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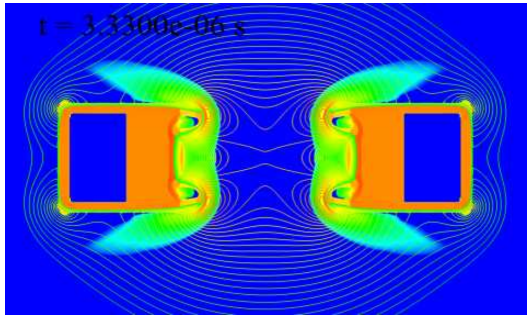


# An ALE Approach to XMHD

Duncan A. McGregor and Allen C. Robinson

Computational Multiphysics

Sandia National Laboratories

MultiMat 2017

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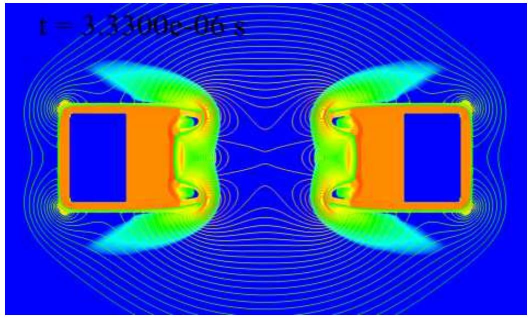


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ARL

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# Acknowledgements

E. Love for consultation on Predictor Corrector and R3D

R. Quadros for consultation on R3D

T. Mattsson for supporting this work

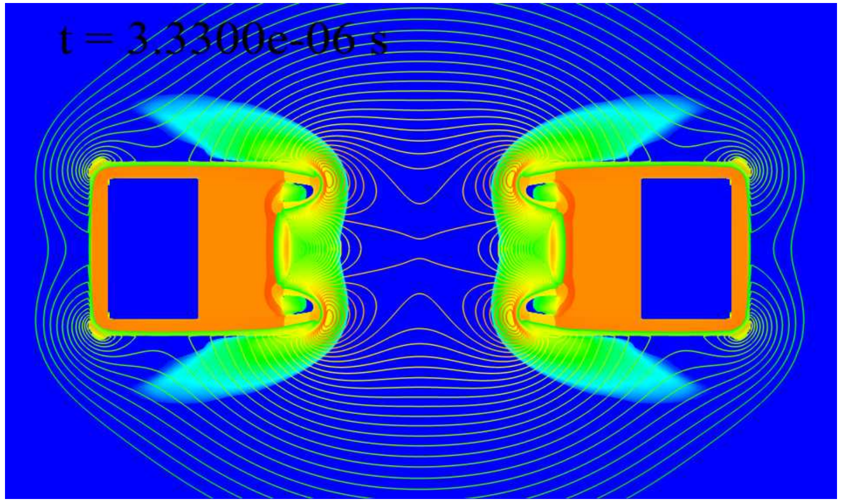
# Z Science with ALEGRA

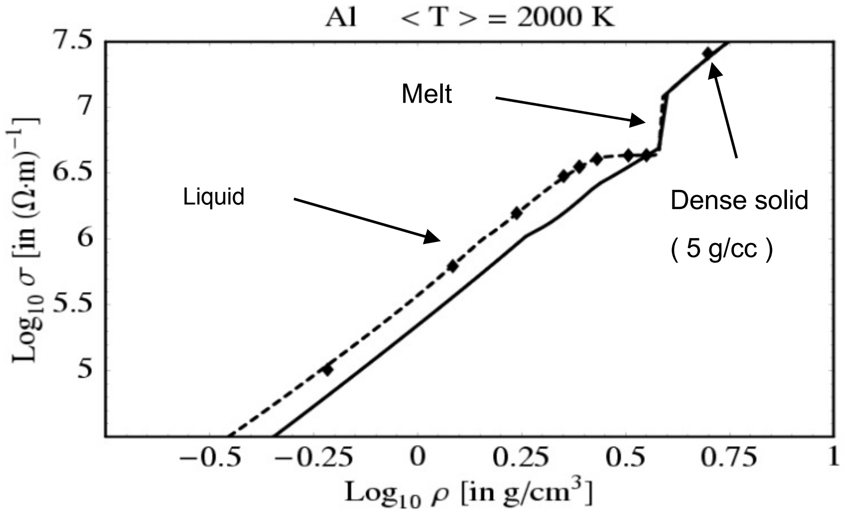
1. Using DFT models to produce material properties for ALEGRA in conjunction with appropriate circuit coupled magnetohydrodynamic (MHD) models, predictive design of Z dynamic materials experiments was enabled.

2. This was a clear demonstration that multiscale physics modeling could be extremely effective.

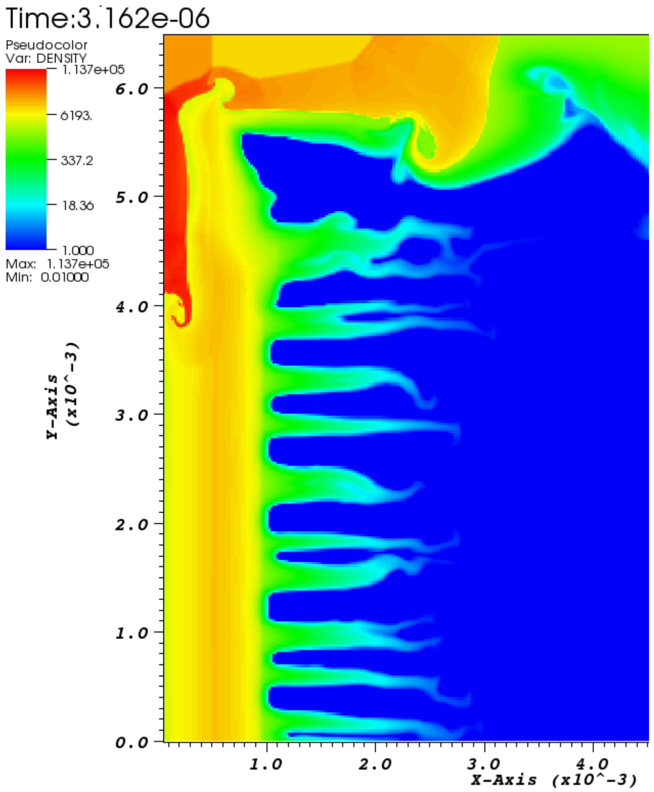
3. In the warm dense matter regime ALEGRA is a powerful tool for simulating MHD physics

**2D Simulation Plane of Two-sided Strip-line (Lemke)**



# However, Low Density Regions Matter




"Eddy" experiment on stagnation: the current flow in low density regions affects the dynamics

