SAND2018-2496PE

Improving the fidelity of simulations of power flow and target design on Sandia’s Z machine

An Efficient Generalized Ohm’s Law Modeling Approach in a Traditional Lagrangian-Eulerian Computational Framework

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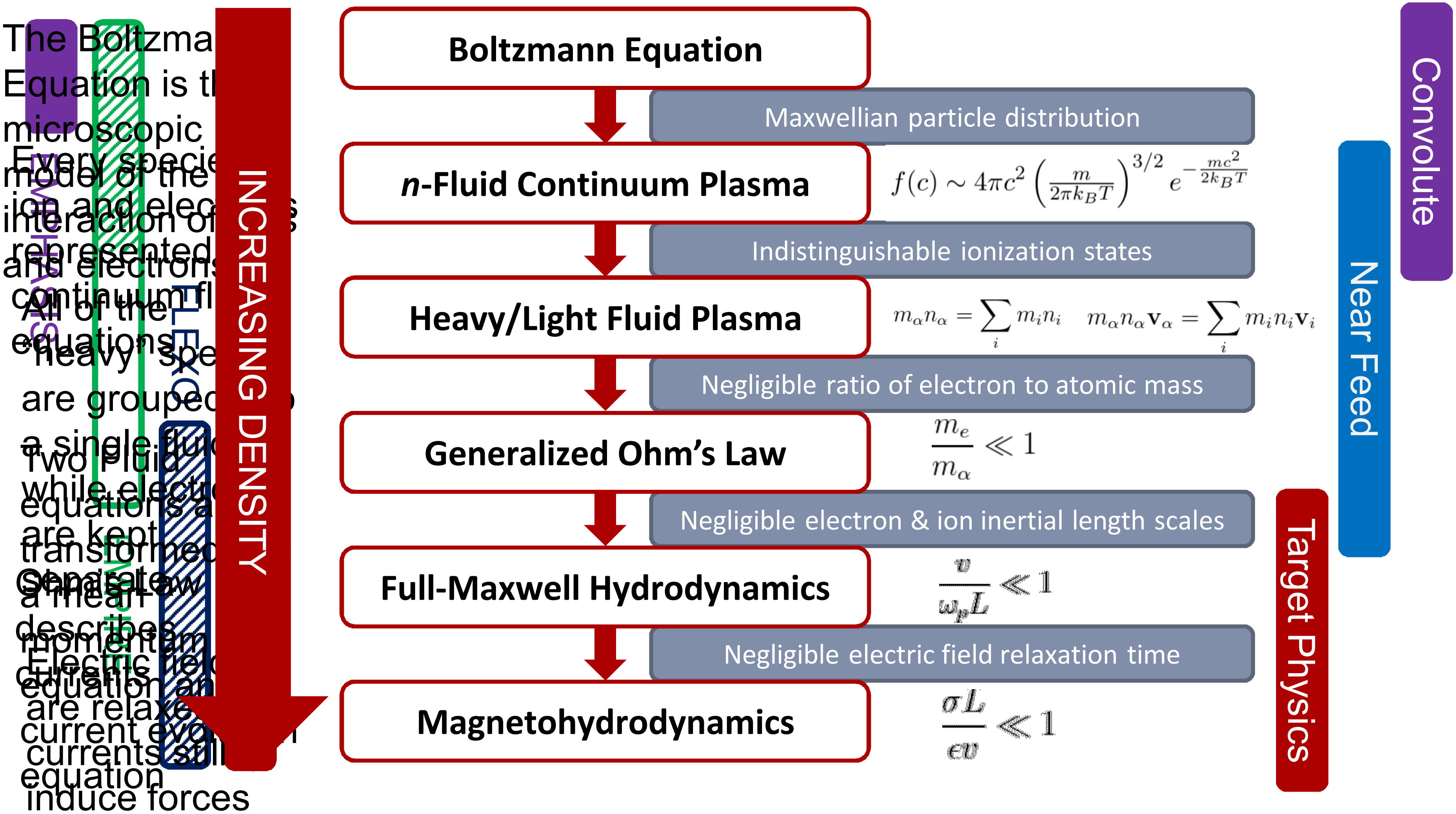
NNSA Seminar

March, 2018

Z spans a broad range of plasma conditions and demands codes which span a large range of physics



Sandia Codes

Physical Approximation

Region of Z

The Boltzma
Equation is t
microscopic
model of the
interaction of
and electrons

Every specie
ion and elec s
represented
continuum fl
equations

All of the
"heavy" spe
are grouped o
a single flui
while electr
are kept
separate

Two Fluid
equations a
transformed
a mean
momentum
equation an
current evo n
equation

Ohm's Law
describes
currents

Electric fiel
are relaxe
currents still
induce forces

Boltzmann Equation

Maxwellian particle distribution

***n*-Fluid Continuum Plasma**

$$f(c) \sim 4\pi c^2 \left(\frac{m}{2\pi k_B T}\right)^{3/2} e^{-\frac{mc^2}{2k_B T}}$$

Indistinguishable ionization states

Heavy/Light Fluid Plasma

$$m_\alpha n_\alpha = \sum_i m_i n_i \quad m_\alpha n_\alpha \mathbf{v}_\alpha = \sum_i m_i n_i \mathbf{v}_i$$

Negligible ratio of electron to atomic mass

Generalized Ohm's Law

$$\frac{m_e}{m_\alpha} \ll 1$$

Negligible electron & ion inertial length scales

Full-Maxwell Hydrodynamics

$$\frac{v}{\omega_p L} \ll 1$$

Negligible electric field relaxation time

Magnetohydrodynamics

$$\frac{\sigma L}{\epsilon v} \ll 1$$

Application of ALEGRA MHD has accelerated experimental progress on Z since the late 1990's

- Early 3D simulation work with the focus on Z wire array shots
- Lemke, et. al. envision dynamic materials experiments (DMP) and desire to design loads for studying material behavior.

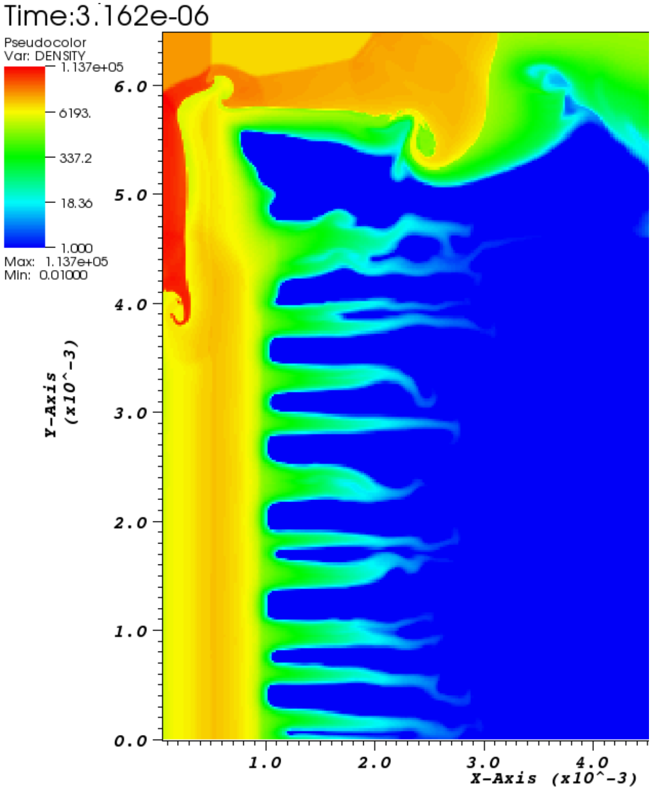
- Early 3D nodal discretizations of magnetic diffusion in ALEGRA clearly display spurious modes. ALEGRA 2D with return current boundary conditions starts to provide useful simulations for Z dynamic material shots.
- Desjarlais, Cochran, et. al., begin to improve the Lee Moore electrical conductivity model for the warm dense matter regime and begin to use DFT-MHD computations for guidance.

