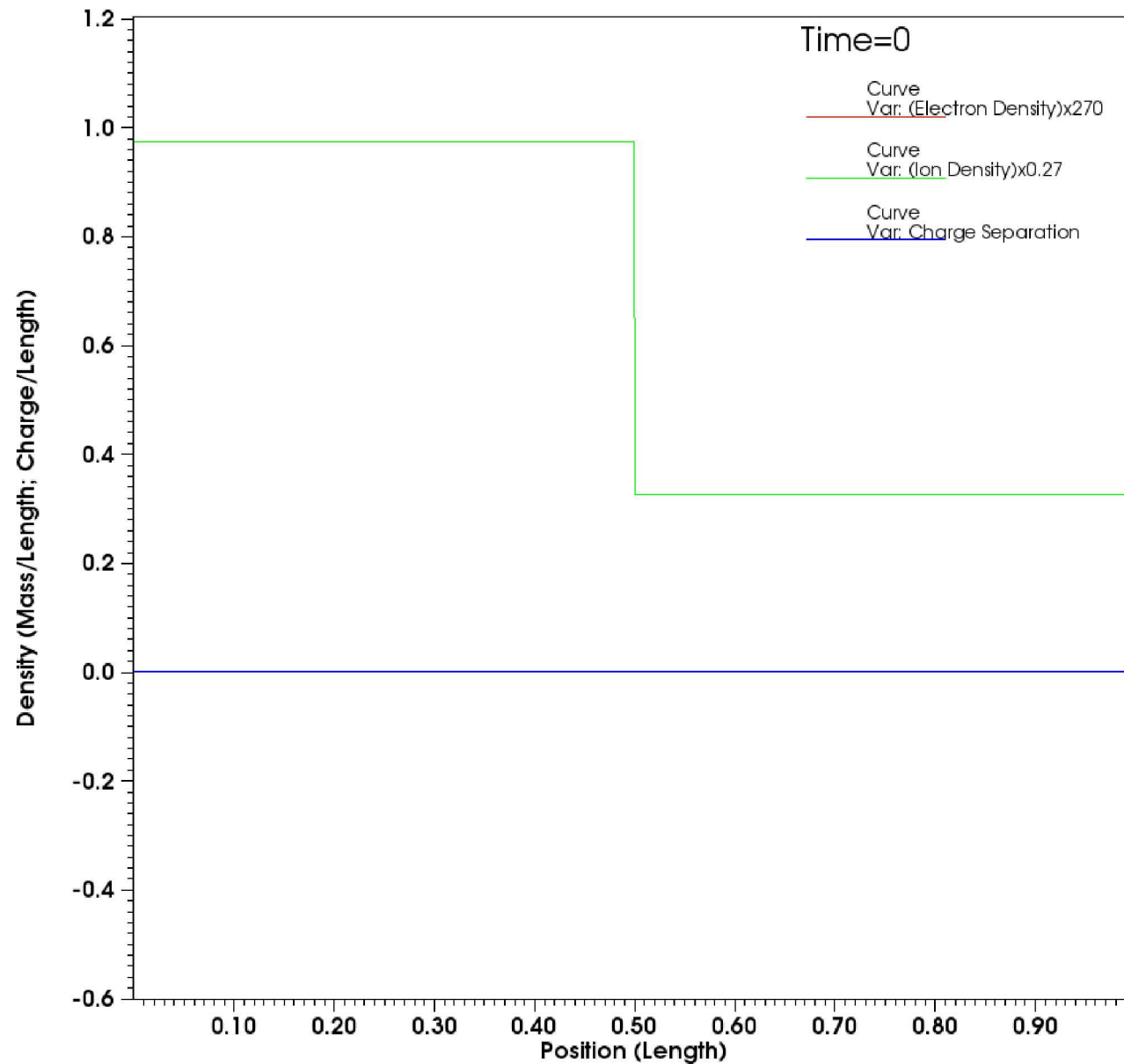


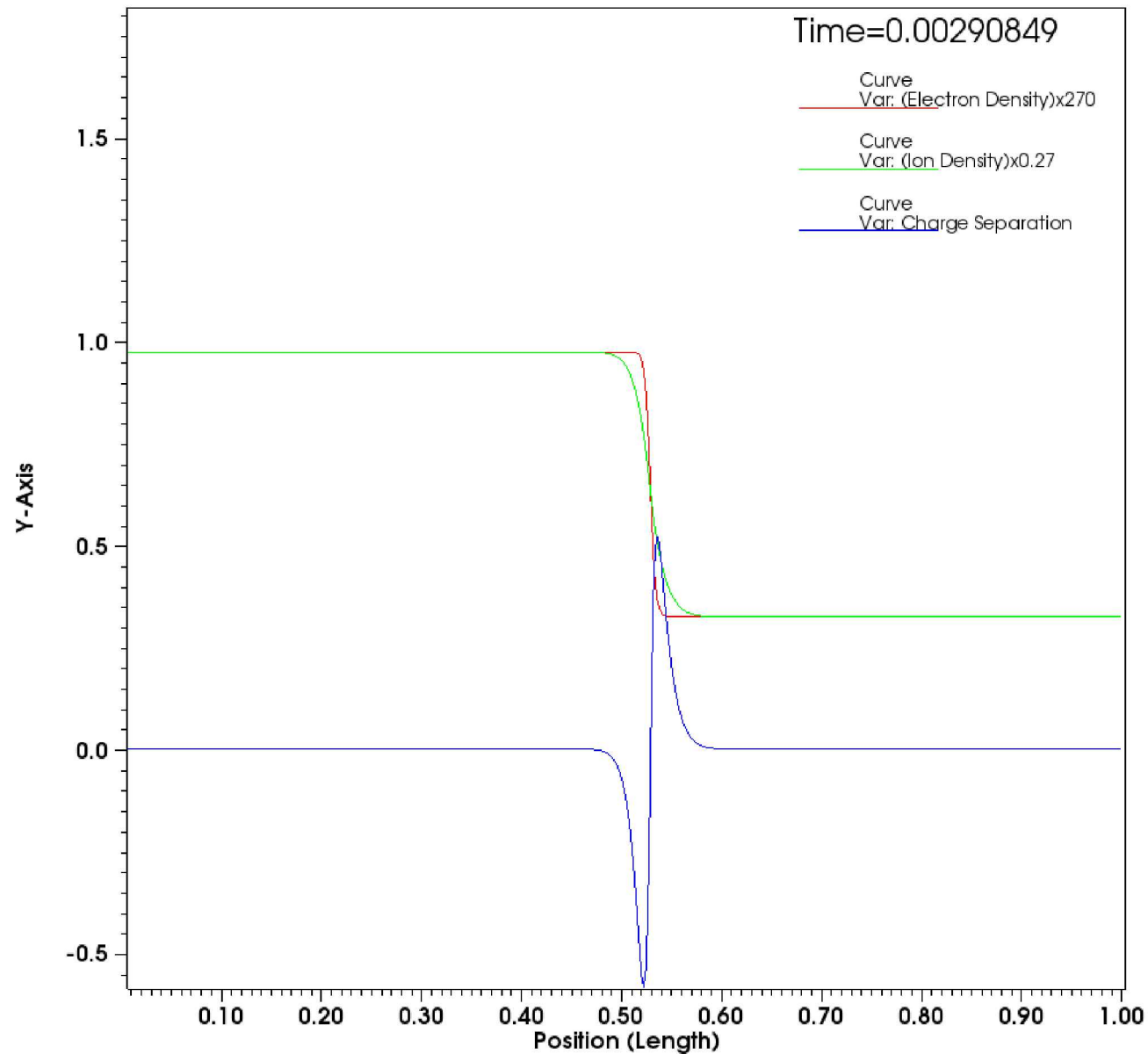
Figure 1: Evolution of a two fluid (ion and electron) contact discontinuity. The left panel shows the initial condition, the center panel the evolution of the discontinuity for stationary fluids and the right panel the evolution when the fluids advect. *Numerical* diffusion results in a net charge being created in the static case, while the same *numerical* effect results in a net current (and hence an electric field) being created in the advecting case.

- Problem: two fluid contact discontinuity (a discontinuity in plasma density at constant pressure).
- Initial state is charge neutral, with an ion to electron mass ratio of $1/1836$.
- Fluids are at constant pressure: no force acting on the gas
- Temperatures of the ions and electrons are different
- Upwind finite volume scheme: numerical diffusion is applied in a fashion proportional to the sound speed
- After ten sound crossing times; the ions and electrons have spread out on the grid due to numerical diffusion, forming a net charge.