Source: Peterson & Mattson

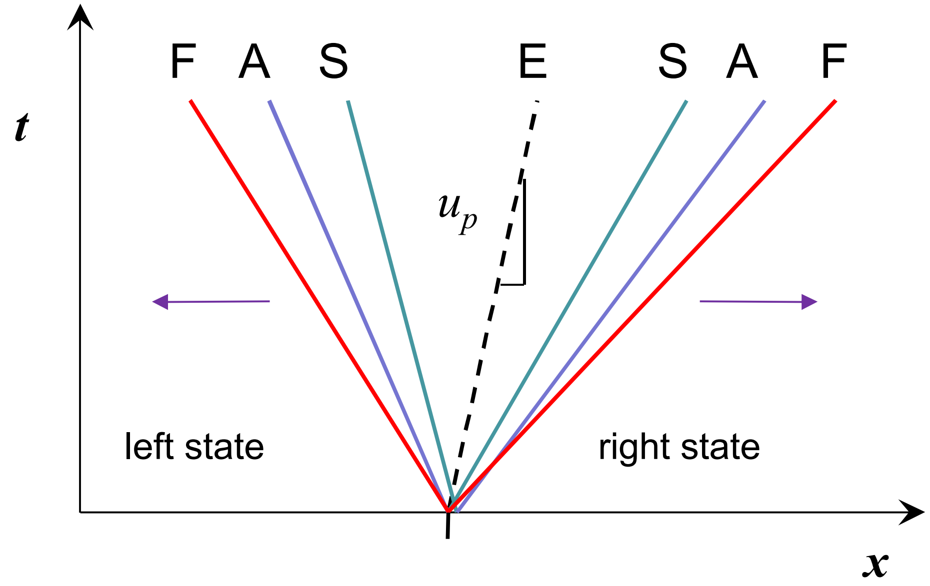
- Current density and forces in low density regions have significant effects on the physics.
- To make ALEGRA work in low density regions we presently require many "knobs"
  - i.e. density and conductivity floors, Lorentz force ceilings, etc which have to be chosen by an analysist to produce *reasonable results*
  - *How do we know the results are reasonable if expert judgement is necessary to assign values?*
- *The standard MHD model has issues…*
- We have MHD and EM propagation behavior. We need a better set of equation options.

# Computational Problems Issues with MHD

- Operator splitting requires an ideal MHD step
- Ideal MHD step requires a positive density

$$\left(u, u \pm \sqrt{\alpha^2 + \frac{|\mathbf{B}|^2}{\mu\rho}}\right)$$

- Magnetic diffusion step requires a positive conductivity even in "void"
- We care about resolving physics in low density regions.
- We have an explicit Lagrangian step which depends on fast magnetosonic speeds!




**To push beyond the warm dense region we will require more physics! Maxwell-Ampere and Generalized Ohm's Law**

# The Physicist's Answer: Add More Physics

- Stagnation experiments for MagLif do not capture torsion at stagnation caused by the Hall Effect.
- MHD assumptions don't hold in low density regions so maybe we shouldn't assume them.
  - Do not neglect displacement currents
- Generalized Ohm's Law starts from change of variables of the from the Two Fluid system
- Without additional assumptions the system is equivalent to the two fluid system.
  - People often assume *at least*
    - $m_e \ll m_\alpha$ » and quasi neutrality

$$\dot{\rho} = -\rho \mathrm{div}\mathbf{v}$$
$$\rho\dot{\mathbf{v}} = \mathrm{div}\mathbb{T} + q\mathcal{E} + \mathcal{J} \times \mathbf{B}$$
$$\overset{\star}{\mathbf{B}} = -\mathbf{curl}\ \mathcal{E}$$
$$\overset{\star}{\mathbf{D}} + \mathcal{J} = \mathbf{curl}\mathcal{H}$$
$$\dot{\mathbf{J}} + \mathbf{J}\mathrm{div}\mathbf{v} = \mathrm{div}\mathbb{T}_J + \epsilon\omega_p^2(\mathcal{E} - \sigma^{-1}\mathcal{J}) + \frac{e}{m_e}\mathcal{J} \times \mathbf{B}$$
$$\mathrm{div}\mathbf{D} = q$$
$$\mathrm{div}\mathbf{B} = 0$$
$$\mathcal{E} = \mathbf{E} + \mathbf{v} \times \mathbf{B}$$
$$\mathcal{H} = \mathbf{H} - \mathbf{v} \times \mathbf{D}$$
$$\mathcal{J} = \mathbf{J} - q\mathbf{v}$$
$$\overset{\star}{\mathbf{B}} = \partial_t\mathbf{B} - \mathbf{curl}\ \mathbf{v} \times \mathbf{B}$$
$$\overset{\star}{\mathbf{D}} = \partial_t\mathbf{D} - \mathbf{curl}\ \mathbf{v} \times \mathbf{D} + q\mathbf{v}$$

The Eulerian DG code PERSEUS (Seyler of Cornell, Martin of SNL, et al.) has very promising results using these physics.

# An incremental increase in complexity

- Instead of considering the full generalized Ohm's law to begin with we started slightly simpler.
- Some people refer to the system as a single fluid plasma.
- We have been floating the name Maxwell Hydrodynamics or Full Maxwell Hydrodynamics

- Does not neglect displacement currents
- Assumes classical Ohm's law.

$$\dot{\rho} = -\rho \operatorname{div} \mathbf{v}$$
$$\rho \dot{\mathbf{v}} = \operatorname{div} \mathbb{T} + q\mathcal{E} + \sigma \mathcal{E} \times \mathbf{B}$$
$$\overset{\star}{\mathbf{B}} = -\mathbf{curl}\ \mathcal{E}$$
$$\overset{\star}{\mathbf{D}} + \sigma \mathcal{E} = \mathbf{curl} \mathcal{H}$$

Attracted to the system because of desirable characteristic and dispersive properties for the linearization

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho\\u\\p\\E\\B\end{bmatrix} + \frac{\partial}{\partial x}\begin{pmatrix} u & \rho & & & \\ & u & \frac{1}{\rho} & & \\ & \rho\alpha^2 & u & & \\ & & & & c_0^2 \\ & & & 1 & \end{pmatrix}\begin{bmatrix}\rho\\u\\p\\E\\B\end{bmatrix} - \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sigma}{\rho}B & \frac{\sigma}{\rho}E \\ 0 & 0 & 0 & \sigma(\gamma-1)(2E-B) & -\sigma(\gamma-1)E \\ 0 & 0 & 0 & -\sigma & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}\begin{bmatrix}\rho\\u\\p\\E\\B\end{bmatrix} = \mathbf{0}$$

Characteristic Speeds $(\pm c, u, u \pm \alpha)$

Dispersion Relation $(\omega - ku)(\omega - k(u+\alpha))(\omega - k(u+\alpha))(\omega^2 + \mathrm{i}\frac{\sigma}{\epsilon_0}\omega - c_0^2 k^2) = 0$