- Robinson et al implement compatible elements and develop 3D *constrained transport remap*.
- Lots of work on robustness in basic ALEGRA hydro algorithms.

- Practice of building electrical conductivity tables by fitting LMD to a mixture of experimental data and quantum molecular dynamics simulations becomes more routine.
- Low density high Alfven wave speed force cutoff knob is available.

- Combination of accurate material models and high quality numerics lead to ALEGRA's hardening as a MHD design tool in continuous use today.
- *Still lacking truly acceptable solutions to low density problem.*

Low density regions matter greatly for modeling experiments on Z accurately



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

Source: Peterson & Mattsson

- 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 floors, Lorentz force floors, etc which have to be chosen by an analysis to produce *reasonable results*
    - *How do we know the results are reasonable if expert judgement is necessary to assign values?*

- This problem exhibits behavior like MHD and EM propagation. Need codes that do both!

Why is the present state - resistive MHD Model – limiting progress?

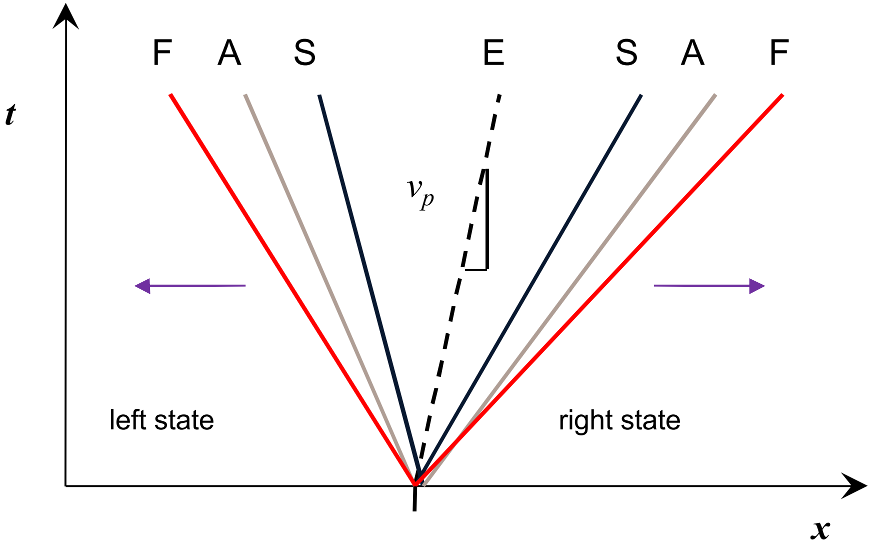
$$\dot{\mathbf{x}} = \mathbf{v}$$

$$\rho\dot{\mathbf{v}} = \operatorname{div}\mathbb{T} + \mathbf{curl}\,\mu^{-1}\mathbf{B}\times\mathbf{B}$$

$$\rho\dot{\varepsilon} = \mathbb{T} : \nabla\mathbf{v} + \sigma|\mathcal{E}|^2$$

$$\overset{\star}{\mathbf{B}} = -\,\mathbf{curl}\,\mathcal{E}$$

$$\sigma\mathcal{E} = \mathbf{curl}\,\mu^{-1}\mathbf{B}$$



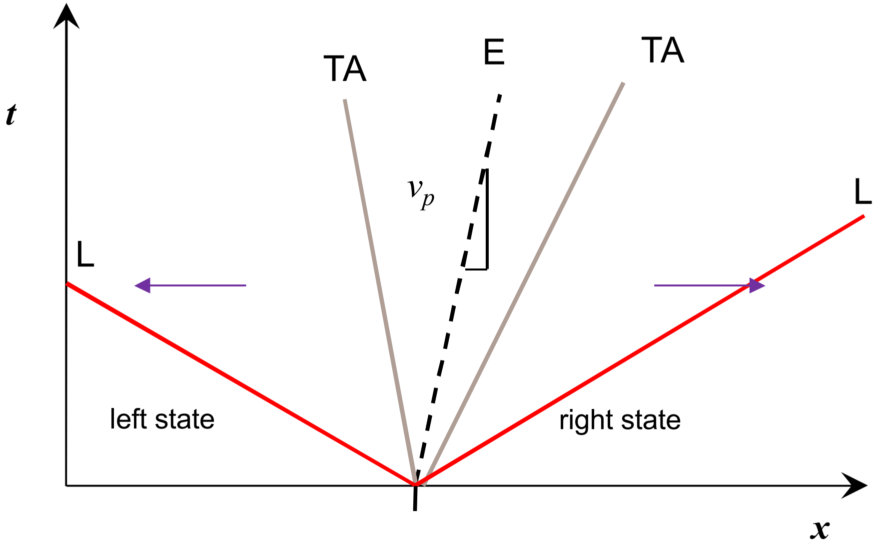
- Classical operator splitting uses an ideal MHD step
- *Ideal MHD step requires a positive density*

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

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

Full Maxwell Hydrodynamics adds terms in the physics that makes solutions stable at low density

$$
\begin{aligned}
\dot{\mathbf{x}} &= \mathbf{v} \\
\rho\dot{\mathbf{v}} &= \operatorname{div}\mathbb{T} + q\mathcal{E} + \sigma\mathcal{E}\times\mathbf{B} \\
\rho\dot{\varepsilon} &= \mathbb{T} : \nabla\mathbf{v} + \sigma|\mathcal{E}|^2 \\
\overset{\star}{\mathbf{B}} &= -\,\mathbf{curl}\,\mathcal{E} \\
\epsilon_0\overset{\star}{\mathcal{E}} &= -\sigma\mathcal{E} + \mathbf{curl}\,\mu^{-1}\mathbf{B} \\
\dot{q} + q\operatorname{div}\mathbf{v} &= -\operatorname{div}\sigma\mathcal{E}
\end{aligned}
$$



- Reintroducing electric displacements to MHD results in a system with desirable characteristics:

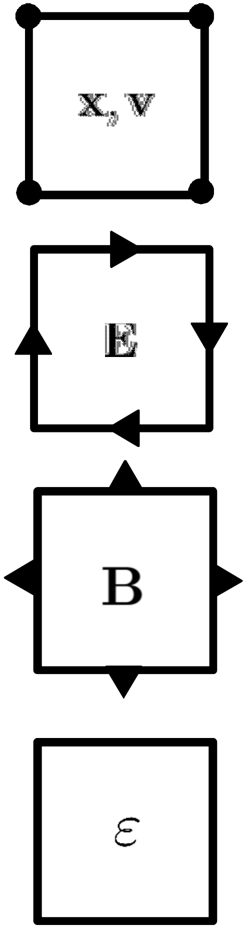
$$(v, v \pm \alpha, \pm c)$$

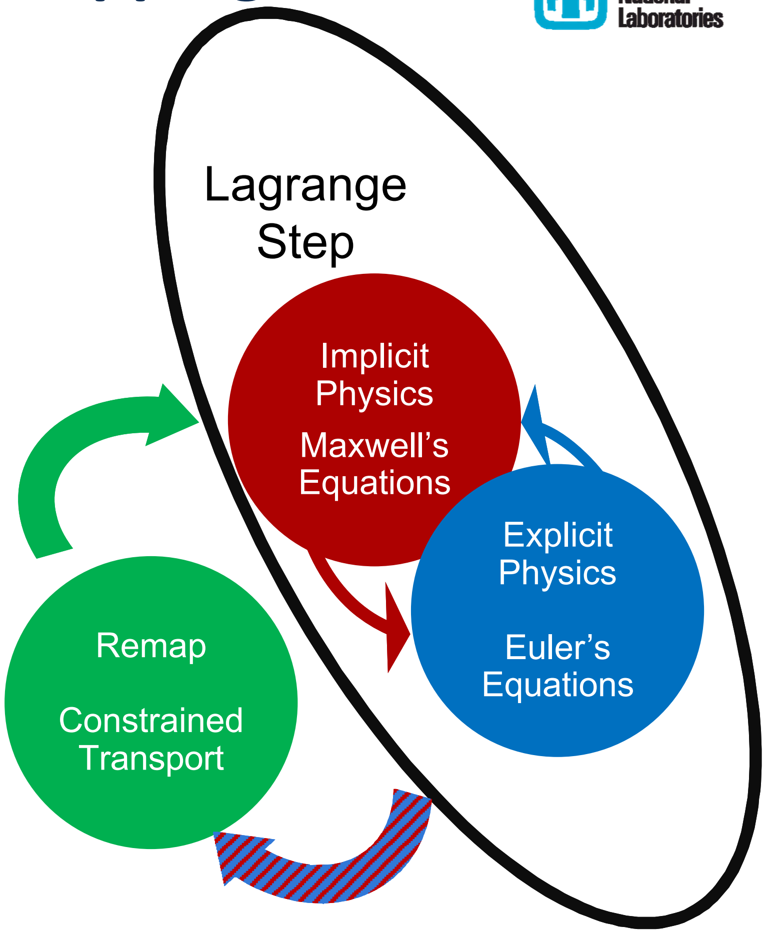
- *Model is linearly stable at arbitrarily low density.*

- We have spent approximately 15 months designing and testing FMHD in ALEGRA. This has required 2 implementations

Equations are discretized on a grid - mapping fields on cells, edges, and corners

- Compatible finite elements
  - Mass/momentum are conserved
  - **B** is divergence free
  - Charge is conserved
- Explicit Hydro, Implicit Maxwell's equations in the Lagrangian step
  - IMEX rather than operator split
  - Provably stable at the hydro CFL
  - No fast magnetosonic time step restriction.
- Asymptotic preserving implicit methods – recover MHD behavior when $\frac{\Delta t \sigma}{\epsilon} \gg 1$
- Remap conserves divergence conditions on **E** and **B** as well as mass and momentum





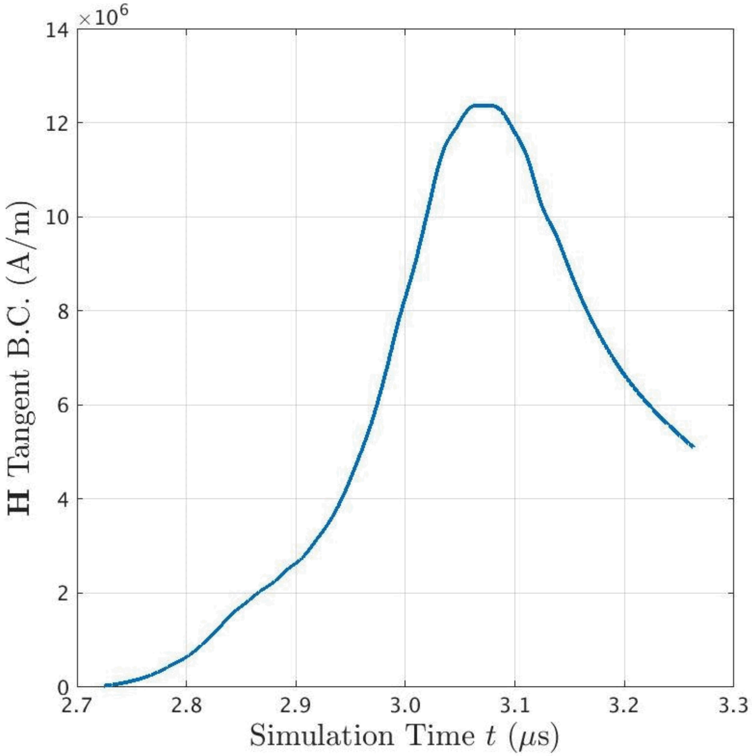
Explicit: $u^{n+1} = u^n + \Delta t f(u^n)$ *Cheap, Unstable*

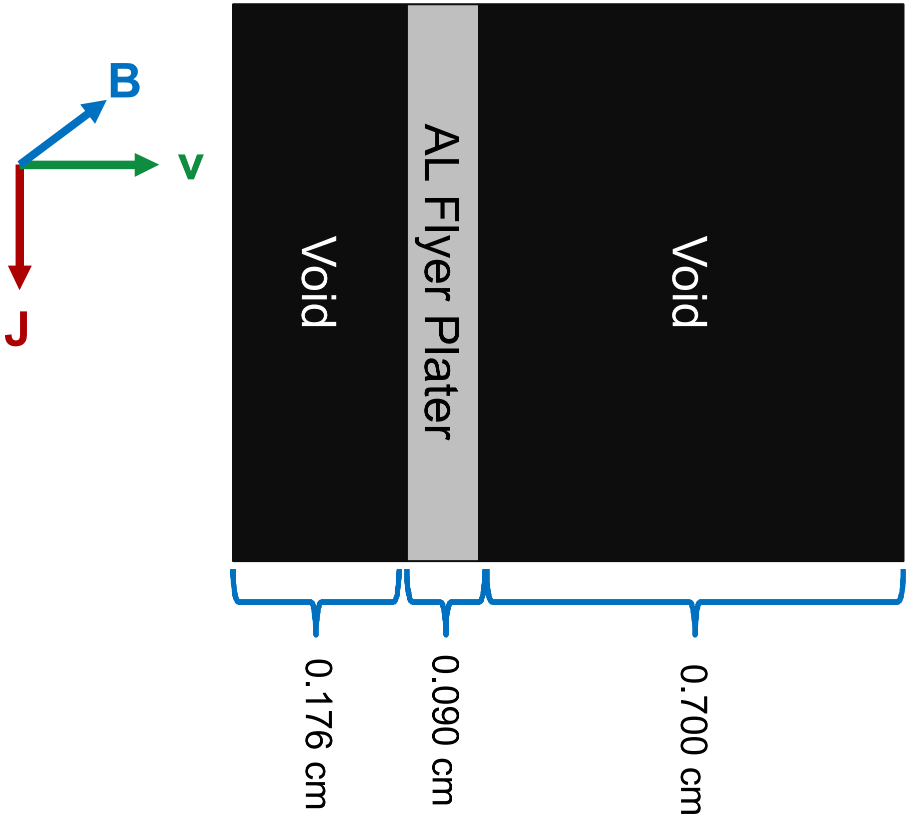
Implicit: $u^{n+1} = u^n + \Delta t f(u^{n+1})$ *Expensive, Stable*