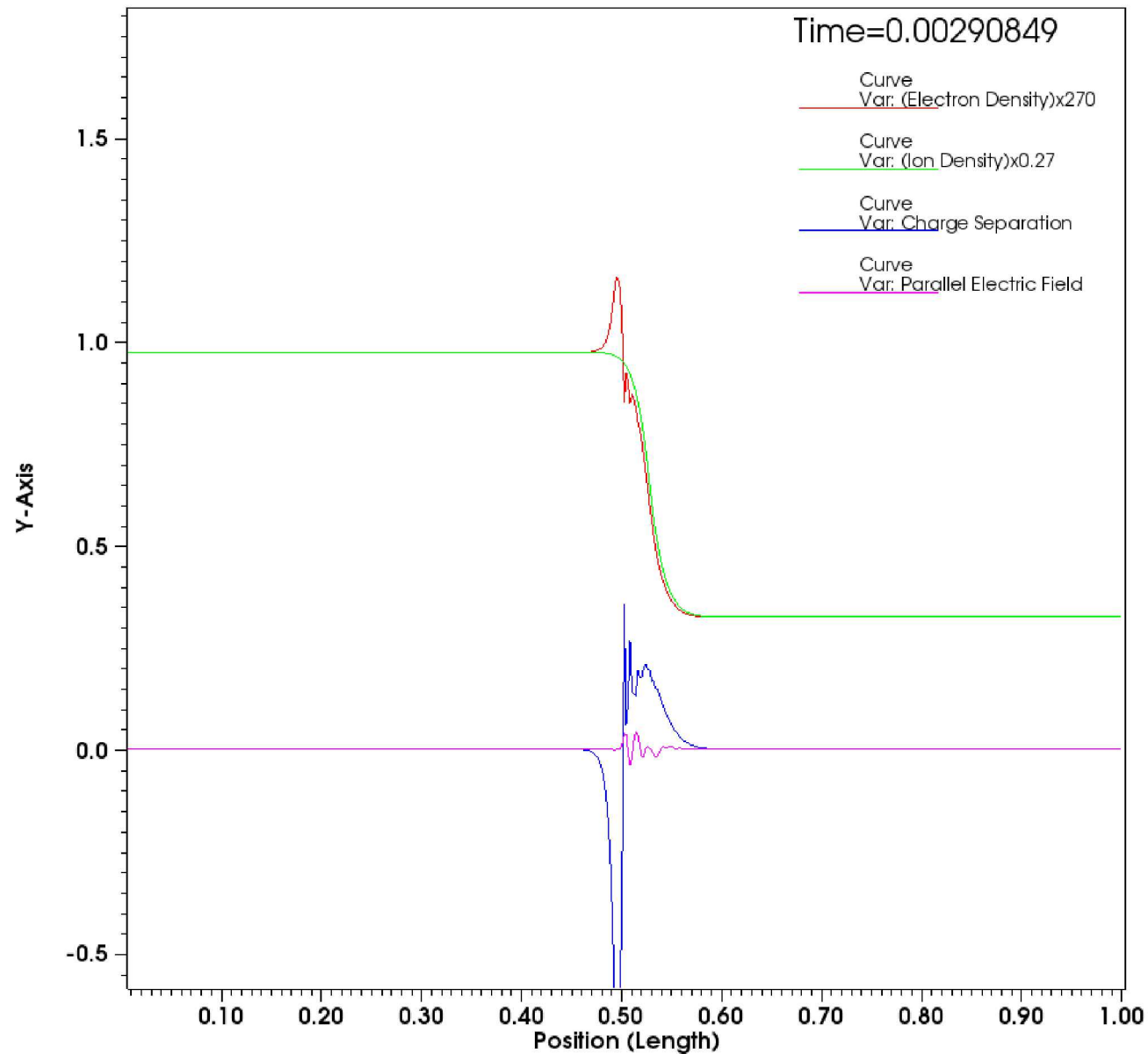
Controlling Numerical Charge Separation



Controlling Numerical Charge Separation



Controlling Numerical Charge Separation



Controlling Numerical Charge Separation

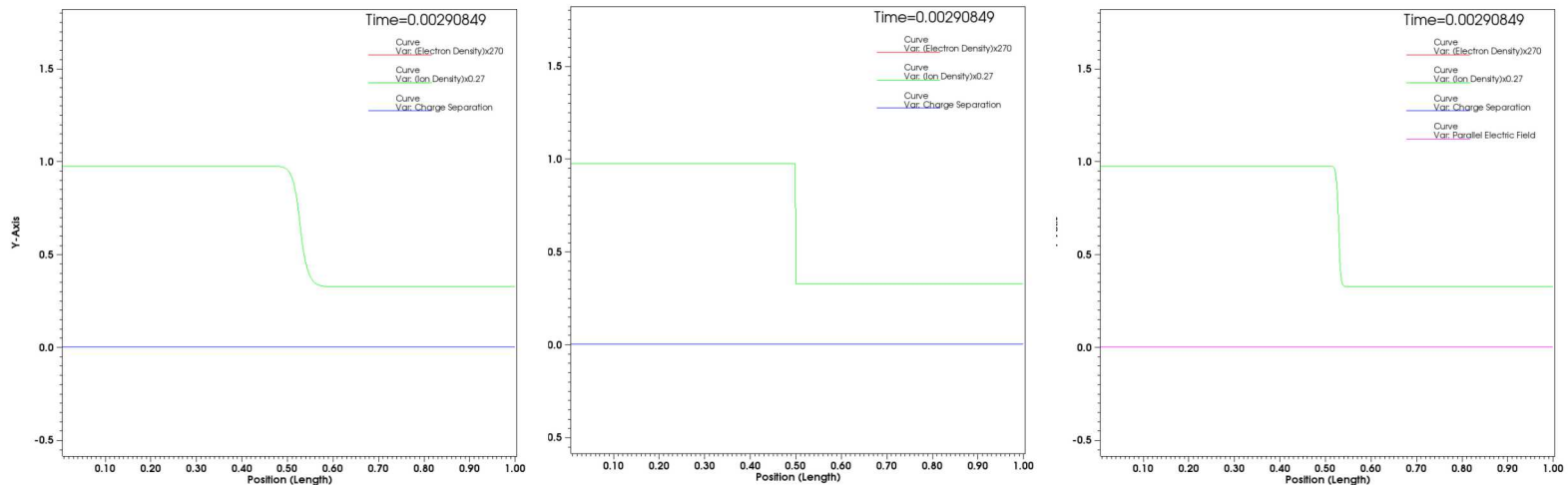
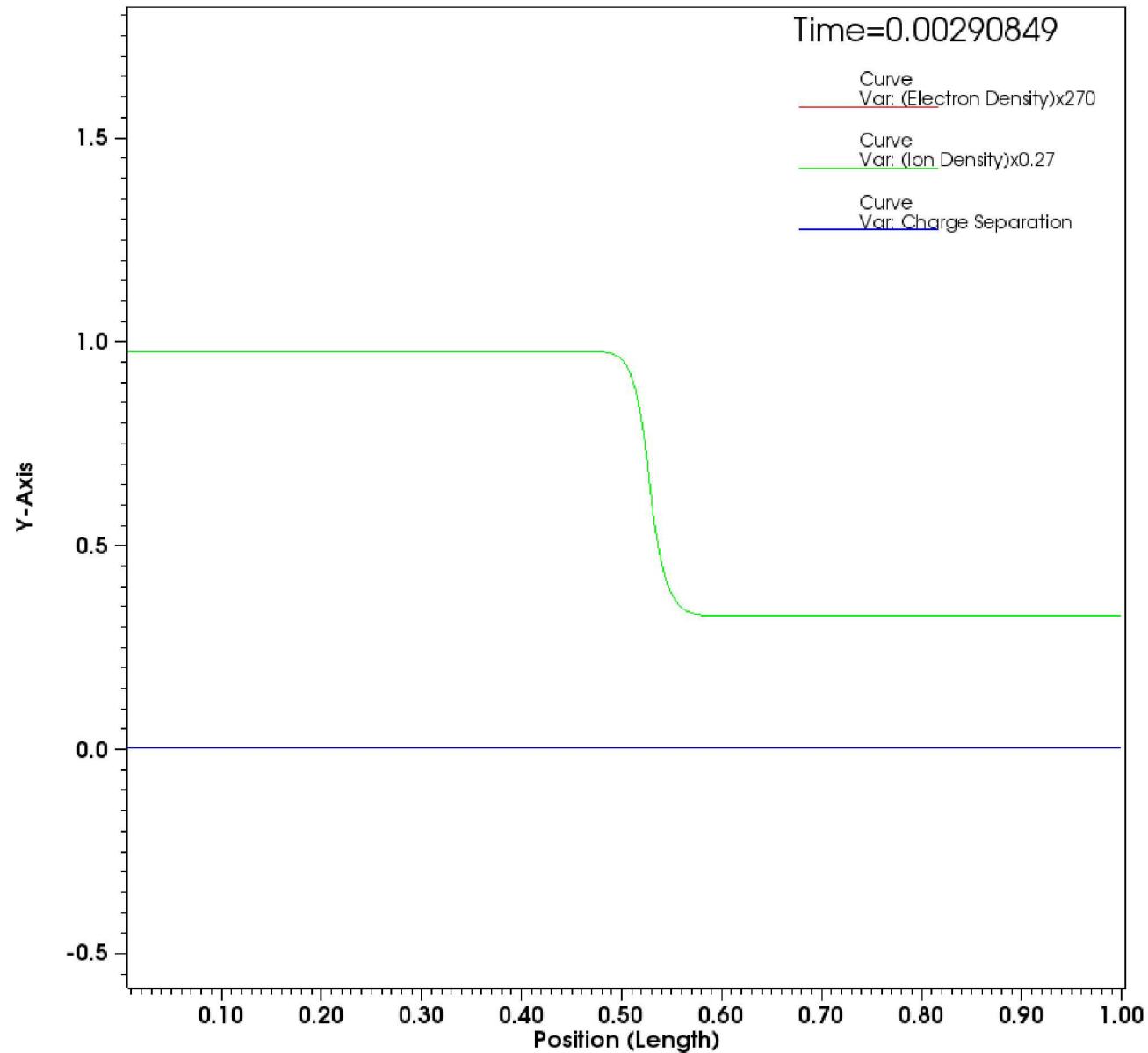


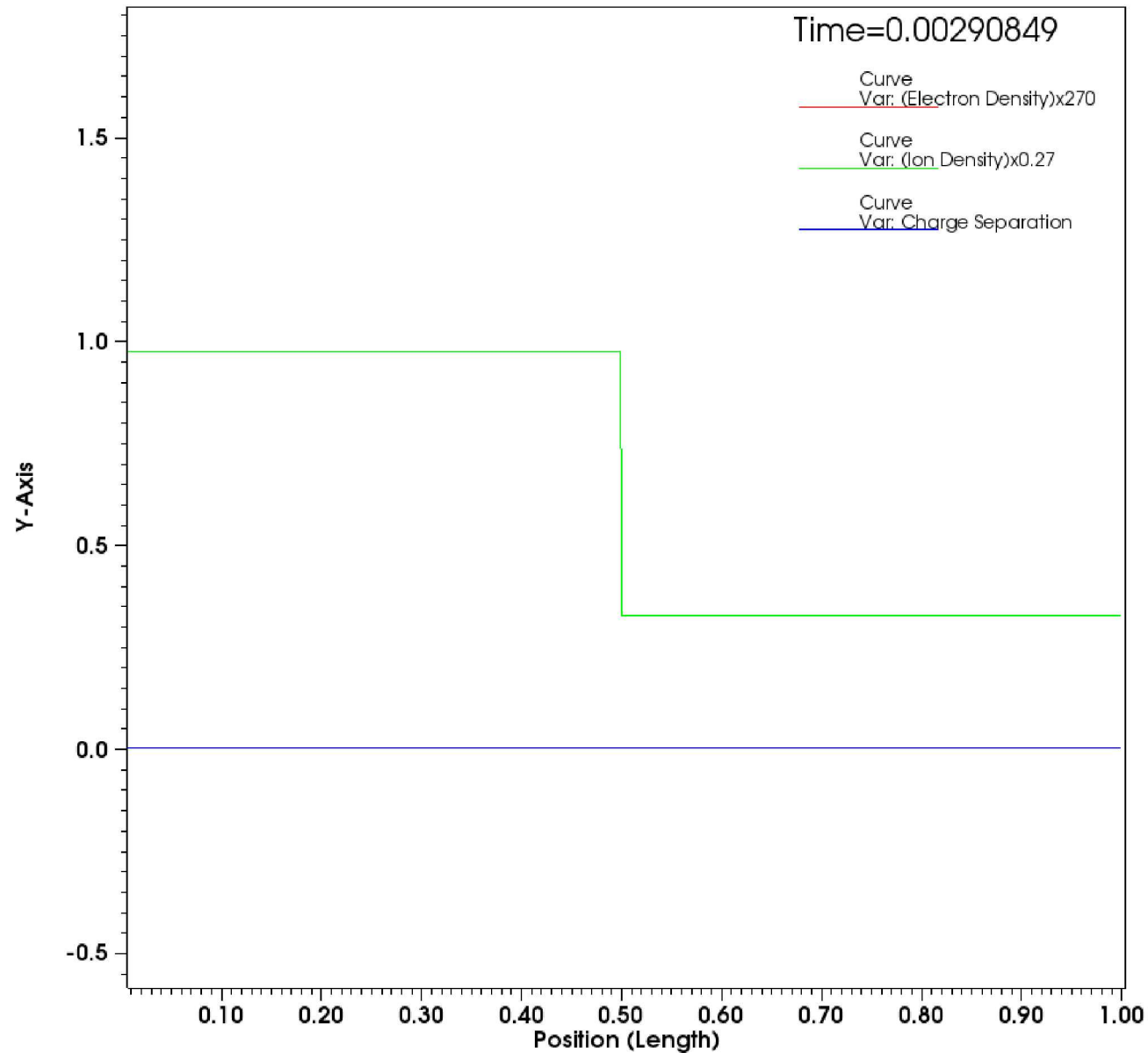
Figure 2: Evolution of a two fluid (ion and electron) contact discontinuity. The left panel shows the evolution for stationary ion and electron fluids using equal temperatures and the HLLC Riemann solver, the center panel the evolution for stationary ion and electron fluids using unequal temperatures and the HLLC Riemann solver and the right panel the evolution for the HLLC case where the fluid advects.

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- Contact discontinuity is now resolved by the scheme, numerical charge separation effects removed.