# Deriving a Lagrangian Internal Energy Balance Law for Maxwell Hydro

**Kinetic Energy:** $\mathrm{U}_K = \frac{1}{2}\int_V \rho|\mathbf{v}|^2$

Kinetic energy can be found by dotting the momentum equation with **v,** integrating, and add scaling of mass equation.

$$\frac{d}{dt}\mathrm{U}_K = \int_V (q\mathbf{E} + \sigma\mathbf{E}\times\mathbf{B})\cdot\mathbf{v} - \mathbb{T} : \nabla\mathbf{v}\; dV + \int_{\partial V} \mathbb{T}\mathbf{v}\cdot dA$$

**Electromagnetic Energy:** $\mathrm{U}_{EM} = \frac{1}{2}\int_V \epsilon|\mathbf{E}|^2 + \mu^{-1}|\mathbf{B}|^2$

Start with the frame invariant Poynting theorem

$$\overset{\star}{\mathbf{B}}\cdot\mathcal{H} + \overset{\star}{\mathbf{D}}\cdot\mathcal{E} + \mathcal{J}\cdot\mathcal{E} + \mathrm{div}\mathcal{E}\times\mathcal{H} = 0$$

$$\frac{d}{dt}\mathrm{U}_{EM} = -\int_V \sigma|\mathcal{E}|^2 + (q\mathbf{E} + \sigma\mathbf{E}\times\mathbf{B})\cdot\mathbf{v}dV - \int_{\partial V} \mathbb{T}_{EM}\mathbf{v} + \mathcal{E}\times\mathcal{H}\cdot dA$$

Integrate and expand terms *very* carefully.
This is not as easy as it looks.

$$\frac{d}{dt}\mathrm{U}_I = \int_V \mathbb{T} : \nabla\mathbf{v} + \sigma|\mathcal{E}|^2 + \rho s\; dV - \int_{\partial V} q\cdot dA$$

**Internal Energy:** $\mathrm{U}_I = \int_V \rho\varepsilon$

We assume its balance law cancels all remaining internal contributions (Joule heating and mechanical work)

This work extends a similar calculation by Robinson for Ideal/Resistive MHD but the application to Full Maxwell systems is new

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Mechanical Work

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Lorentz Force Work

Mechanical Work

$$\frac{d}{dt}\mathrm{U}_{EM} = -\int_V \sigma|\mathcal{E}|^2 + \boxed{(q\mathbf{E} + \sigma\mathbf{E}\times\mathbf{B})\cdot\mathbf{v}}\, dV - \int_{\partial V} \mathbb{T}_{EM}\mathbf{v} + \mathcal{E}\times\mathcal{H}\cdot dA$$

$$\frac{d}{dt}\mathrm{U}_I = \int_V \boxed{\mathbb{T} : \nabla\mathbf{v}} + \sigma|\mathcal{E}|^2 + \rho s\, dV - \int_{\partial V} q\cdot dA$$

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Mechanical Work

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Joule Heating

$$\frac{d}{dt}\mathrm{U}_I = \int_V \boxed{\mathbb{T} : \nabla\mathbf{v}} + \boxed{\sigma|\mathcal{E}|^2} + \rho s\, dV - \int_{\partial V} q\cdot dA$$

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# ALEGRA's Resistive MHD Time integration

1. Predictor Corrector for Hydrodynamics/Ideal MHD
2. Split out diffusion solves and joule heating

Hydro

$$
\begin{cases}
\rho_{(i)}^{n+1/2}\mathbf{u}_{(i+1)}^{n+1} = \mathbf{u}^n - \Delta t \nabla p_{(i)}^{n+1/2} \\
\mathbf{x}_{(i+1)}^{n+1} = \mathbf{x}^n + \Delta t \mathbf{u}_{(i+1)}^{n+1/2} \\
p_{(i+1)}^{n+1} = p^n - \Delta t \rho_{(i+1)}^{n+1/2} (\alpha_{(i+1)}^{n+1/2})^2 \operatorname{div} \mathbf{u}_{(i+}^{n+} \\
\rho_{(i+1)}^{n+1} = \rho^n - \Delta t \rho_{(i+1)}^{n+1/2} \operatorname{div} \mathbf{u}_{(i+1)}^{n+1/2}
\end{cases}
$$

Ideal MHD

$$
\begin{cases}
\rho_{(i)}^{n+1/2}\mathbf{u}_{(i+1)}^{n+1} = \mathbf{u}^n - \Delta t \left( \nabla p_{(i)}^{n+1/2} - \mu^{-1} \operatorname{curl} \mathbf{B}_{(i)}^{n+1/2} \times \mathbf{B}_{(i)}^{n+1/2} \right) \\
\mathbf{x}_{(i+1)}^{n+1} = \mathbf{x}^n + \Delta t \mathbf{u}_{(i+1)}^{n+1/2} \\
p_{(i+1)}^{n+1} = p^n - \Delta t \rho_{(i+1)}^{n+1/2} (\alpha_{(i+1)}^{n+1/2})^2 \operatorname{div} \mathbf{u}_{(i+1)}^{n+1/2} \\
\rho_{(i+1)}^{n+1} = \rho^n - \Delta t \rho_{(i+1)}^{n+1/2} \operatorname{div} \mathbf{u}_{(i+1)}^{n+1/2} \\
\mathbf{B}_{(i+1)}^{n+1} = \mathbf{B}^n - \Delta t \left( \mathbf{B}_{(i+1)}^{n+1/2} \cdot \nabla \mathbf{u}_{(i+1)}^{n+1/2} - \mathbf{B}_{(i+1)}^{n+1/2} \operatorname{div} \mathbf{u}_{(i+1)}^{n+1/2} \right)
\end{cases}
$$

Magnetic Diffusion

$$
\begin{cases}
\mu\sigma \mathbf{E}^{n+1} + \Delta t \operatorname{curl}\operatorname{curl} \mathbf{E}^{n+1} = \operatorname{curl} \mathbf{B}^n \\
\mathbf{B}^{n+1} = \mathbf{B}^n - \Delta t \operatorname{curl} \mathbf{E}^{n+1} \\
\varepsilon^{n+1} = \varepsilon^n + \Delta t \sigma |\mathbf{E}^{n+1}|^2
\end{cases}
$$

- We discretize mass, magnetic flux, and energy using Reynold's Transport
- This is the equivalent Eulerian system

# 1D, Linear, Time Discrete stability analysis

Stability Analysis

1. Linearize the system
2. Reduce to 1 dimension
3. Fourier Transforms in space

Hydro

$$\begin{cases} u^{n+1}_{(i+1)} = u^n - \frac{\Delta t}{2\rho} \mathrm{i}k(p^{n+1}_{(i)} + p^n) \\ x^{n+1}_{(i+1)} = x^n + \frac{\Delta t}{2}(u^{n+1}_{(i+1)} + u^n) \\ p^{n+1}_{(i+1)} = p^n - \frac{\Delta t}{2} \mathrm{i}k\rho\alpha^2(u^{n+1}_{(i+1)} + u^n) \end{cases}$$