IMEX: $u^{n+1} = u^n + \Delta t (f_1(u^n) + f_2(u^{n+1}))$

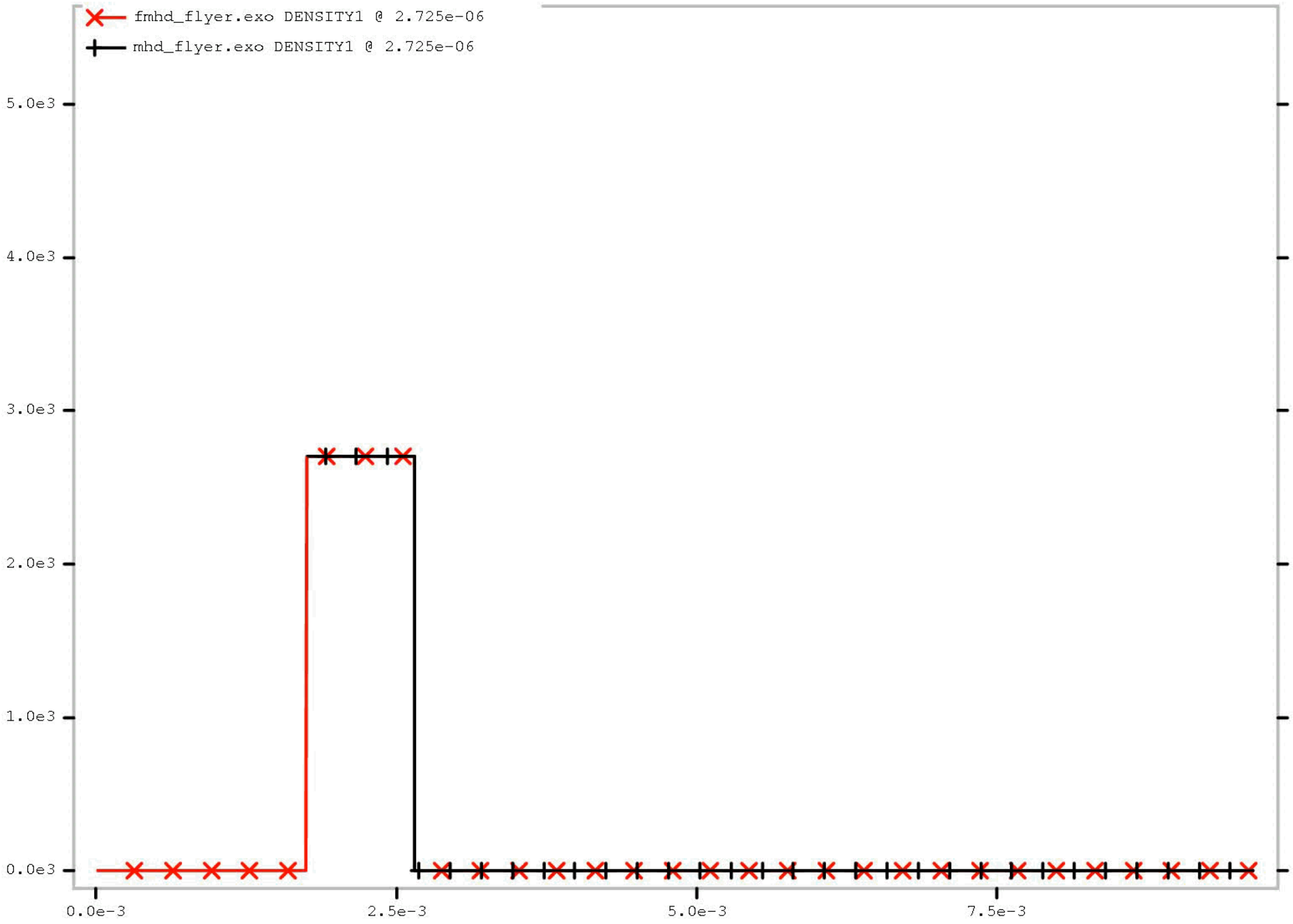
Prototype problem for a well-diagnosed experiment on Z – a magnetically accelerated flyer