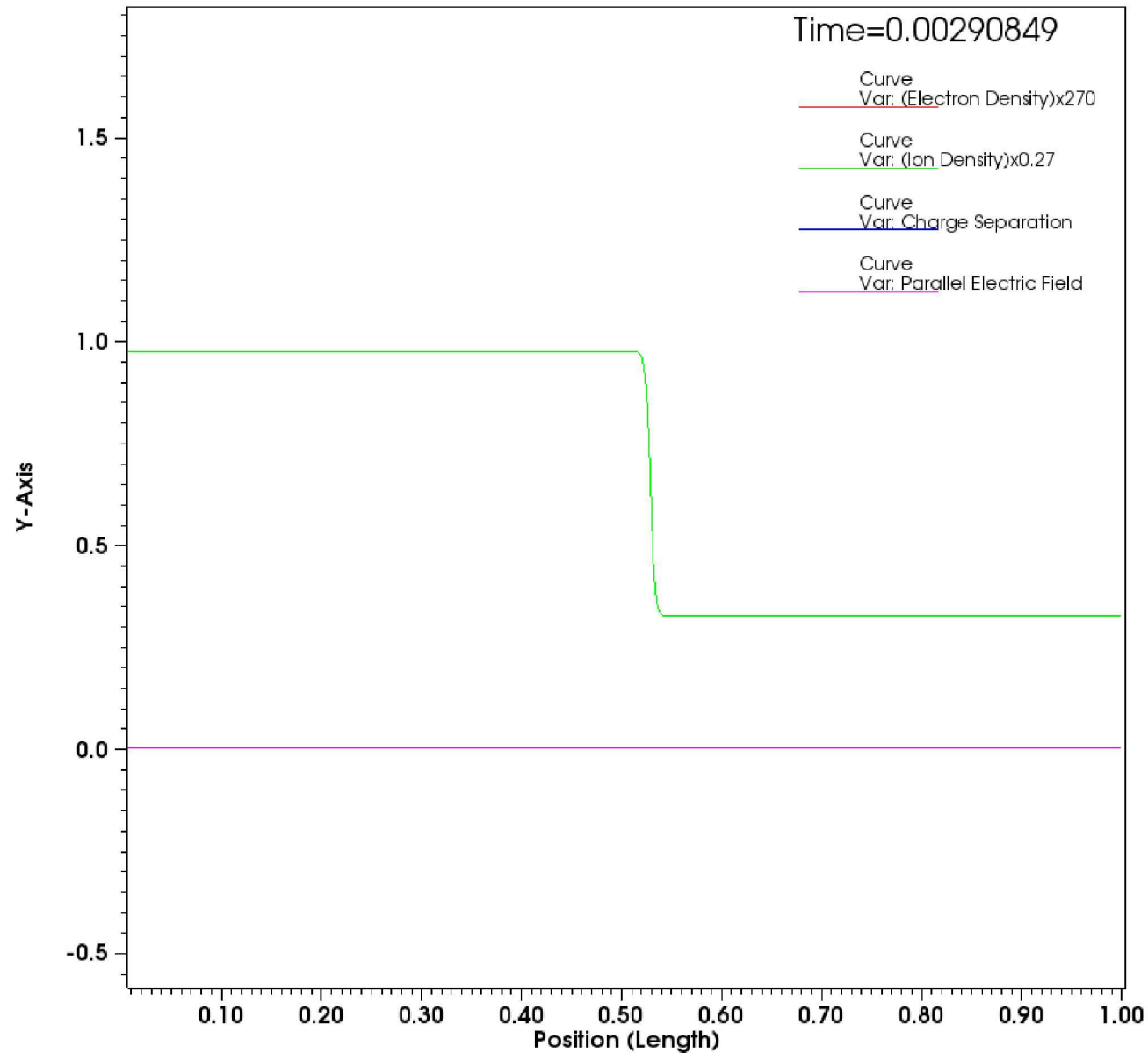
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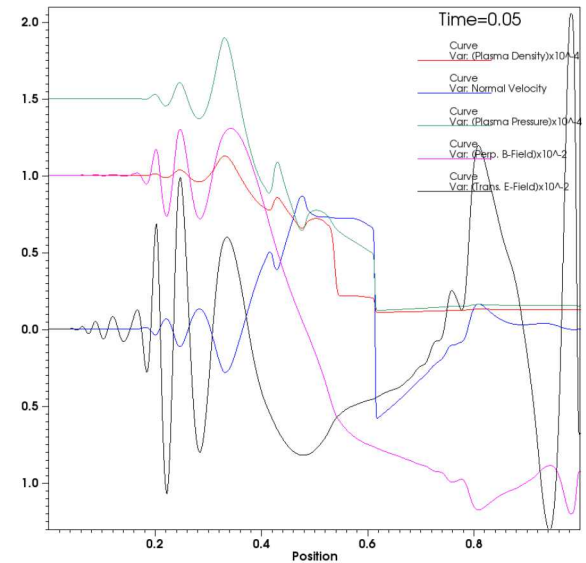
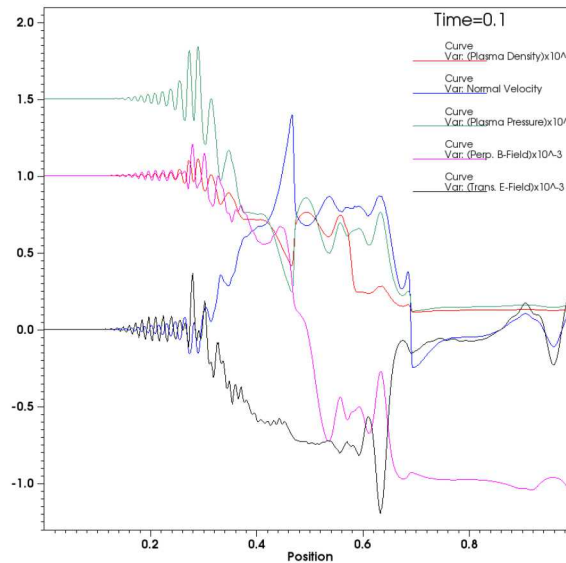
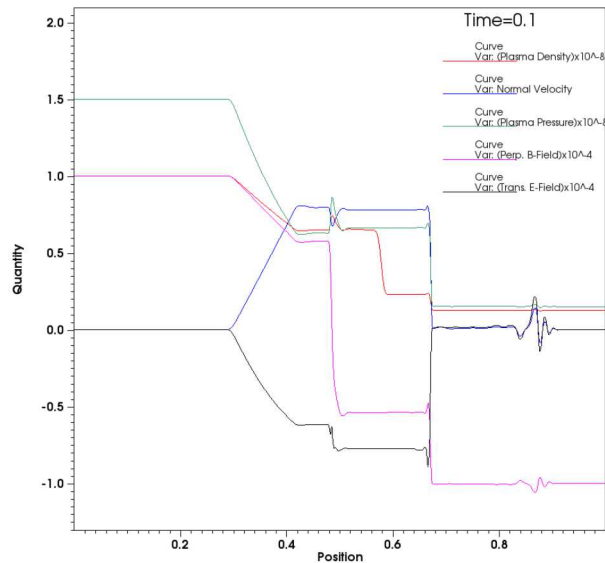


Controlling Numerical Charge Separation



Controlling Numerical Charge Separation





Example problems:

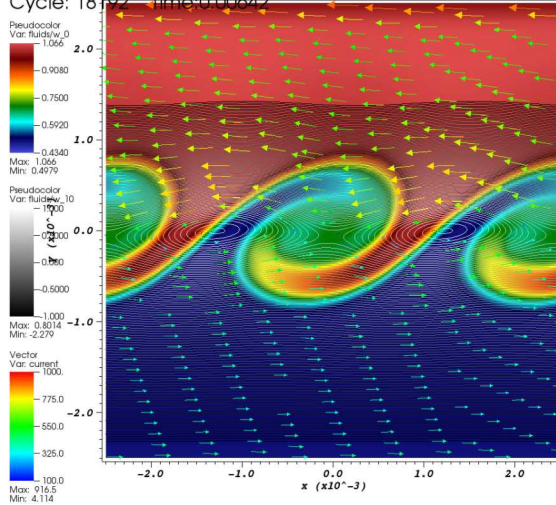
- Classic 'Brio-Wu' shock-tube:
 - MHD regime
 - Hall MHD regime
 - Multi-fluid regime
- Electron/Ion shear instabilities:
 - Ions linearly unstable to Kelvin-Helmholtz
 - Electrons non-linearly unstable.

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)

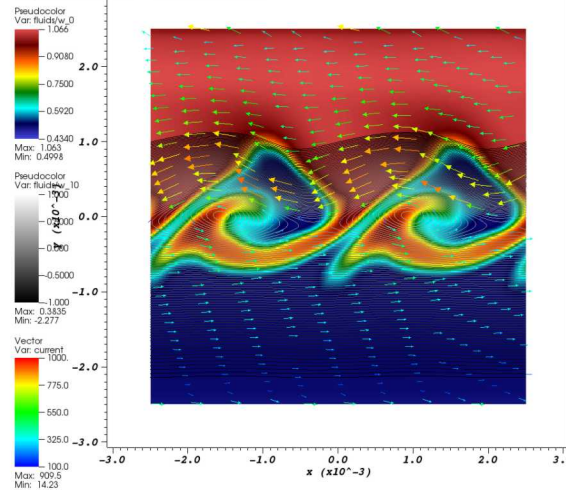


DB: electronShearInstability_642.h5
Cycle: 18192 Time: 0.00642



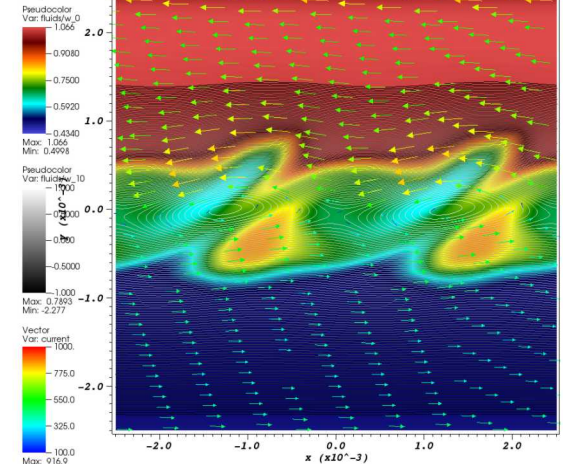
user: beckwith
Fri May 29 08:19:11 2015

DB: electronShearInstability_520.h5
Cycle: 15481 Time: 0.0052



user: beckwith
Fri May 29 15:04:10 2015

DB: electronShearInstability_937.h5
Cycle: 25861 Time: 0.00937



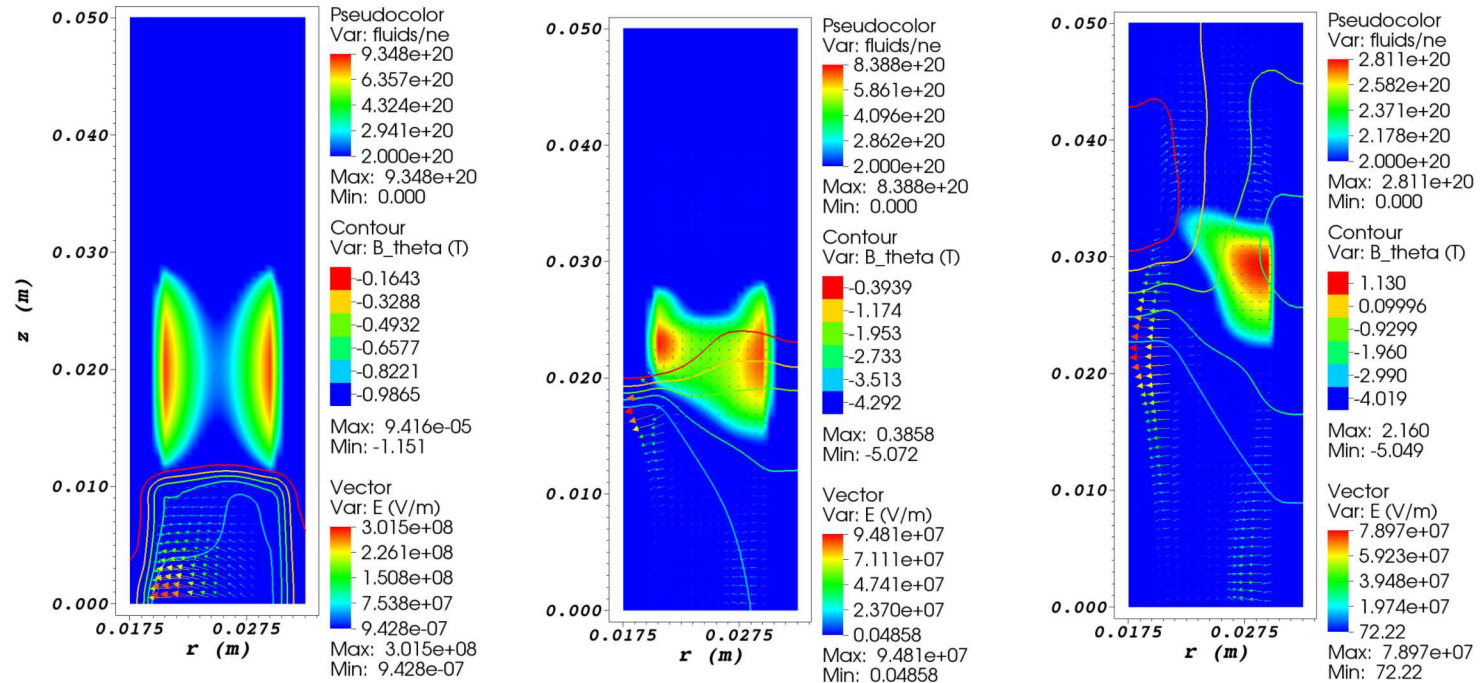
user: beckwith
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Semi-Implicit two-fluid simulation of plasma opening switch:

- 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.