Ideal MHD

$$\begin{cases} u^{n+1}_{(i+1)} = u^n - \frac{\Delta t}{2\rho} \mathrm{i}k\left((p^{n+1}_{(i)} + p^n) + \mu^{-1} B_0(B^{n+1}_{(i)} + B^n)\right) \\ x^{n+1}_{(i+1)} = x^n + \frac{\Delta t}{2}(u^{n+1}_{(i+1)} + u^n) \\ p^{n+1}_{(i+1)} = p^n - \frac{\Delta t}{2} \mathrm{i}k\rho\alpha^2(u^{n+1}_{(i+1)} + u^n) \\ B^{n+1}_{(i+1)} = B^n - \frac{\Delta t}{2} \mathrm{i}k B_0(u^{n+1}_{(i+1)} + u^n) \end{cases}$$

4. Rewrite as matrix equations

$$\xi^{n+1}_{(i+1)} = \mathbb{A}_1 \xi^{n+1}_{(i)} + \mathbb{A}_0 \xi^n \qquad \xi^{n+1}_{(2)} = \mathbb{A}\xi^n, \quad \mathbb{A} = \mathbb{A}_0 + \mathbb{A}_1(\mathbb{A}_0 + \mathbb{A}_1)$$

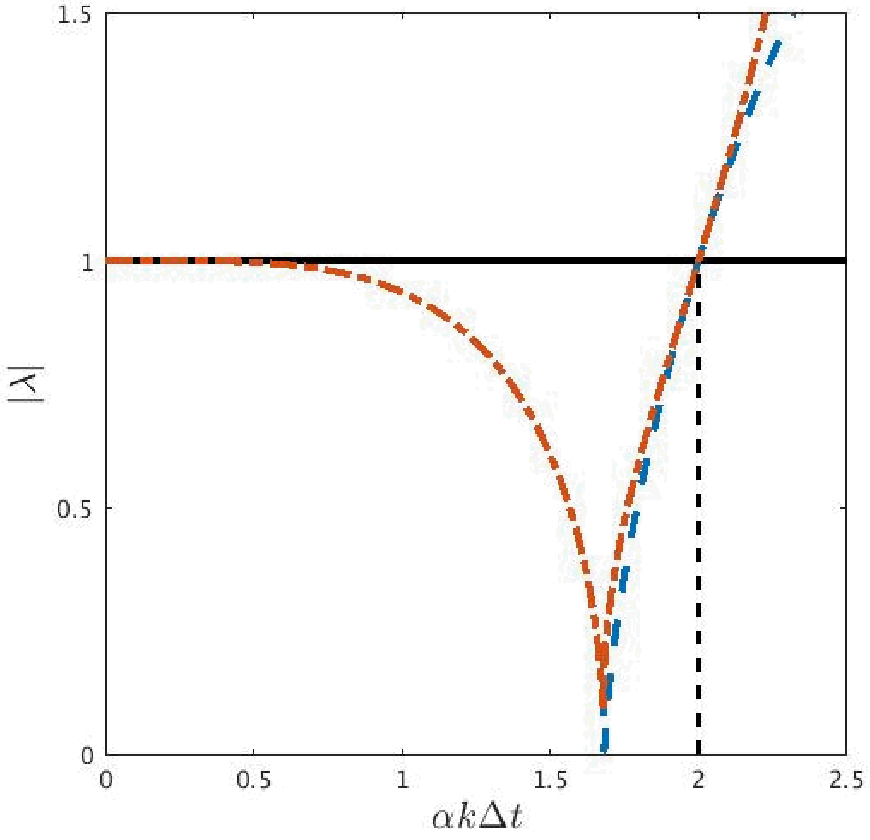
5. Spectral radius of $\mathbb{A}$ less than 1 implies stability
6. Largest wave number supported lowest order FEM is

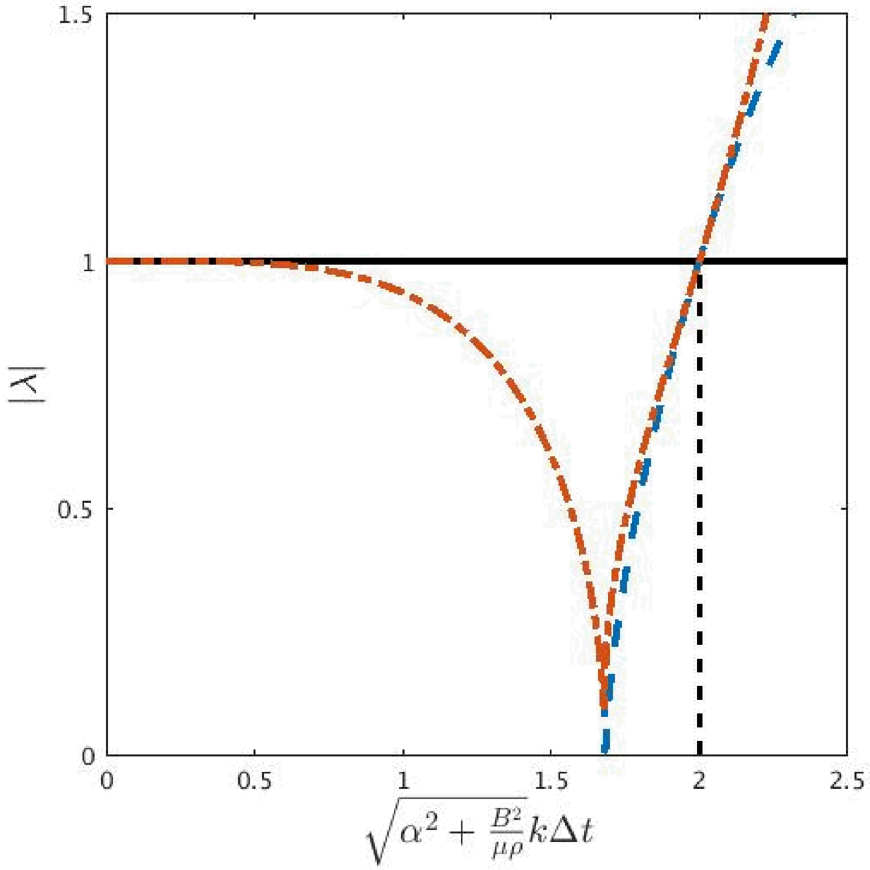
$$k_{\max} = \frac{1}{2h}$$



This reproduces and extends the analysis found Love, Rider, and Scovazzi, J. Comput. *Phys.* 228.20 (2009): 7543-7564.

# Stability of Predictor Corrector




Note similar stability bounds involving the speed of sound and fast magnetosonic speed for predictor corrector.