Z1929_1D_opt_tr4



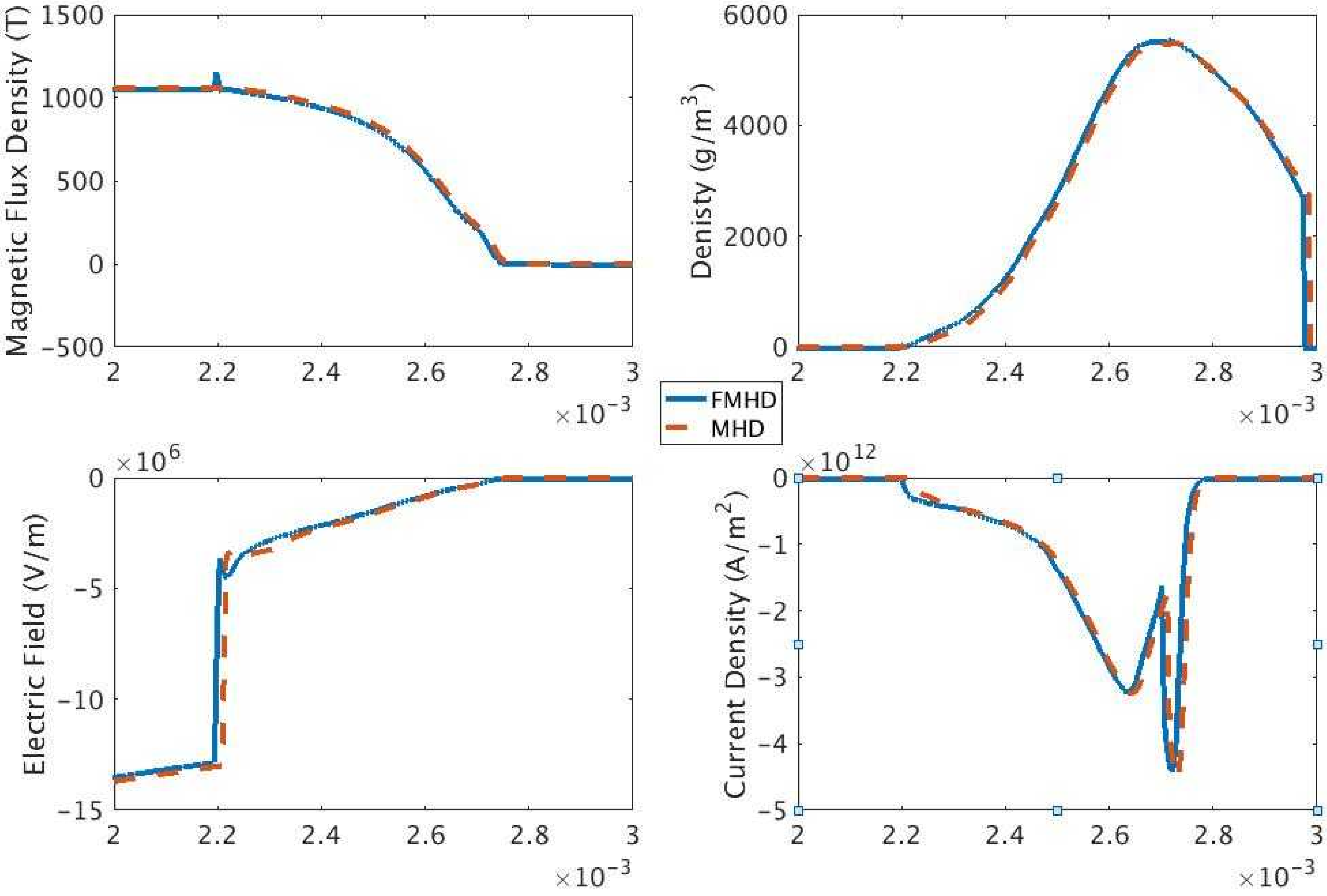


Prototype problem for a well-diagnosed experiment on Z – a magnetically accelerated flyer



MHD FMHD

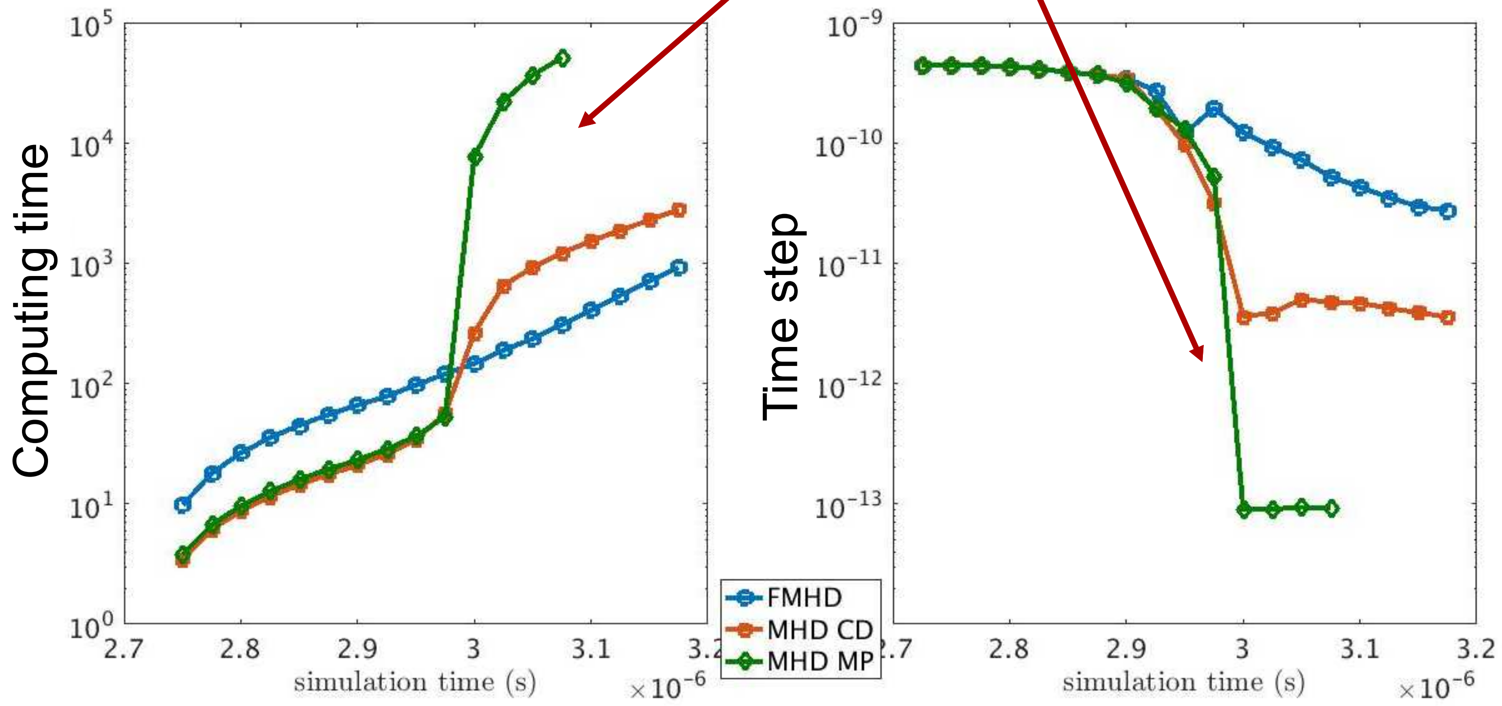
Prototype problem for a well-diagnosed experiment on Z – a magnetically accelerated flyer



Key findings from the FMHD simulations of a Z experiment

- *Recovers the MHD behavior in the right limit*
  - Low density behavior is as expected slightly different
- *Is significantly faster*
  - >5x speed up compared to midpoint
  - >2x compared to central difference
- Conserves charge