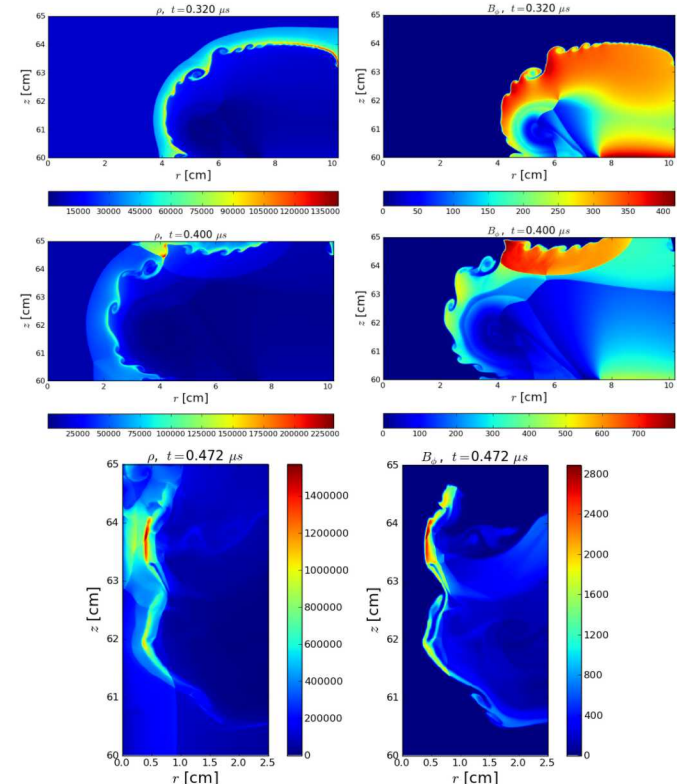
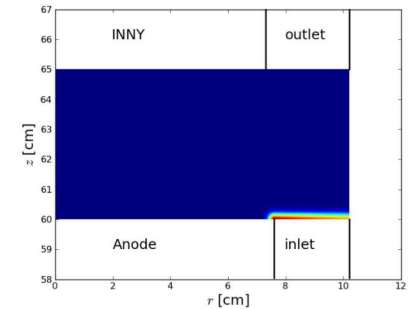
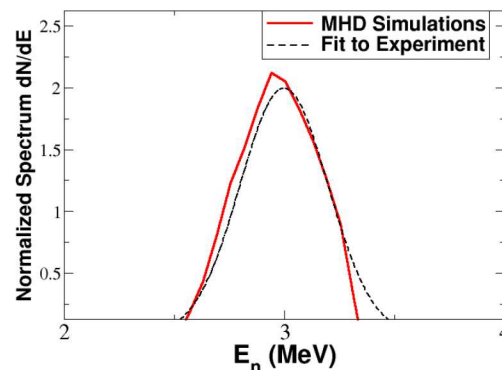
Mechanisms for pinch formation, ion acceleration and subsequent neutron production in Dense Plasma Focus are not well-understood

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...



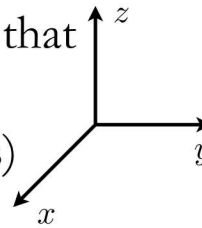


Understanding *how* the electromagnetic field penetrates into the plasma is a key aspect of understanding the operation of the plasma opening switch

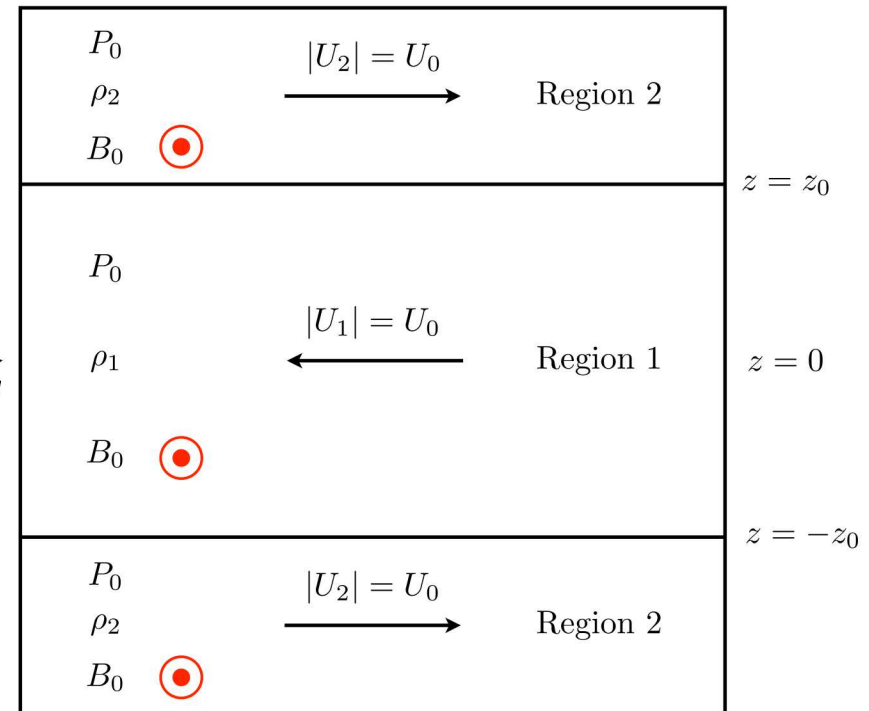
- By studying this as a prototype problem physics, we can remove the influence of boundary conditions

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

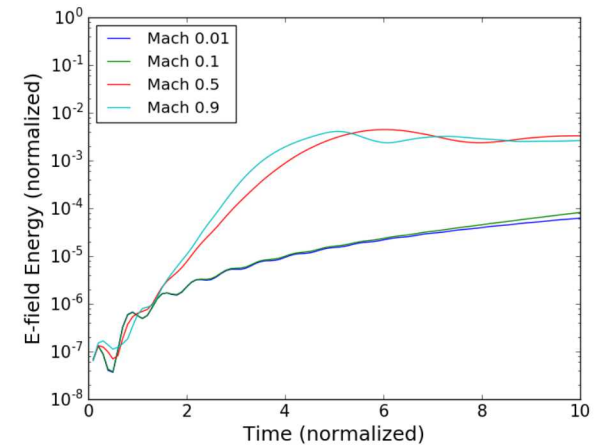
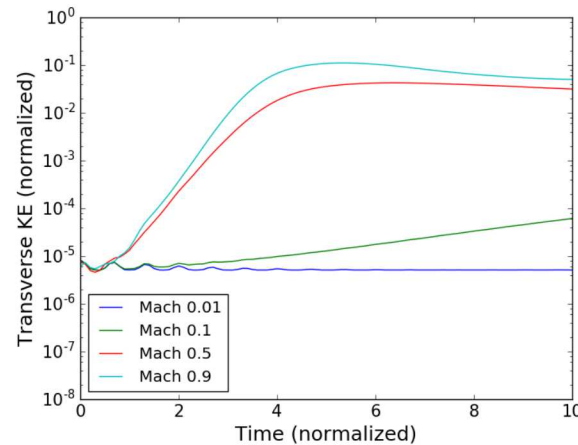
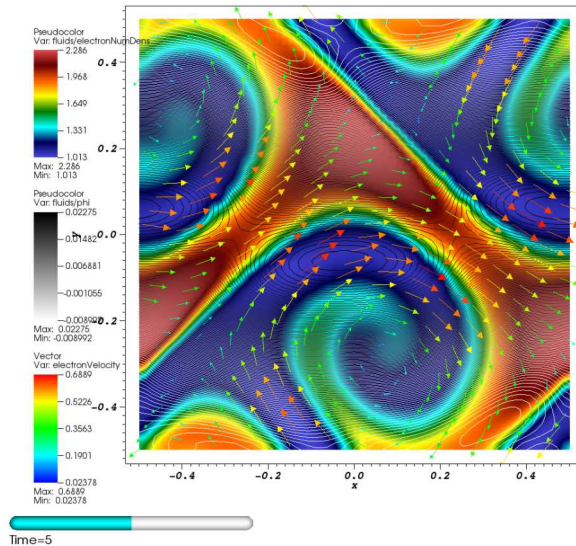
- Compressibility (transonic flows)
- Magnetic field amplification & turbulent energy cascades
- Dynamo activity (two-fluid flows)
 - Electrons can be KHI *unstable* when ions are *stable*
- Relativistic (finite Lorentz factor) effects



Salvesen et al. (2014)



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



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 \ll electron inertial length

Electric potential computed based on charge separation as diagnostic.

Results:

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



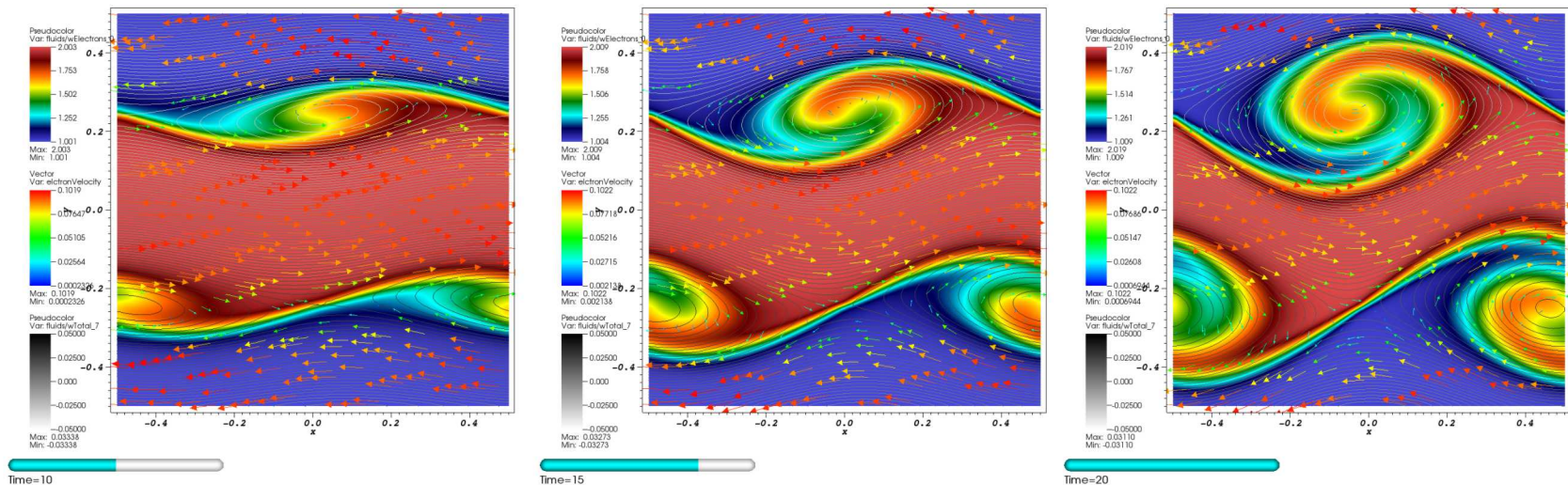
Subsonic EKH: electric field amplified to equipartition with transverse kinetic energy, implies that generated electric field can influence formation of shear flow

- 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 collocated with electron vortices