# Magnetic Diffusion

$$\int \sigma \mathbf{E}^{n+1} \cdot \boldsymbol{\Phi} + \Delta t \mu^{-1} \,\mathbf{curl}\,\mathbf{E}^{n+1} \cdot \mathbf{curl}\,\boldsymbol{\Phi} \; dV = \int \mu^{-1} \mathbf{B}^{n} \,\mathbf{curl}\,\boldsymbol{\Phi} \; dV$$

$$\mathbf{B}^{n+1} = \mathbf{B}^{n} - \Delta t \,\mathbf{curl}\,\mathbf{E}^{n+1}$$

1. Compatible discretization, **E** on edges and **B** on faces
2. Implicit Euler and solve for **E**
3. Update **B** using the strong compatible curl

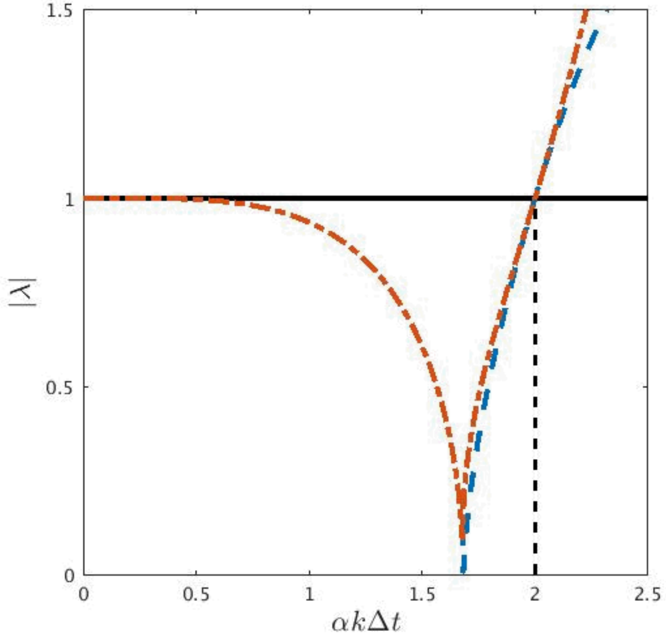
4. Most of this problem really boils down to preconditioning the matrix system

$$\frac{\sigma}{\Delta t} \mathbb{M}_{\mathcal{E}} + \mu^{-1} \,\mathbf{curl}_h^T \,\mathbb{M}_{\mathcal{F}} \,\mathbf{curl}_h$$

5. When $\frac{\sigma}{\Delta t} \ll 1$ large null space makes the system very ill conditioned but this large null space is necessary!

# Predictor Corrector for Maxwell Hydrodyanmics

$$
\begin{aligned}
&(\tfrac{\epsilon}{\Delta t} + \sigma)E^{n+1}_{(i+1)} - \tfrac{\Delta t}{\mu}\mathrm{curl}B^{n+1}_{(i+1)} = \tfrac{\epsilon}{\Delta t}E^n \\
&B^{n+1}_{(i+1)} + \Delta t\mathrm{curl}E^{n+1}_{(i+1)} = B^n \\
&\rho_0 v^{n+1}_{(i+1)} = \rho_0 v^n - \Delta t\nabla p^{n+1/2}_{(i)} + \Delta t(q_0 E^{n+1/2}_{(i+1)} + \sigma E^{n+1/2}_{(i+1)} \times B^{n+1/2}_{(i+1)}) \\
&x^{n+1}_{(i+1)} = x^n + \Delta t v^{n+1/2}_{(i+1)} \\
&p^{n+1}_{(i+1)} = p^n - \Delta t\rho_0\alpha^2\mathrm{div}v^{n+1/2}_{(i+1)} + \Delta t\sigma\gamma|E^{n+1/2}_{(i+1)}|^2
\end{aligned}
$$

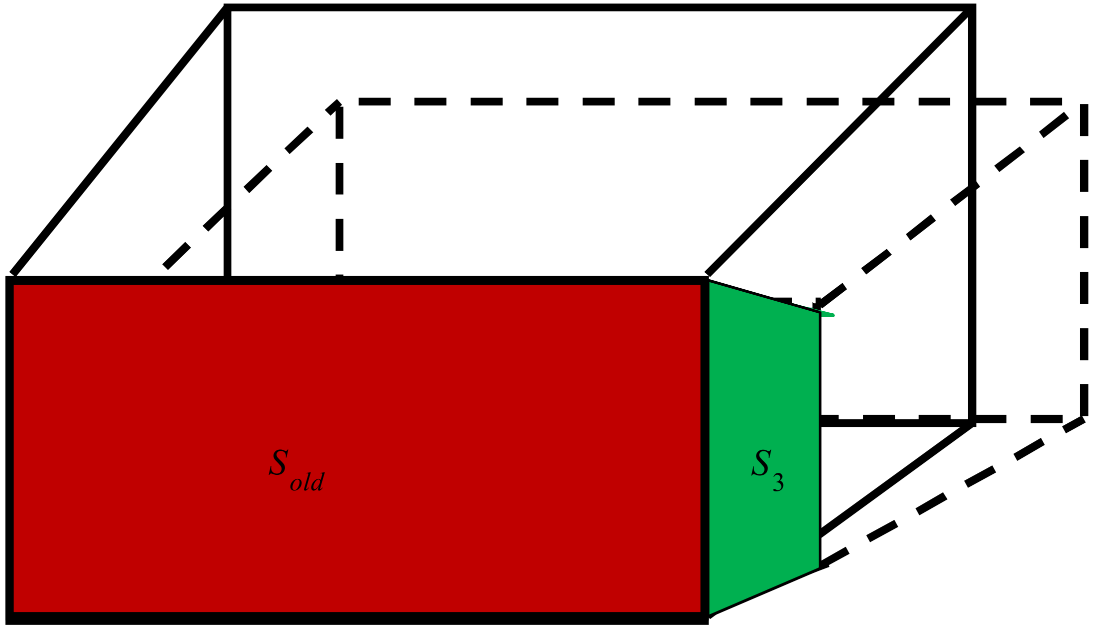



- Operator splitting a la ALEGRA MHD leads to an **unstable** system.
- An implicit field solve in the Lagrangian step recovers **hydro stability limit!**
- Requires two fields solves on the **Lagrangian Mesh!**
- **Electric Displacement flux** is the Galilean Invariant. Simplest approach requires discrete Hodge Starr.