The wall-time speed-up is due to the ability to maintain long time-steps



Projected Impact of the FMHD implementation

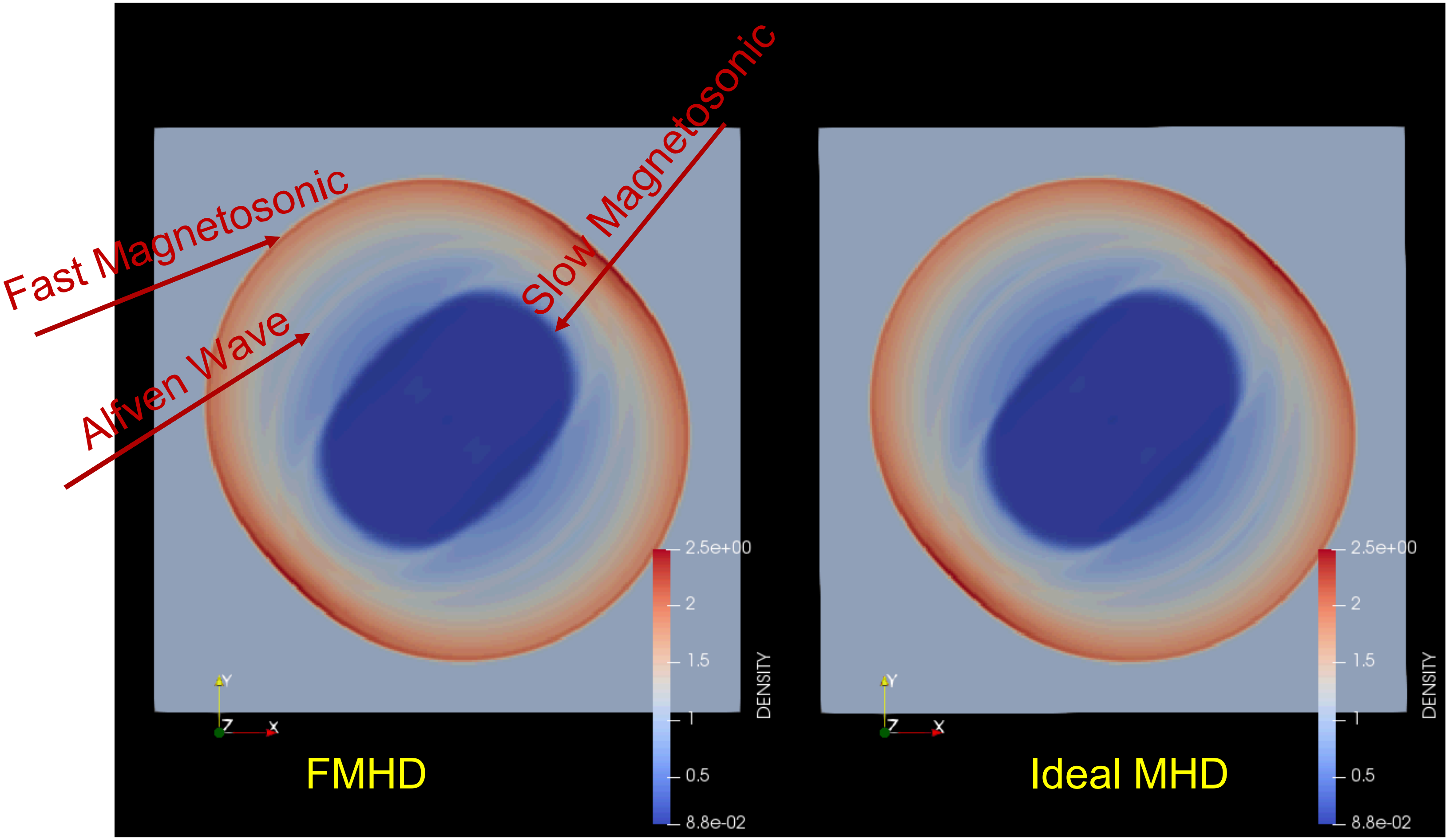
- *A 5x speed up accelerates progress*
  - 1 Work Week -> 1 Day, 1 Month -> 1 Week
  - Uncertainty quantification (5x more data points for the same compute time)
  - Buys room to the computational budget to add additional physics (GOL)

- *FMHD has improved robustness*
  - FMHD does *not require*:
    - Conductivity floors
    - Maximum Alfven speed force limiting
  - May require time step adjustments for solver precision reasons.
  - Reduce analyst time to set up problem

$$\frac{1}{2}\frac{\text{Fast Magnetosonic Wave Speed}}{\text{Thermoacoustic Wave Speed}}$$

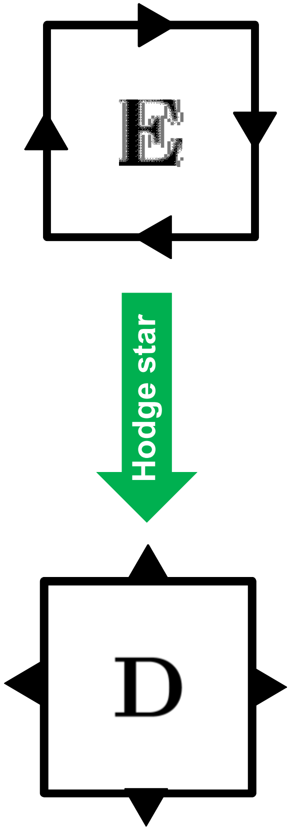
- FMHD adds new physics
  - Coulomb Forces