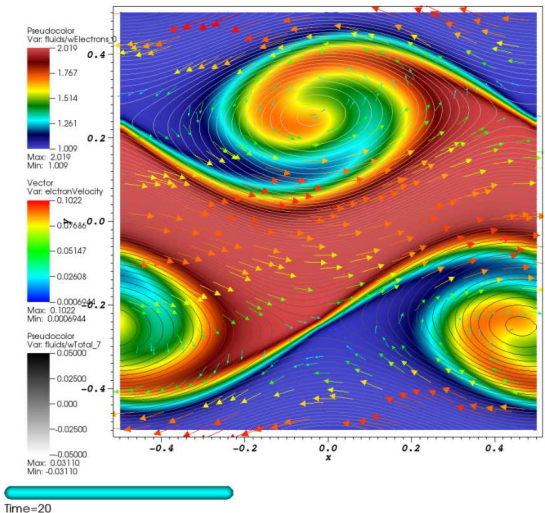
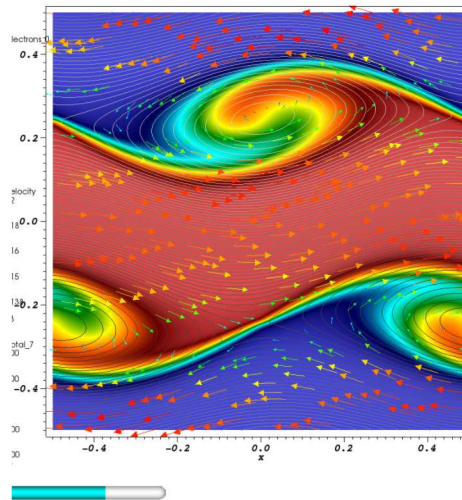
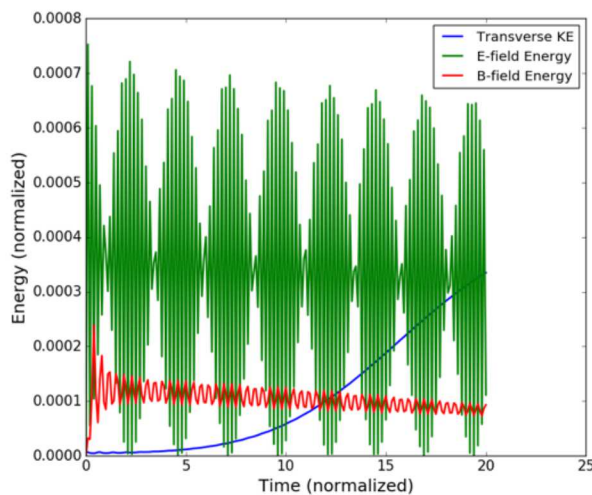
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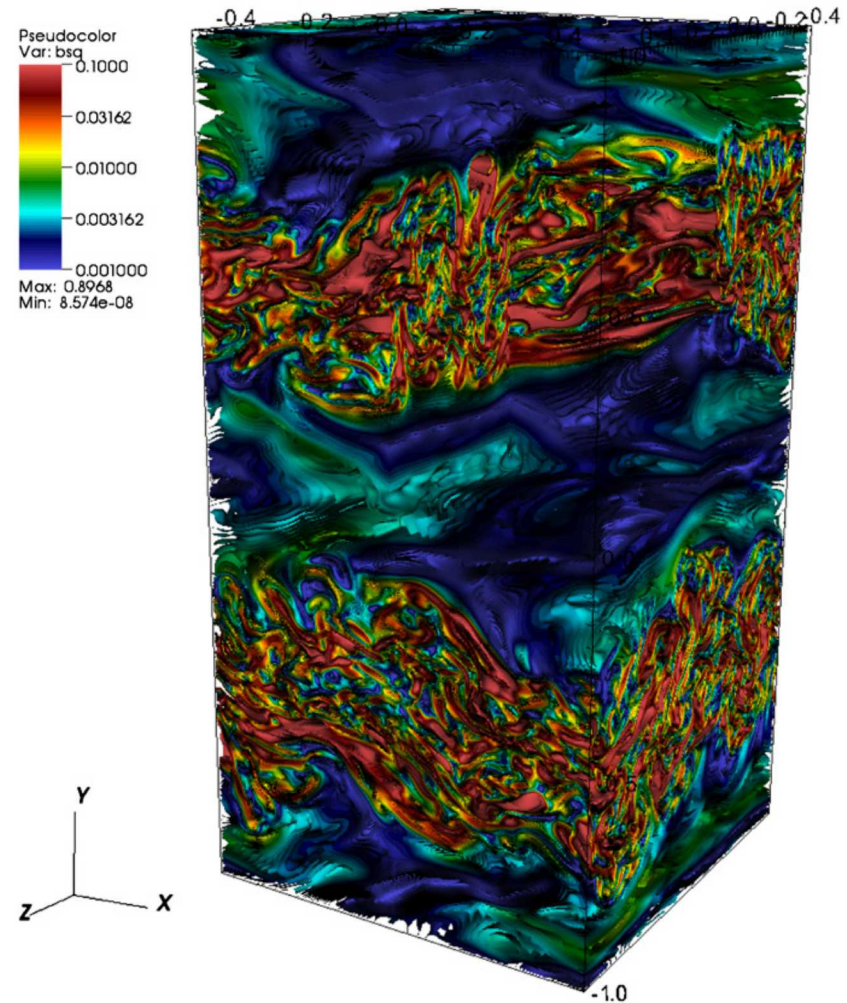


Simulations of turbulence can rarely resolve the dissipation scale. How can we trust them?

- 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)

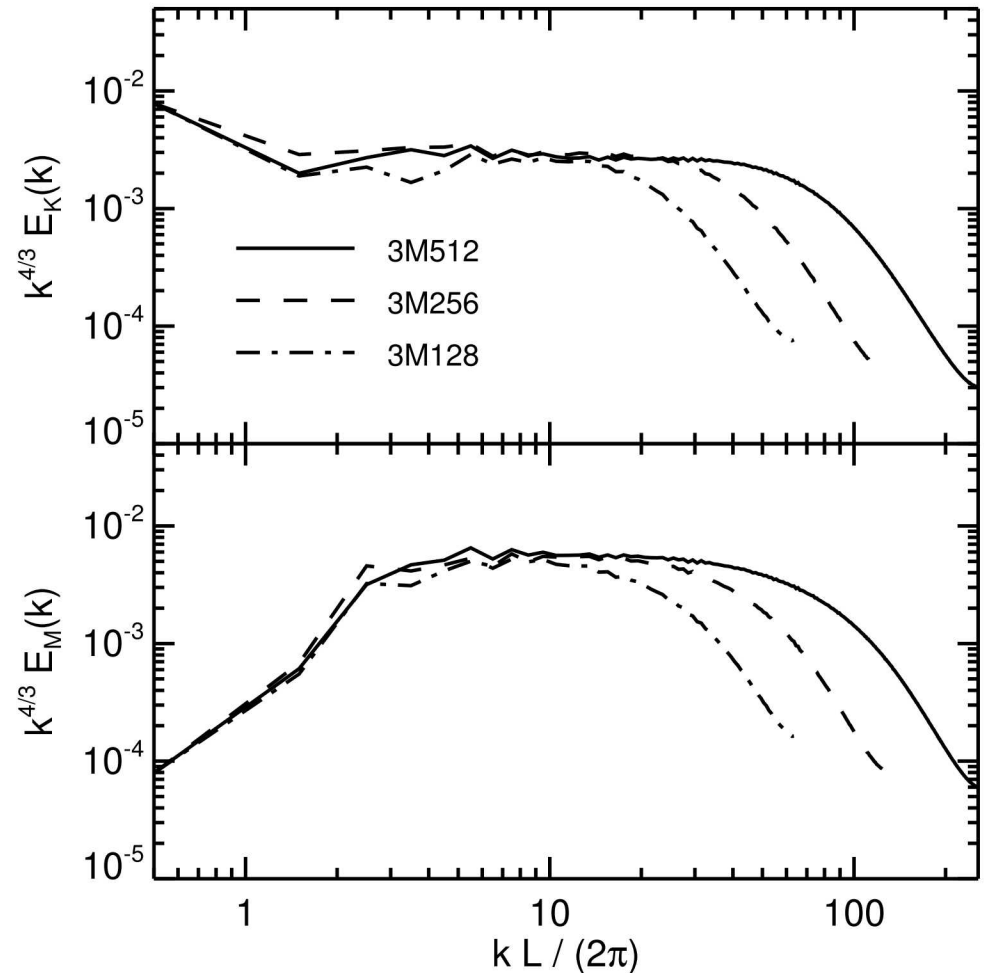


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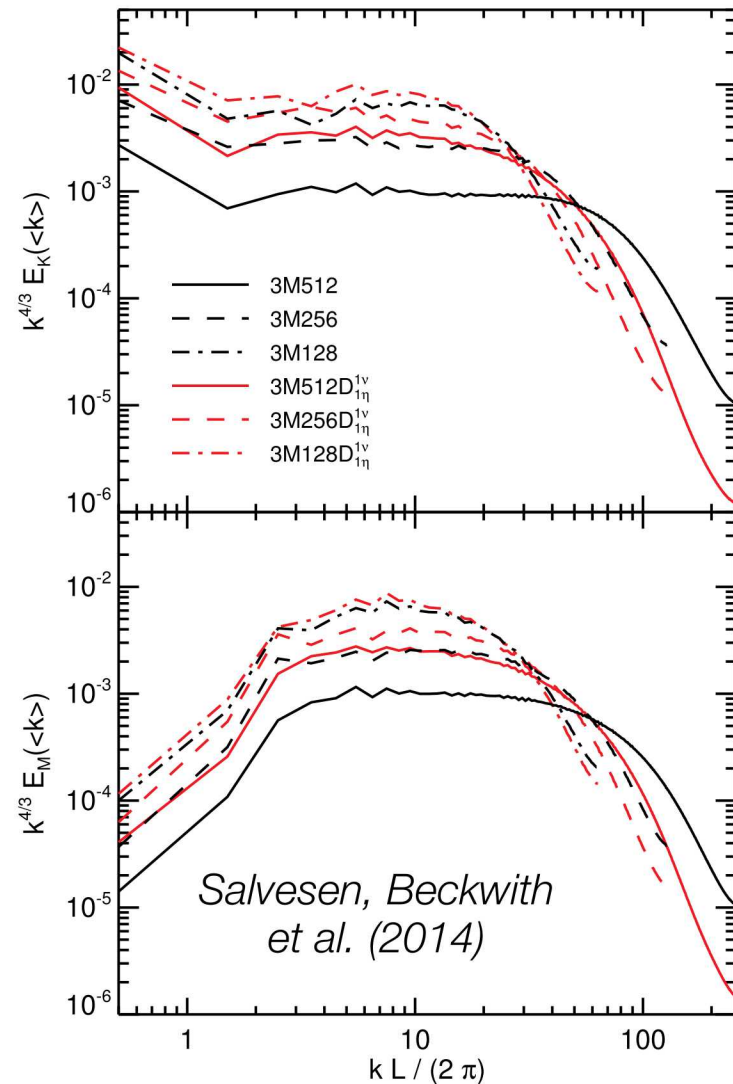


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Add Navier-Stokes shear viscosity and Ohmic resistivity to decaying turbulence model.

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



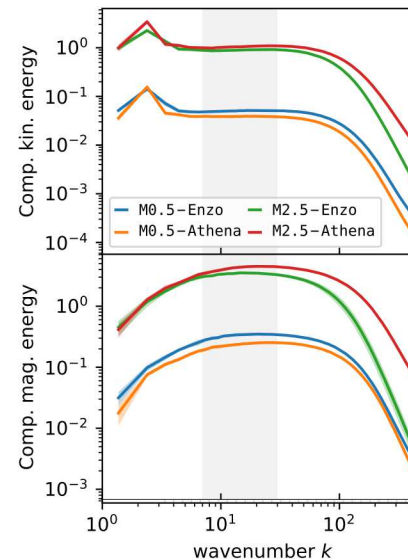


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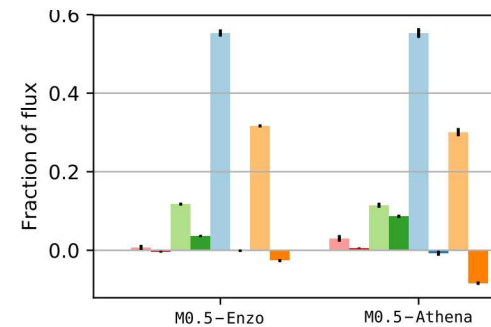
More recently, we have developed analysis tools for energy transfer in MHD turbulence that enable both cross-code comparison and comparison against analytic theory across a range of Mach numbers.



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 (Debligny et al. 2005).



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

Grete, O'Shea
Beckwith &
Christlieb (2017)



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.