Seems very similar to IMEX (e.g. SSP(2,2,2))
2D von Neumann analysis seems prudent

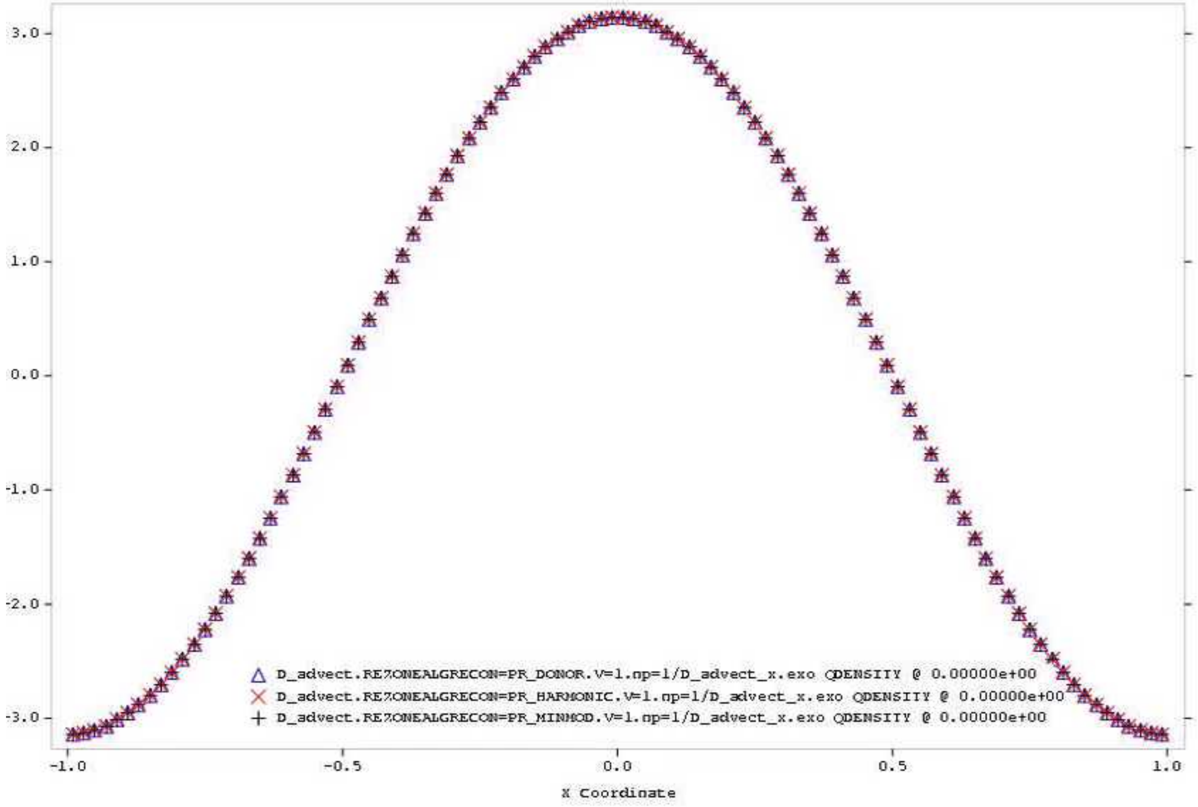
# 2-Form remap

$$\frac{\partial \mathbf{D}}{\partial t} + \boxed{\nabla \times (\mathbf{D} \times \mathbf{v})} + \boxed{\mathbf{v}(\nabla \cdot \mathbf{D})}$$




New electric displacement flux is the oriented sum of swept edge contributions which do not change the charge plus swept volume contributions which do. This is simply the divergence theorem (generalized Stoke's theorem).

# Face Element Remap Results




Harmonic
Minmod
Donor – Low Order

- A high order volume remap contribution for face element has been implemented.
- The volume contribution is associated with the through-face flux rather than the flux passing through the swept-edge faces in the standard div free CT algorithm.
- Below comparison of low and high order remap of charge density. Note much reduced charge diffusion for high order algorithms.

# Discrete Maxwell's Equations with a Hodge Star

Electric Displacement **(D)** is really the frame invariant of the system for Galilean invariant Maxwell.
We have preconditioners for (M + curl curl) systems:

$$\int_\Omega \left(\tfrac{\epsilon}{\Delta t} + \sigma\right) \mathbf{E}_h^{n+1} \cdot \boldsymbol{\Psi}_h + \tfrac{\Delta t}{\mu} \mathbf{curl} \mathbf{E}_h^{n+1} \cdot \mathbf{curl} \boldsymbol{\Psi}_h \, dV = \int_\Omega \mathbf{D}_h^{n+1} \cdot \boldsymbol{\Psi}_h + \tfrac{1}{\mu} \mathbf{B}_h^n \cdot \mathbf{curl} \boldsymbol{\Psi}_h \, dV \quad \forall \boldsymbol{\Psi}_h \in \mathcal{E}_h$$

$$\mathbf{B}_f^{n+1} = \mathbf{B}_f^n - \Delta t \sum_{e \in \partial f} o_{e,f} \mathbf{E}_e^{n+1}, \qquad \forall f \in \mathcal{F}$$

$$\int_\Omega \mathbf{D}_h^{n+1} \cdot \boldsymbol{\Phi}_h = \int_\Omega \epsilon \mathbf{E}_h^{n+1} \cdot \boldsymbol{\Phi}_h, \qquad \forall \boldsymbol{\Phi}_h \in \mathcal{F}_h$$

Is this method asymptotic preserving? Does it converge to a solution of Resistive diffusion?
**Simple Verification test for sanity:**

$$\mathbf{B}(t) = e^{-\frac{\pi^2}{\mu\sigma} t} (0, \sin(\pi x), 0)$$
$$\mathbf{D}(t) = \epsilon \frac{\pi}{\mu\sigma} e^{-\frac{\pi^2}{\mu\sigma} t} (0, 0, \cos(\pi x))$$

$$\Omega = [-\tfrac{3}{4}, \tfrac{3}{4}] \times [-1, 1] \times [-1, 1]$$
$$\mathbf{B}(0) = (0, \sin(\pi x), 0)$$
$$\mathbf{D}(0) = (0, 0, 0)$$
$$\mathbf{H} \times \mathbf{n}|_{x = \pm \frac{3}{4}} = \mu^{-1} e^{-\frac{\pi^2}{\mu\sigma} t} (0, \sin(\pi x), 0)$$
$$\mathbf{E} \times \mathbf{n}|_{y = \pm 1} = \frac{\pi}{\mu\sigma} e^{-\frac{\pi^2}{\mu\sigma} t} (0, 0, \cos(\pi x))$$
$$\mathbf{E} \times \mathbf{n}|_{z=1} = \mathbf{E} \times \mathbf{n}|_{z=-1}$$