Qualitative Evidence of Asymptotic Preserving (AP) Property

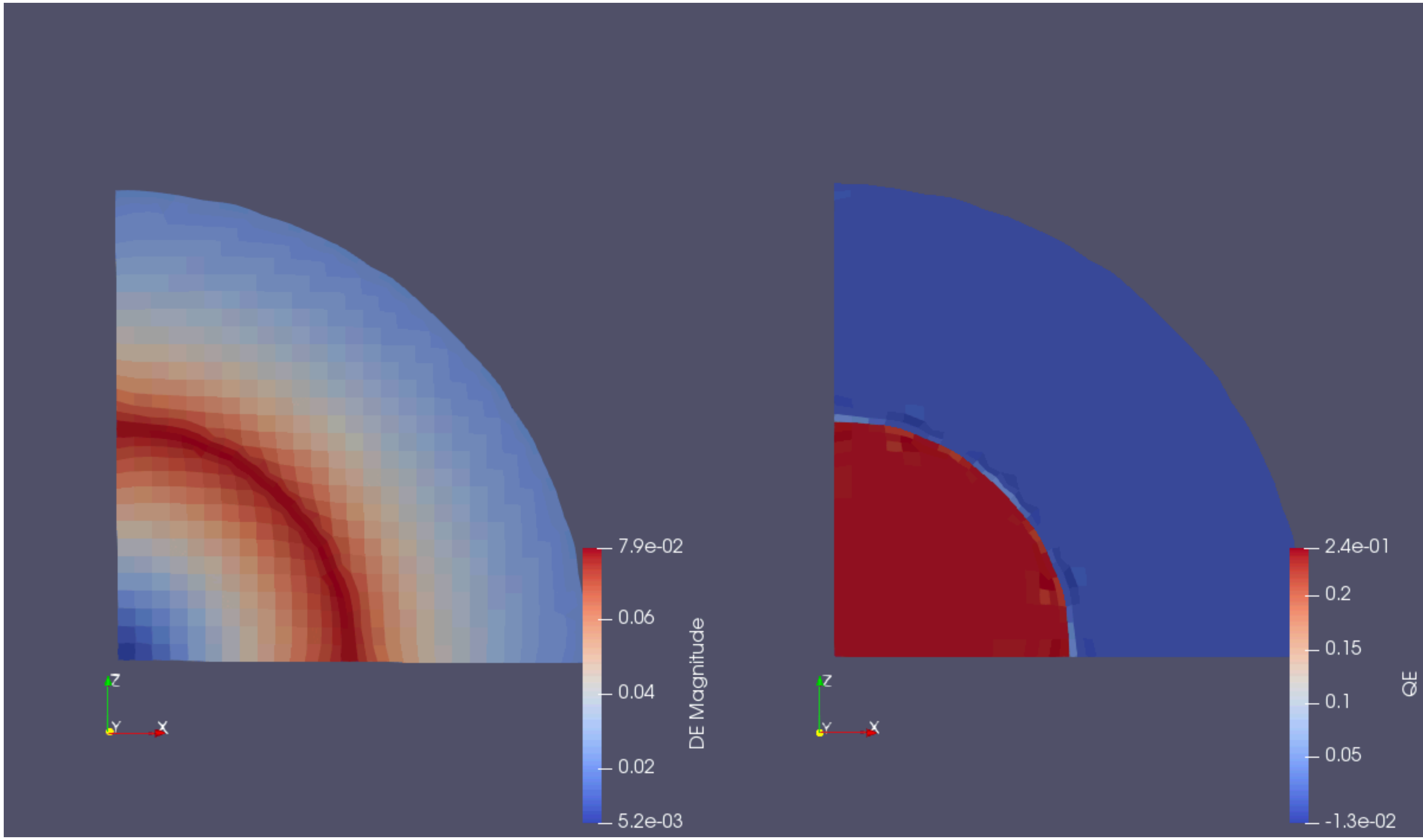


Charged Sphere

Solved for Maxwell's Equations



Remap with Constrained Transport



Charge Conservation

Lie Derivatives describe advection

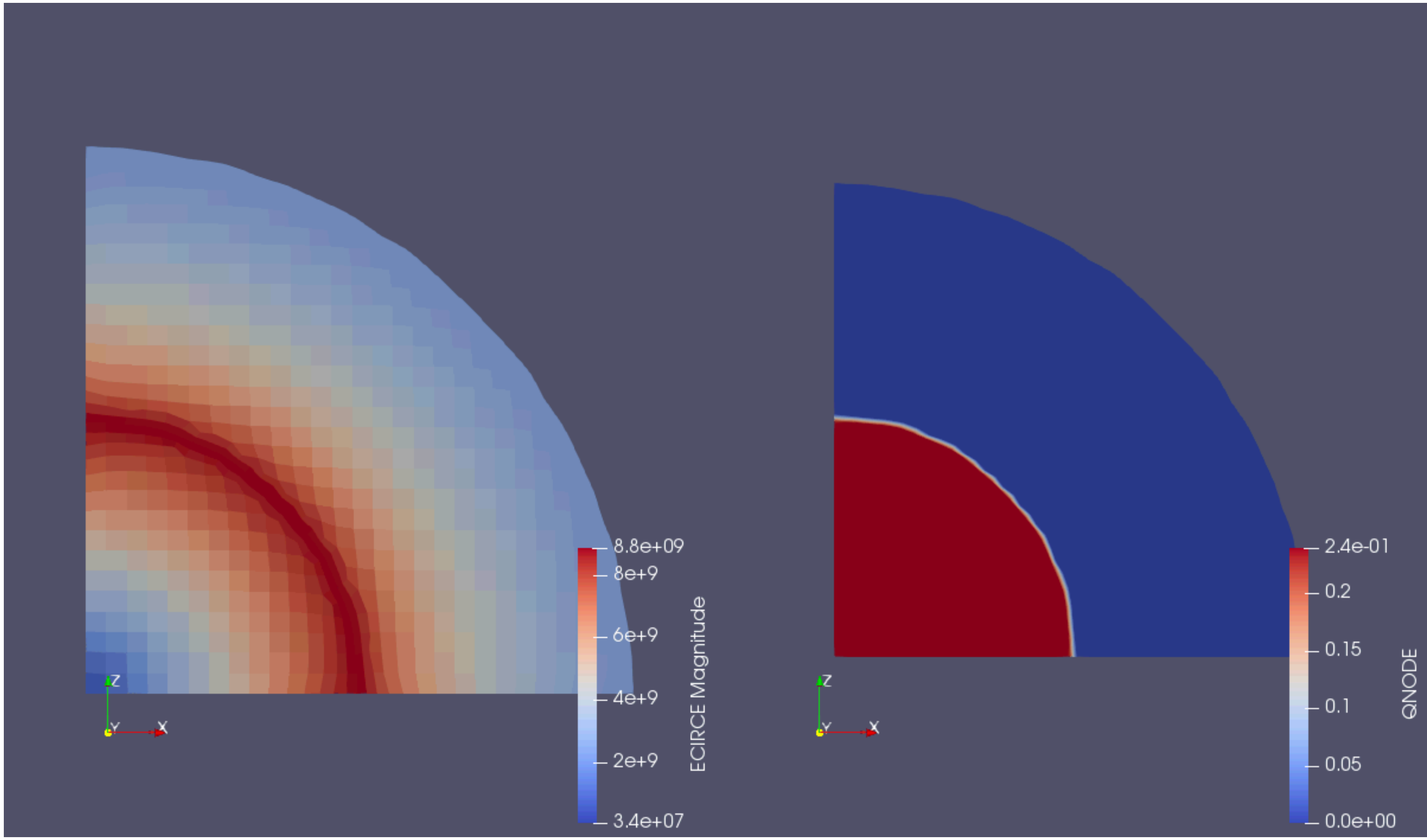
$$\dot{\psi} = (\partial_t + \mathcal{L}^0_{\mathbf{v}})\varphi = \partial_t \varphi + \mathbf{v} \cdot \nabla \varphi$$

$$(\partial_t + \mathcal{L}^1_{\mathbf{v}})\boldsymbol{\Psi} = \partial_t \boldsymbol{\Psi} + \nabla(\mathbf{v} \cdot \boldsymbol{\Psi}) - \mathbf{v} \times \mathbf{curl}\, \boldsymbol{\Psi}$$