Verification that HO algorithms pass standard benchmarks for (e.g.) MHD:

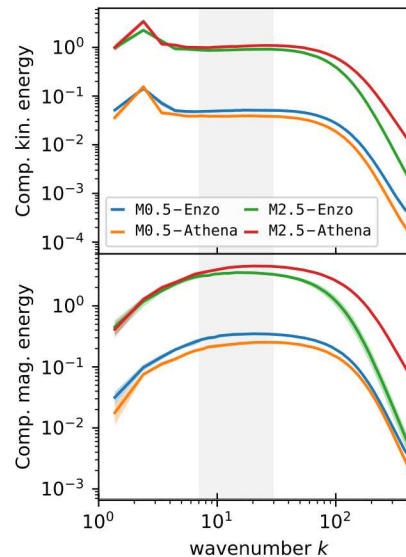
- Includes rigorous tests that divergence-free constraint is preserved in three-dimensions
- Extensive test-suite developed by a range of communities including astrophysics, fusion, etc.

MHD-turbulence is three-dimensional and *non-linear*:

- Requires careful analysis and benchmarking to demonstrate that algorithm can reproduce established results
- e.g. reproduce results established by spectral and analytic methods in non-linear regimes

PoS and DPF will require more than just ideal MHD: hall effect, electron inertia, Braginskii viscosity, equation of state models, boundary conditions, kinetic effects...

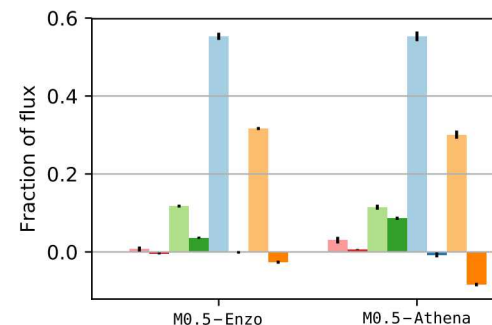
Non-Linear MHD Turbulence Benchmark



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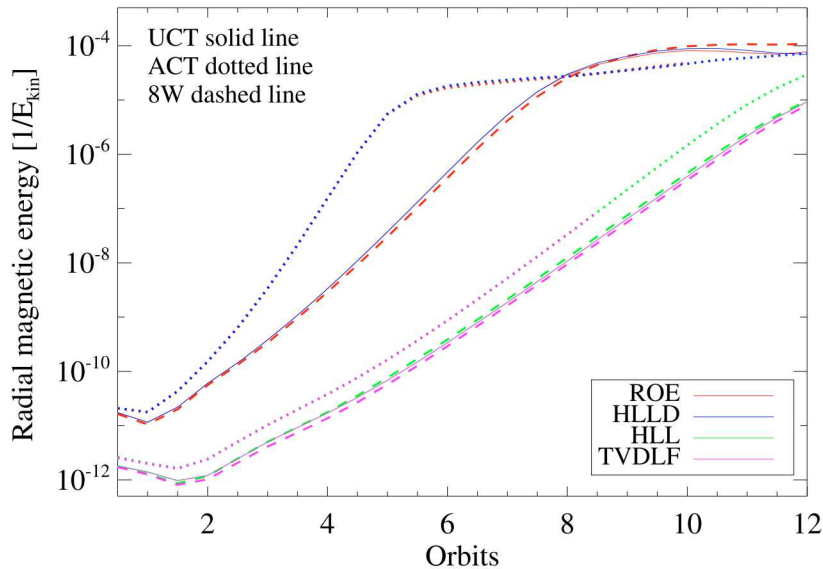
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Why Does (Non-Linear) (MHD) Turbulence Need Special Attention?



Answer: painful experience:

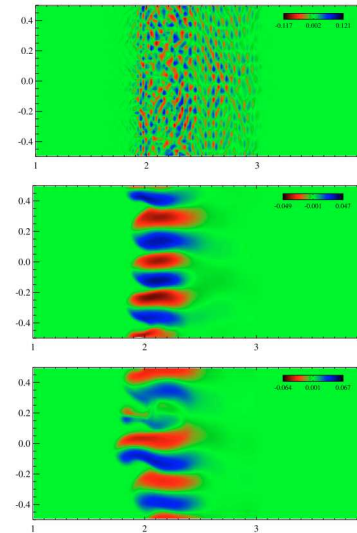
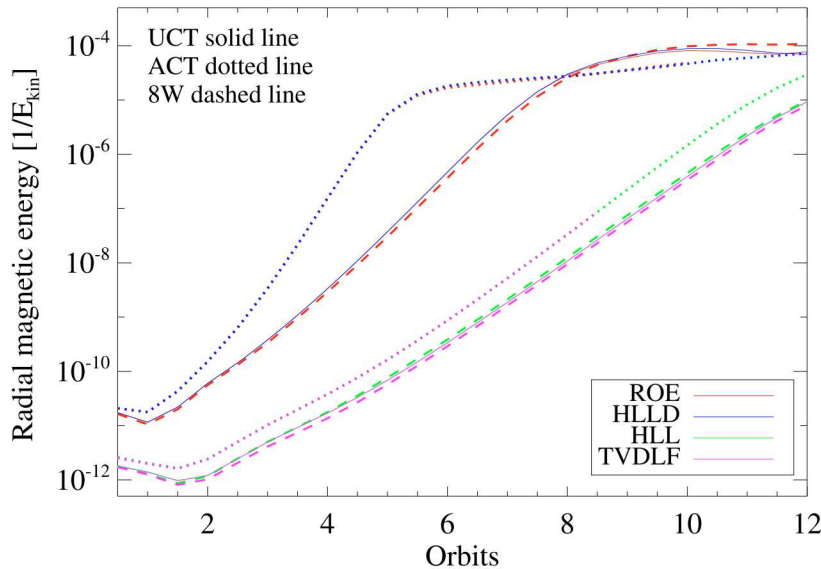
- e.g. magneto-rotational instability (MRI, Balbus & Hawley, 1991).

Compare 3 different methods of computing EMF for induction equation (Flock et al., 2010):

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{v} \mathbf{B}^T - \mathbf{B} \mathbf{v}^T) + \nabla \psi = 0$$

- All pass standard benchmark test suite
- All produce similar non-linear saturation level
- One of these methods is producing numerical garbage.
 - Which one?

Why Does (Non-Linear) (MHD) Turbulence Need Special Attention?



ACT

UCT

Zeus

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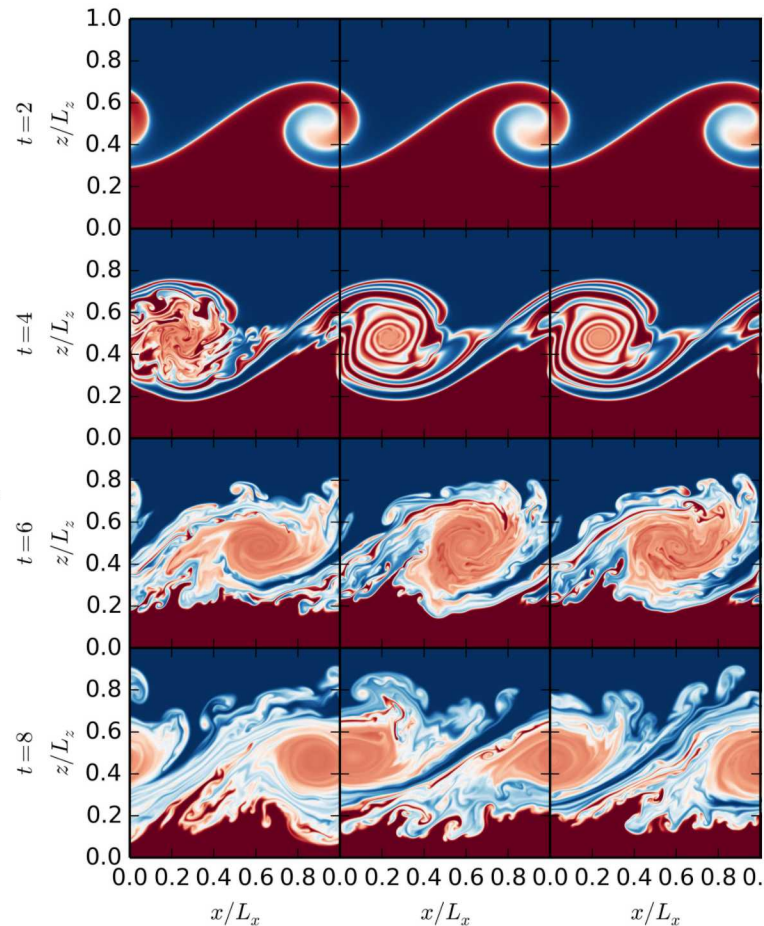


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Compare numerical schemes at fixed Reynolds # and a range of resolutions (Lecoanet et al., 2015):

- Linear growth compares well.
- Non-linear regime?



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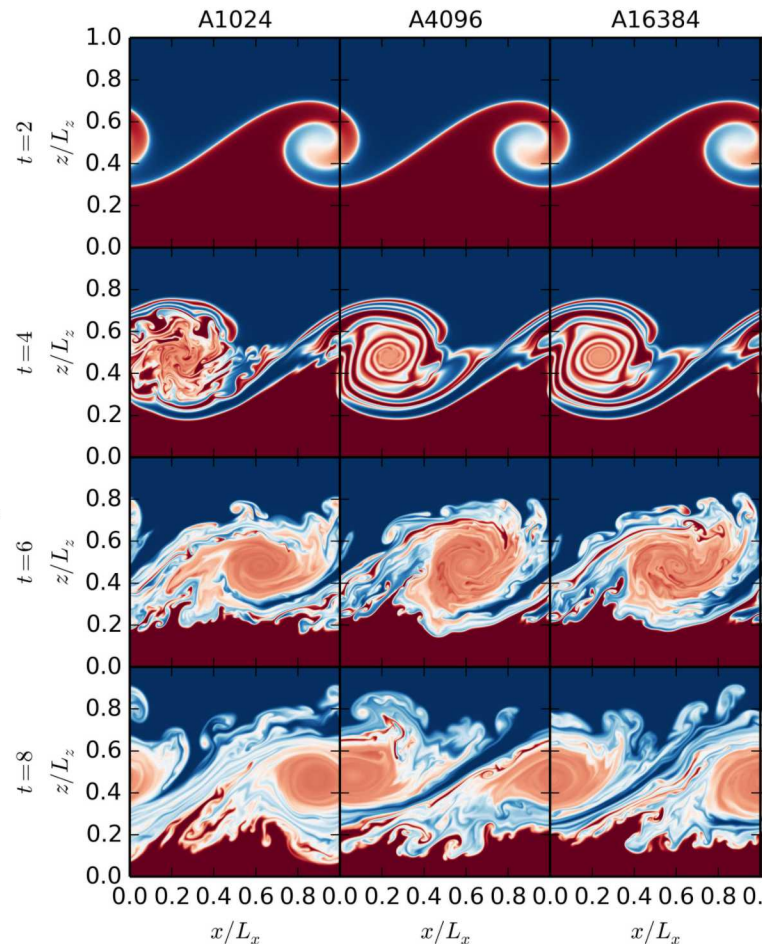