# Results of Verification Problem: Errors and rates at final time

$\mathbf{B}$ Magnetic Flux Density

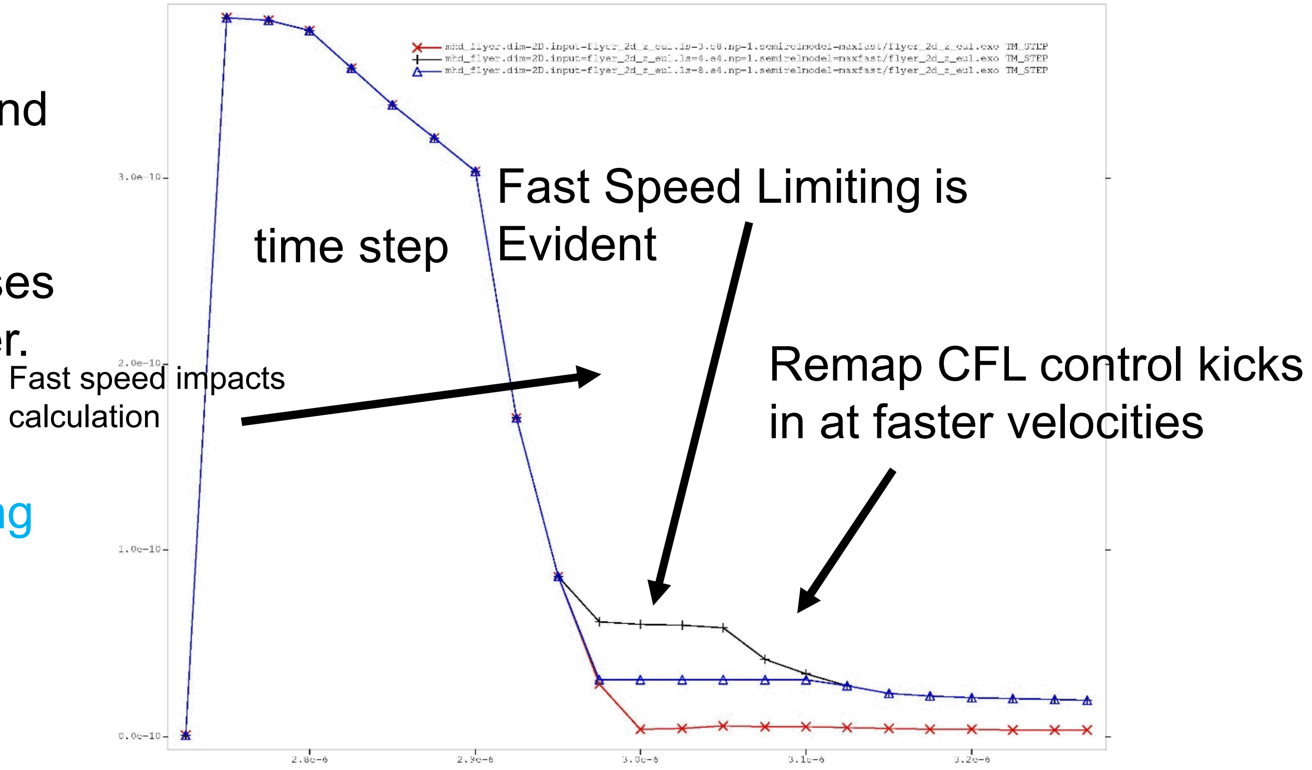
| h | Δt | RL∞ | Rate | RL1 | Rate | RL2 | Rate |
|---|---|---|---|---|---|---|---|
| 0.1000 | 1.00e-1 | 4.96e-01 | -- | 3.53e-01 | -- | 3.82e-01 | -- |
| 0.0500 | 0.25e-1 | 1.53e-01 | 1.69 | 1.08e-01 | 1.70 | 1.16e-01 | 1.70 |
| 0.0025 | 6.25e-2 | 4.06e-02 | 1.91 | 2.88e-02 | 1.91 | 3.10e-02 | 1.91 |
| 0.0125 | 1.56e-2 | 1.03e-02 | 1.97 | 7.31e-03 | 1.97 | 7.87e-03 | 1.97 |

$\mathbf{D}$ Electric Displacement

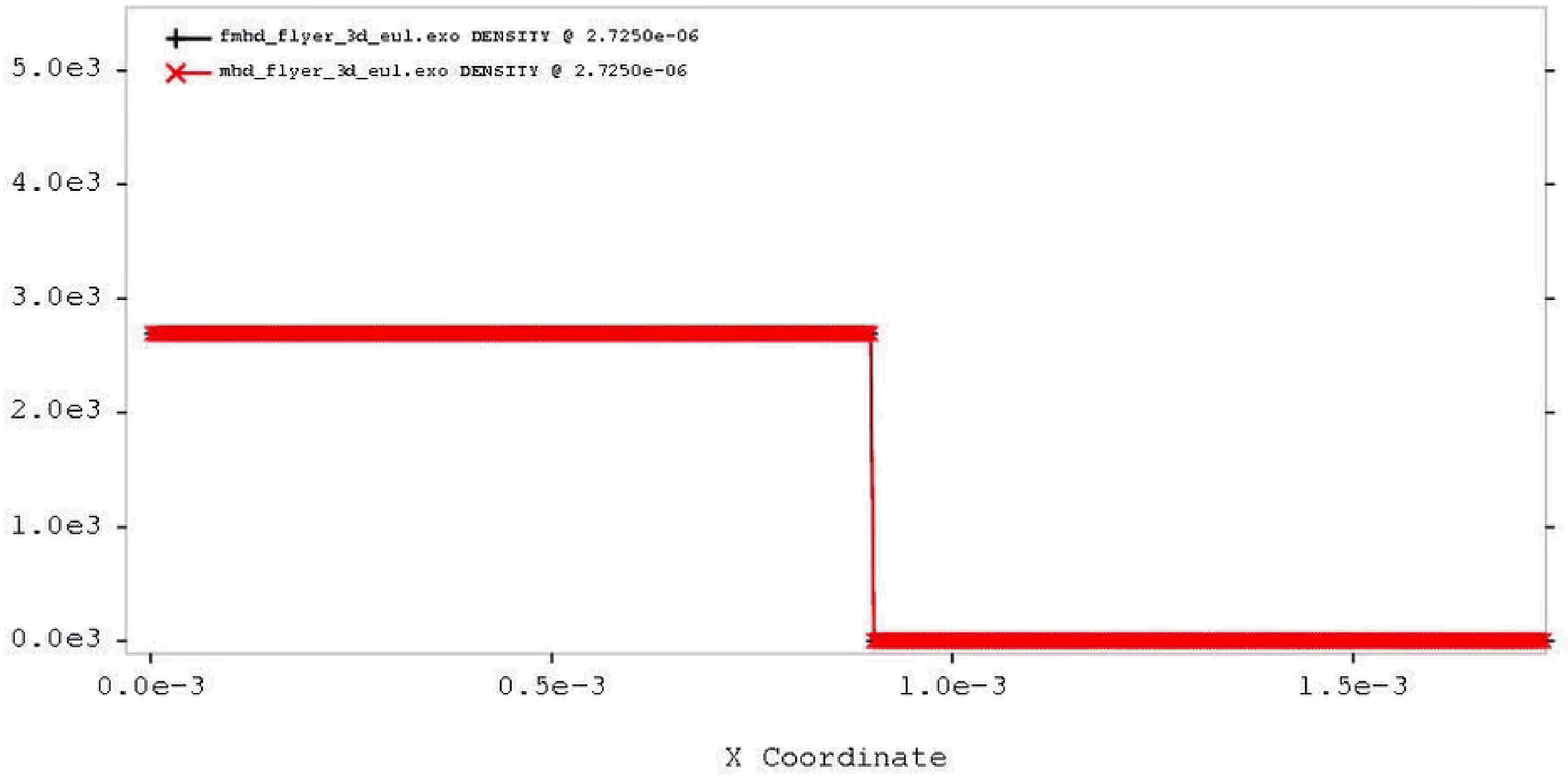
| h | Δt | RL∞ | Rate | RL1 | Rate | RL2 | Rate |
|---|---|---|---|---|---|---|---|
| 0.1000 | 1.00e-1 | 4.23e-01 | -- | 3.73e-01 | -- | 3.78e-01 | -- |
| 0.0500 | 0.25e-1 | 1.33e-01 | 1.66 | 1.18e-01 | 1.65 | 1.19e-01 | 1.67 |
| 0.0025 | 6.25e-2 | 3.56e-02 | 1.90 | 3.17e-02 | 1.89 | 3.18e-02 | 1.90 |
| 0.0125 | 1.56e-2 | 9.10e-03 | 1.98 | 8.07e-03 | 1.97 | 7.87e-03 | 1.97 |