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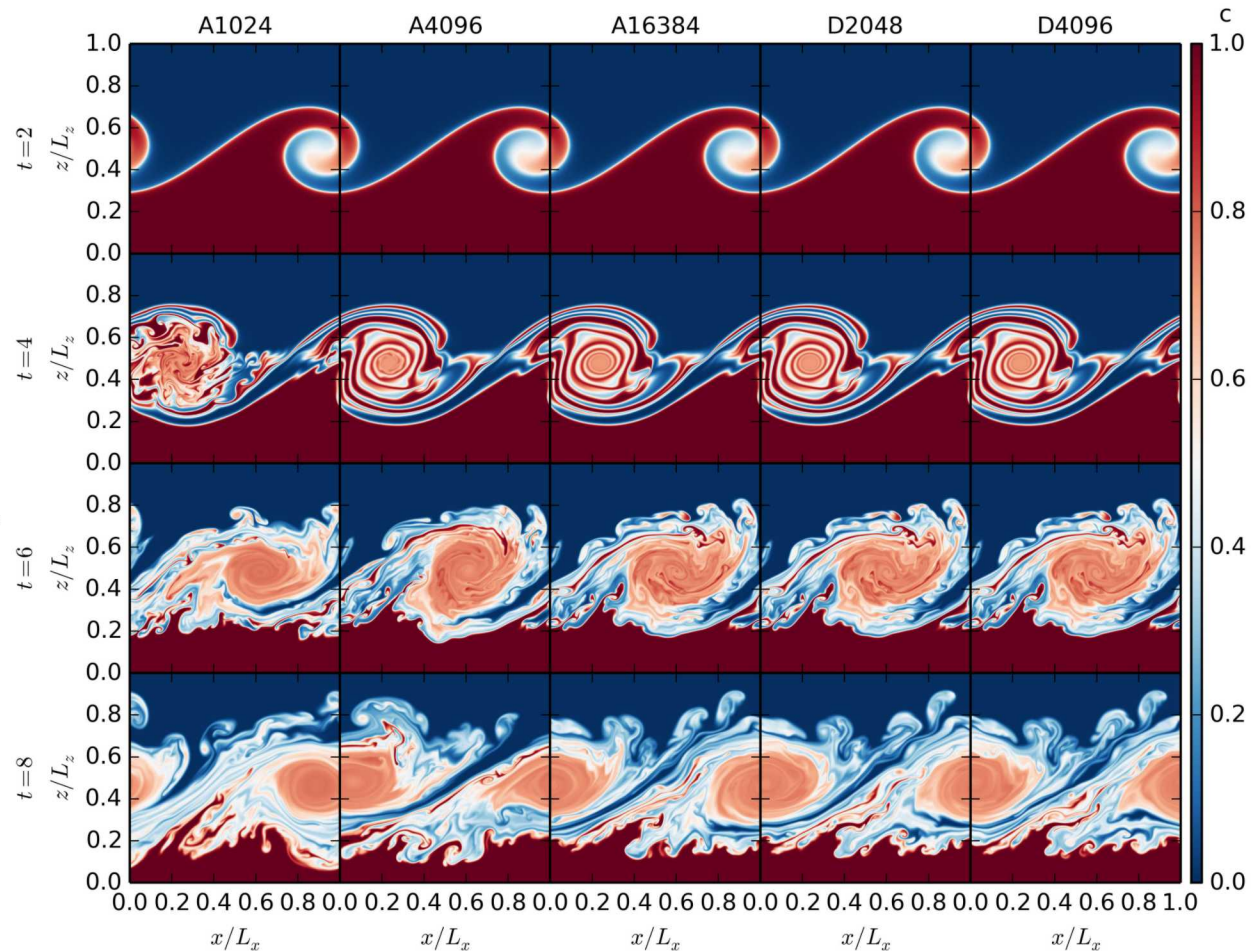


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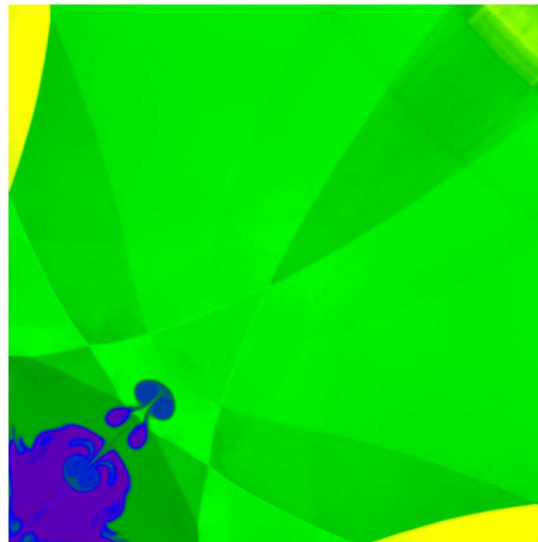
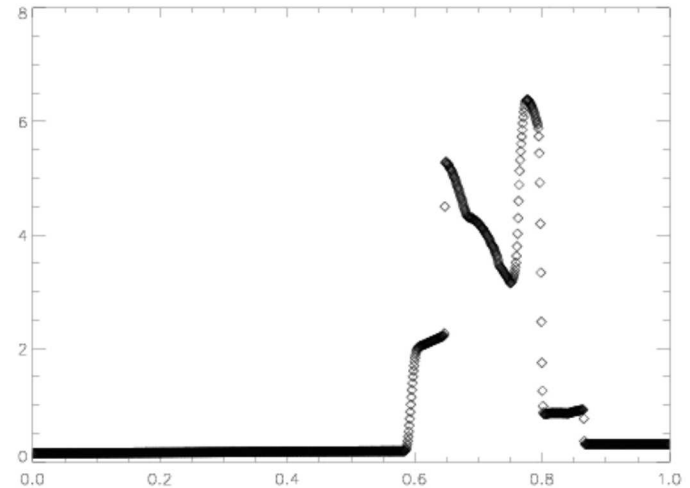
Examine convergence of sound waves in 1D/2D/3D:

- Excellent quantitative test of the accuracy and convergence of algorithm
- Sensitive to both diffusion and dispersion errors
- Very good at detecting coding bugs

Shock tubes:

- Examines codes ability to reproduce jump conditions
- Extend to multi-dimension: preservation of symmetry, allow measurement of numerical diffusivity through comparison to 1d tests

Are these tests sufficient?





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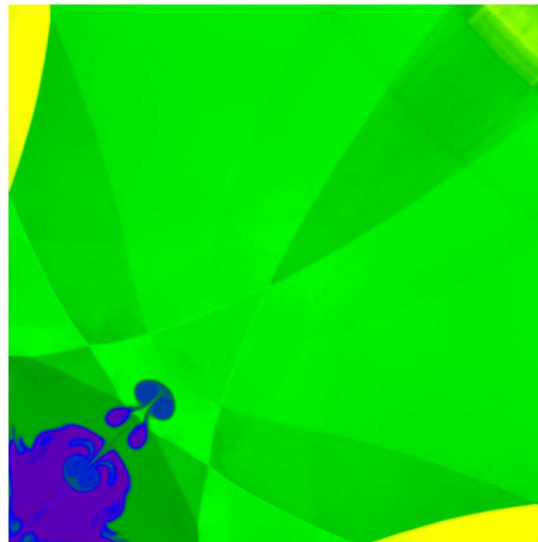
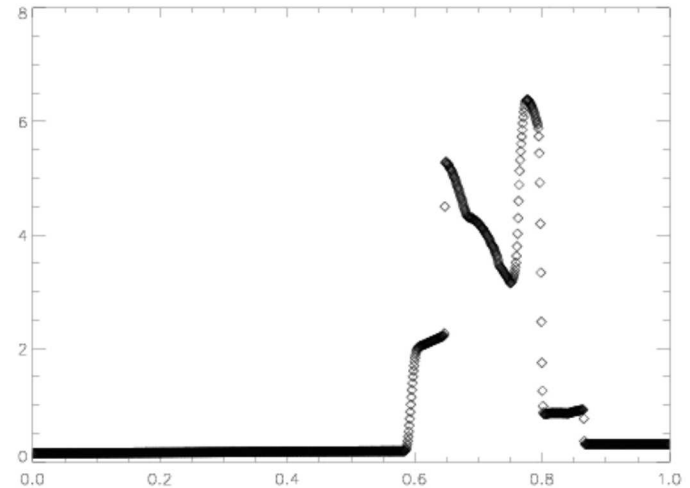
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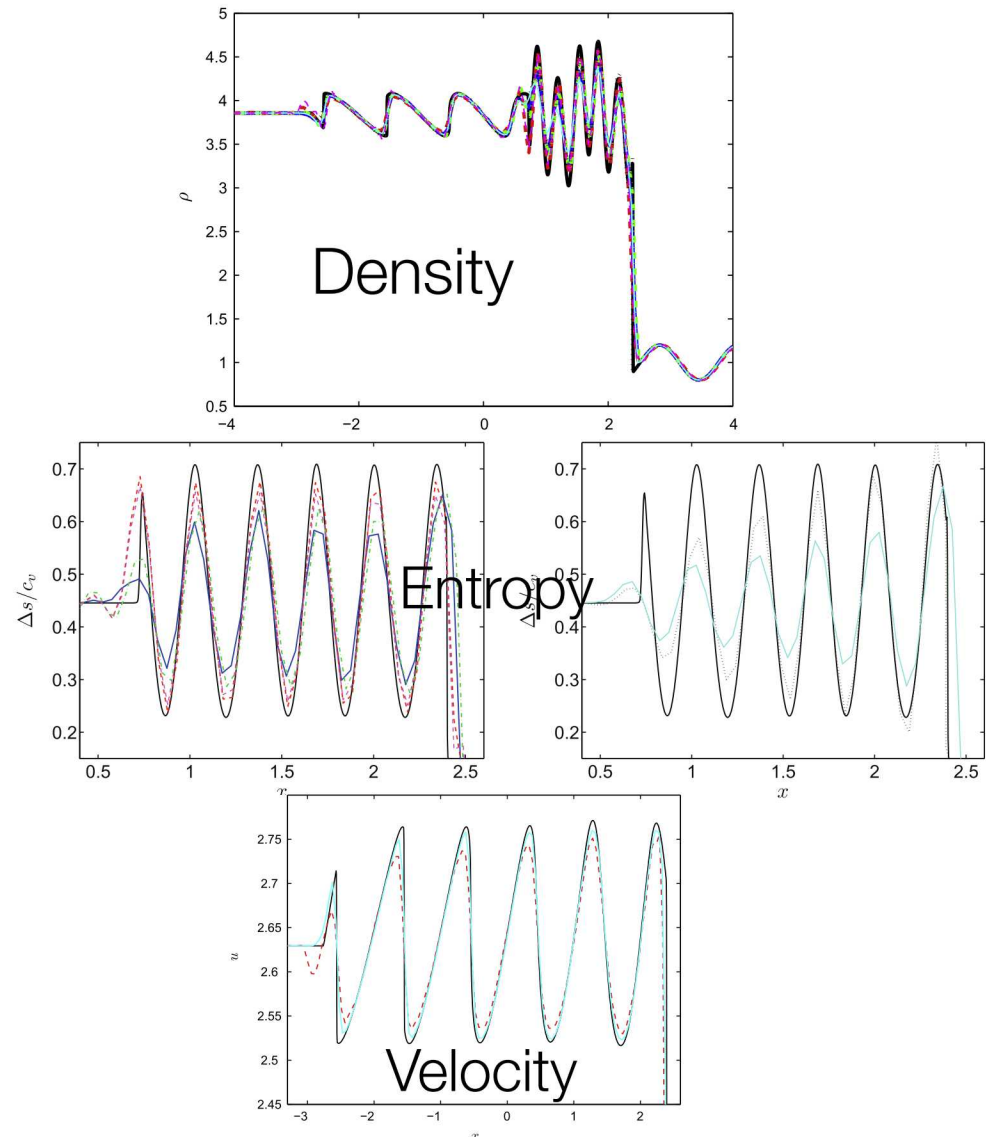


No: we want to understand how algorithms impact performance for ‘real scientific applications’

This kind of study has been performed by the compressible turbulence community, see Johnsen (2009); Kritsuk (2011)

Example: Shu-Osher problem

- 1D idealization of shock-turbulence interaction in which a shock propagates into a perturbed density field.
- Test the capability of an algorithm to accurately capture a shock wave, its interaction with an unsteady density field, and the waves propagating downstream of the shock.
- Allows probe of non-linear behavior of an algorithm on a well-defined problem.
- DG-based AV methods seem to under-resolve the interaction of the shock wave with the density field, even at high order (Yu et al. 2014)





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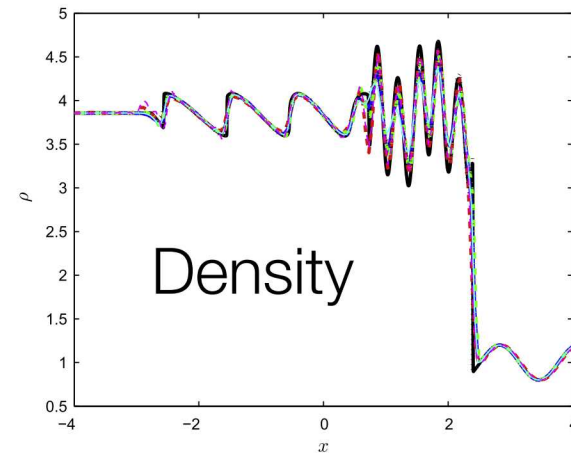
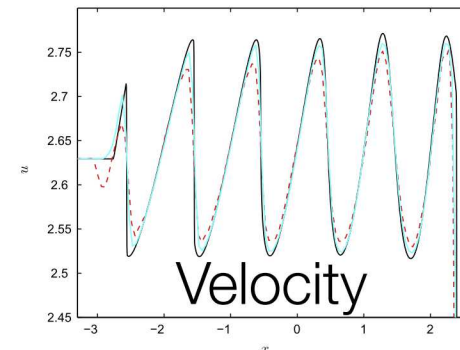


Table 1

Estimated number of operations required to compute the convective terms per grid point per Runge-Kutta substep. The order of accuracy of the central difference and WENO schemes are included in parentheses. For the *Stan* codes, the 11 Runge-Kutta evaluations march the solution forward by two time steps. For the *ADPDIS3D* code, the spatial central base scheme is employed at every Runge-Kutta substep, but the WENO filter step is only employed after the completion of the full time step.