# Synthesis: 1D Flyer Plates

- Prototype for a pulsed power Dynamic Materials Experiment.
- Traditionally solved with ALEGRA MHD
- Initial configuration of Aluminum (Tabular EOS and LMD conductivities) is accelerated by magnetic field push.
- Joule heating ablates the back surface and causes a stream of lower density plasma behind the flyer.
  - Alfvén velocity eats your lunch and the time step crashes if you do nothing
  - Previously could be circumvented by capping the Alfvén velocity and reducing forces



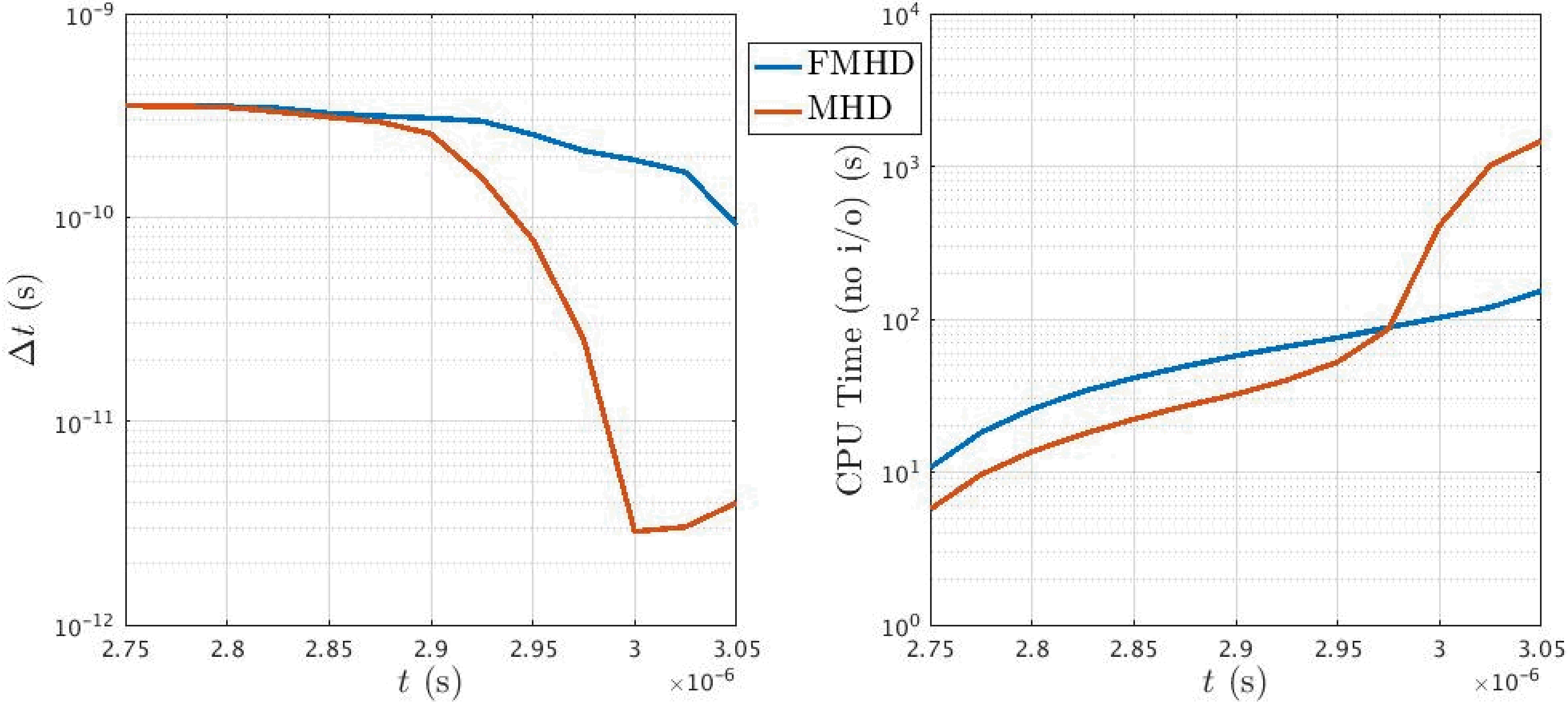
# Preliminary Results : The bad news




The answers on our **very first** test problem are not the same.

FMHD is essentially a research capability needs extensive V&V and more testing

# Preliminary Results : The good news




Predictor Corrector for FMHD is stable at hydrodynamic time steps

Despite requiring **2 ML** solves and **2 CG** solves results in an order of magnitude speed up compared to operator split resistive MHD.

# Closure

1. ALEGRA needs additional physics to meet the demands of next generation pulsed power systems (Z-Next)

2. Generalized Ohm's Law can be formulated in a frame invariant setting and is thus amenable to an ALE approach

3. Working with Maxwell Hydrodynamics we were able to eliminate Fast-Alfvén time step restrictions for more traditional Resistive MHD problems

4. Eliminating variables may make your equations harder to solve.

**Next Steps:**

1. Fix the current implementation and run a large number of ALEGRA-MHD calculations using FMHD.

2. How many low density kludges can be removed by using FMHD?

3. Can we modify SSP(2,2,2) for Lagrangian step to gain second order accuracy in time for no additional solves?

4. Once we're confident in FMHD's implementation we will introduce a GOL and begin iterating again

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