Code	# RK eval.	# Derivative eval. (1st and 2nd)	# Ops/grid point
<i>Stan</i>	11/2	24 and 42	1900
<i>Stan-I</i>	11/2	24 and 42	1900
Central difference (6)	4	33 and 0	1100
Central difference (8)	4	33 and 0	1600
WENO (5)	4	15 and 0	3100
WENO (7)	4	15 and 0	6200





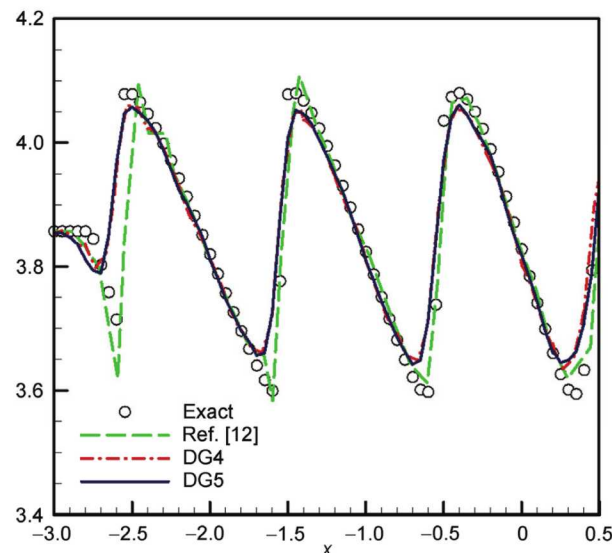
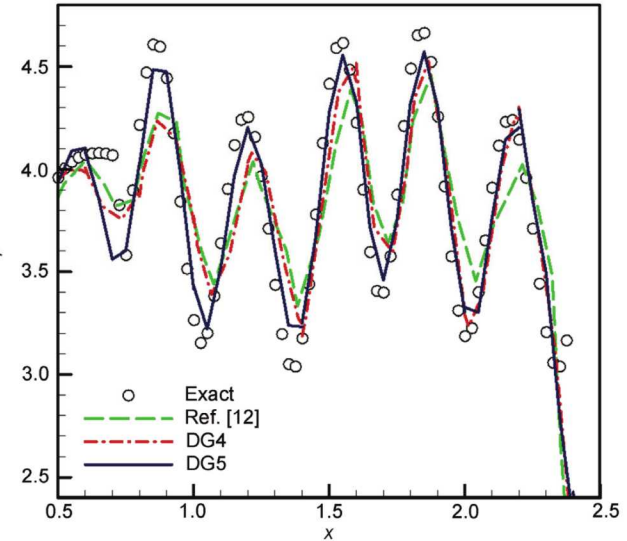
We want to understand how algorithms impact performance for ‘real scientific applications’.

This kind of study has been performed by the compressible turbulence community, see Johnsen et al. (2009); Kritsuk et al. (2011)

Example: Shu-Osher problem

- 1D idealization of shock-turbulence interaction in which a shock propagates into a perturbed density field.
- Test the capability of an algorithm to accurately capture a shock wave, its interaction with an unsteady density field, and the waves propagating downstream of the shock.
- Allows probe of non-linear behavior of an algorithm on a well-defined problem
- DG-based AV methods seem to under-resolve the interaction of the shock wave with the density field, even at high order (Yu et al. 2014)

How many
ops. per grid
point?





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Example: Shu-Osher problem

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- Test the capability of an algorithm to accurately capture a shock wave, its interaction with an unsteady density field, and the waves propagating downstream of the shock.
- Allows probe of non-linear behavior of an algorithm on a well-defined problem
- For smooth flows, nodal DG methods appear to have larger L2 errors than equivalent order FV schemes and requires more DoF (Noguiera et al. 2009)

6.1.3. Results Figure 10 presents a comparison of the convergence performance of the analyzed discretizations. The L_2 errors and convergence rates are broken down in tables V, VI and VII

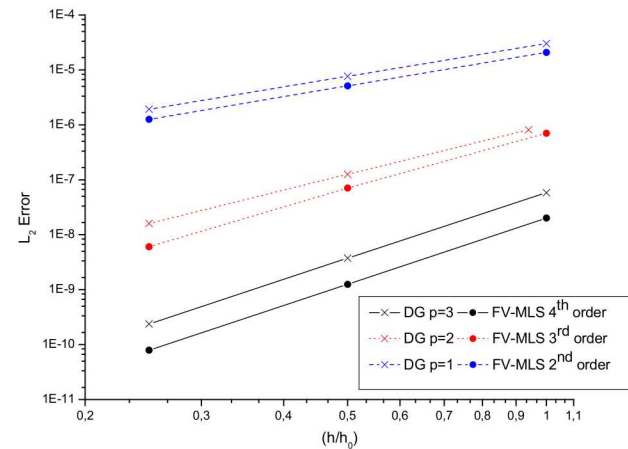


Figure 10. Convergence comparison for different reconstruction/polynomial orders

h/h_0	4 th order					
	dofs DG	Error DG	Order DG	dofs FV-MLS	Error FV-MLS	Order FV-MLS
1	1600	5.80 E-08	-	900	2.02 E-08	-
0.5	6400	3.75 E-09	3.95	3600	1.25 E-09	4.01
0.25	25600	2.38 E-10	3.98	14400	7.89 E-11	3.99

Table V. Convergence rates for the Ringleb flow and fourth order discretizations.

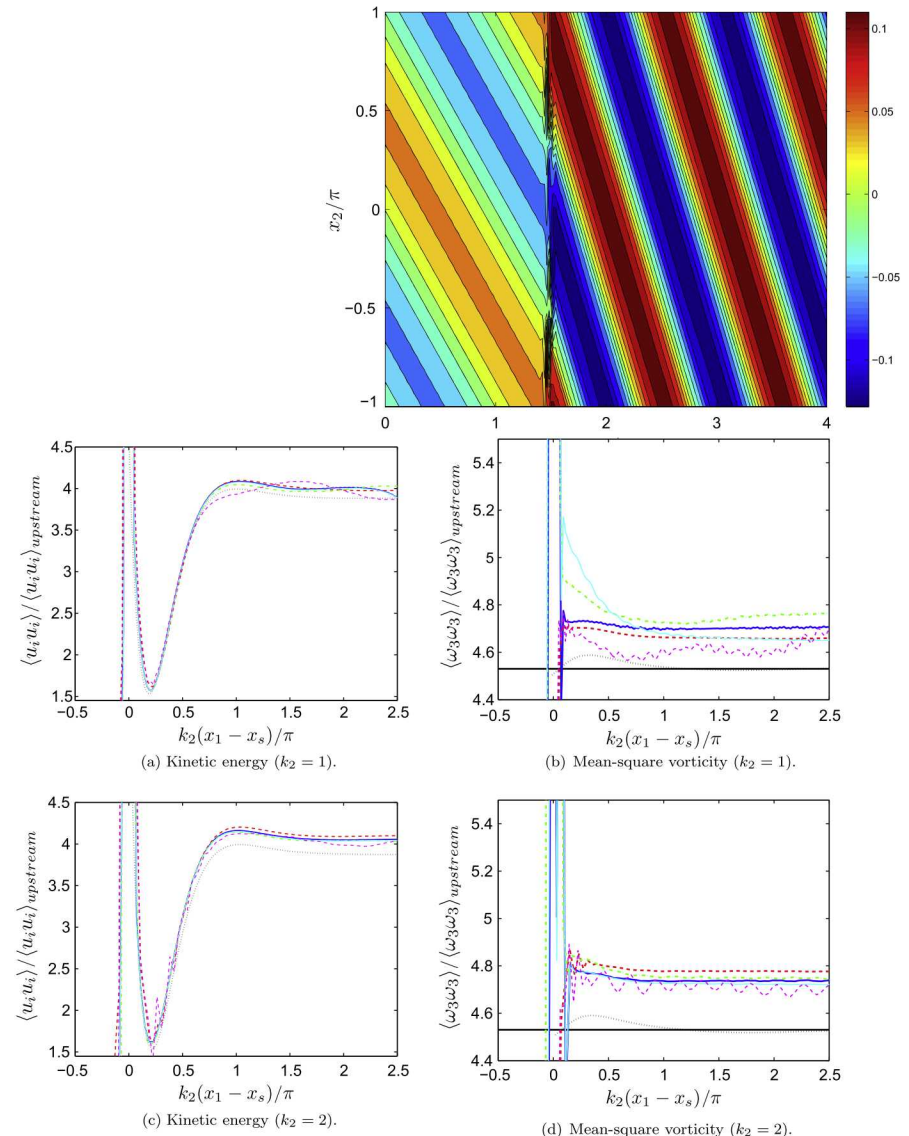


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Example: Shock-vorticity/entropy wave interaction

- Generalization of the Shu–Osher problem to two-dimensions.
- Interaction of a vorticity/entropy wave with a normal shock
- Reveal algorithmic sensitivities to multi-dimensional effects.
- For sufficiently large amplitudes of incidence, significant post-shock oscillations can be produced that are a numerical artifact



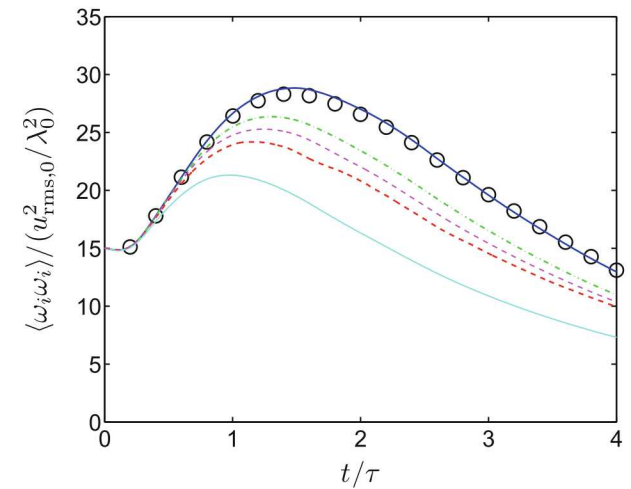


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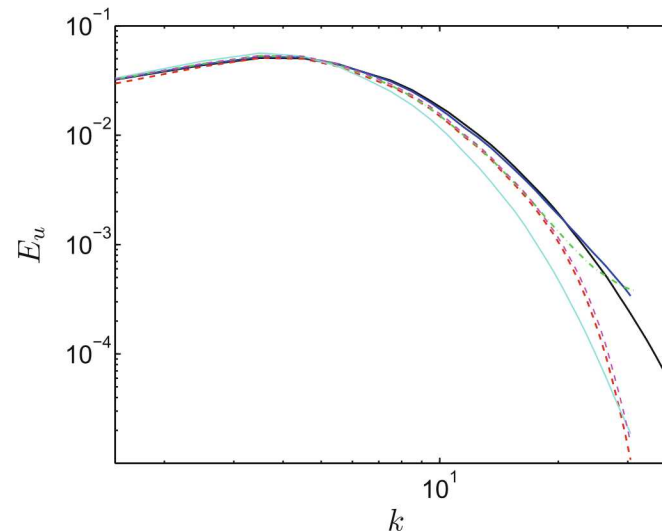
This kind of study has been performed by the compressible turbulence community, see Johnsen (2009); Kritsuk (2011)

Example: Decay of compressible isotropic turbulence

- Probe methods ability to handle ‘randomly’ distributed shocklets as well as the accuracy for broadband motions in the presence of shocks.
- Measurements of large scale flow properties (e.g. enstrophy) and power spectra allow for detailed comparison between performance of the numerical methods
- DG computations of similar problems appear to show existence of small-scale bottlenecks c.f. reference DNS computations



(b) Enstrophy.





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