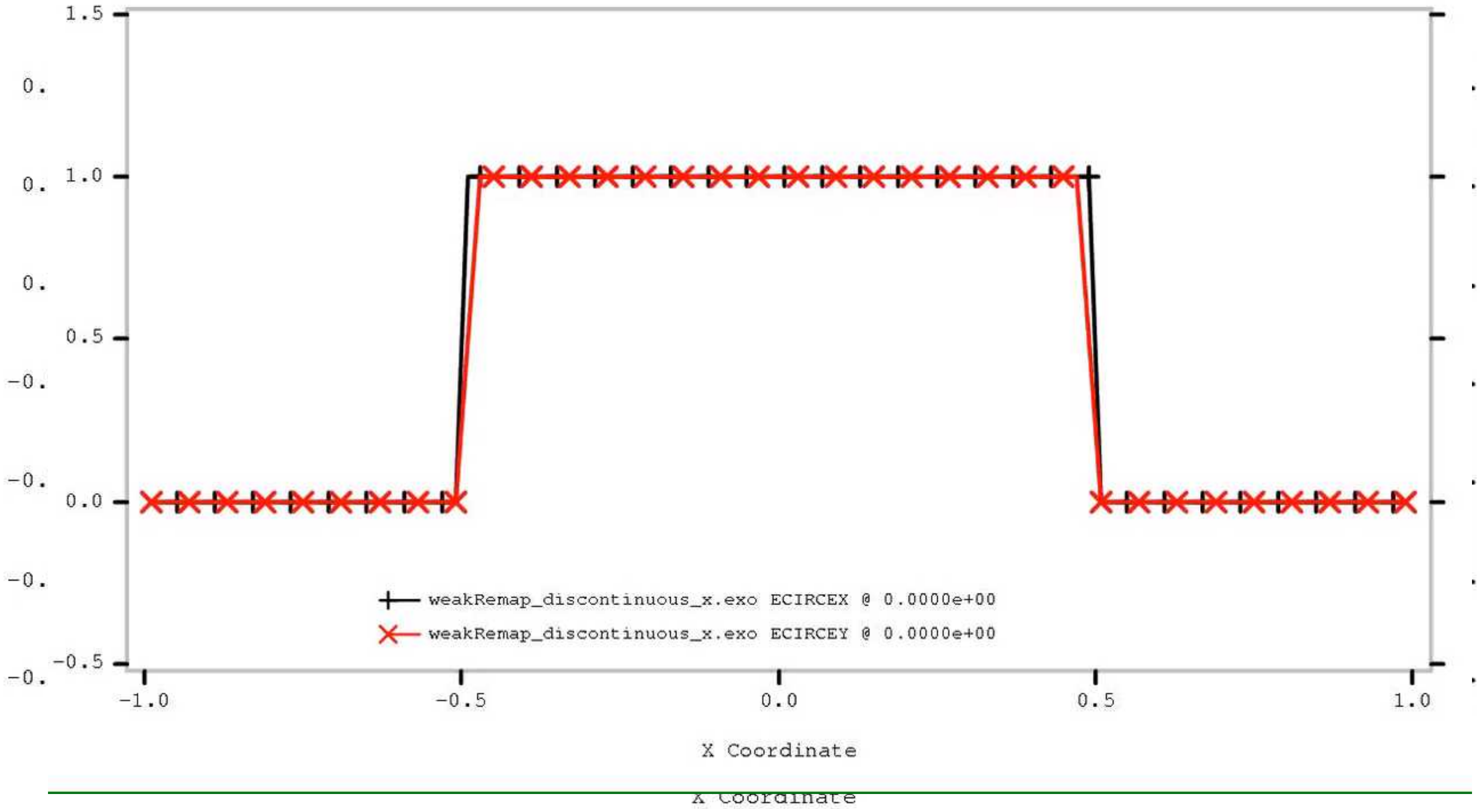
$$\overset{\star}{\boldsymbol{\Phi}} = (\partial_t + \mathcal{L}^2_{\mathbf{v}})\boldsymbol{\Phi} = \partial_t \boldsymbol{\Phi} - \mathbf{curl}(\mathbf{v} \times \boldsymbol{\Phi}) + \mathbf{v}\, \mathrm{div}\, \boldsymbol{\Phi}$$

$$(\partial_t + \mathcal{L}^3_{\mathbf{v}})\psi = \partial_t \psi + \mathrm{div}(\mathbf{v}\psi)$$

Charged Sphere with no Hodge Star



Stability of Weak Remap



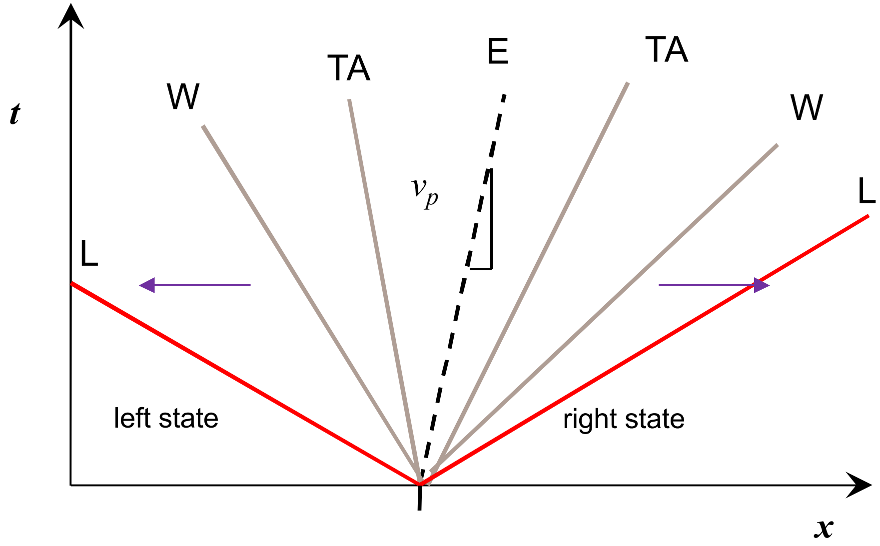
[illegible]

$$\int_{\Omega^\star} \epsilon_0 \mathbf{E}^\star \cdot \mathbf{\Psi} dv = \int_{\Omega^n} \epsilon_0 \mathbf{E}^n \cdot \mathbf{\Psi} dv + \Delta s \int_{\Omega^n} \epsilon_0 \mathbf{E} \cdot (\nabla(\mathbf{w} \cdot \mathbf{\Psi}) - \mathbf{w} \times \mathbf{curl}\, \mathbf{\Psi}) dv$$

$$+ \tau \Delta s^2 \int_{\Omega^n} \epsilon_0 (\nabla(\mathbf{w} \cdot \mathbf{E}^n) - \mathbf{w} \times \mathbf{curl}\, \mathbf{E}^n) \cdot (\nabla(\mathbf{w} \cdot \mathbf{\Psi}) - \mathbf{w} \times \mathbf{curl}\, \mathbf{\Psi}) dv$$

Generalized Ohm's Law Is the Next Step

$$\begin{aligned}
\dot{\mathbf{x}} &= \mathbf{v} \\
\rho\dot{\mathbf{v}} &= \operatorname{div}\mathbb{T} + q\mathcal{E} + \mathcal{J}\times\mathbf{B} \\
\rho\dot{\varepsilon} &= \mathbb{T} : \nabla\mathbf{v} + \mathcal{J}\cdot\mathcal{E} \\
\overset{\star}{\mathbf{B}} &= -\,\mathbf{curl}\,\mathcal{E} \\
\epsilon_0\overset{\star}{\mathcal{E}} &= -\mathcal{J} + \mathbf{curl}\,\mu^{-1}\mathbf{B} \\
\dot{\mathbf{J}} + \mathbf{J}\operatorname{div}\mathbf{v} &= \operatorname{div}\mathbb{T}_j + \epsilon_0\omega_p^2\mathcal{E} - \eta\mathcal{J} - \frac{e}{m_e}\mathcal{J}\times\mathbf{B} \\
\dot{q} + q\operatorname{div}\mathbf{v} &= -\operatorname{div}\mathcal{J} \\
\mathbb{T}_j &= -\mathbf{v}\otimes\mathcal{J} + \frac{1}{en_e}\mathcal{J}\otimes\mathcal{J} + \frac{e}{m_e}p\mathbb{I}
\end{aligned}$$



Includes Hall effect and plasma oscillations.

(Low Risk) Requires η rather than σ, new material model tables

(Med Risk) non-symmetric matrix solves
(Med Risk) Eulerian vs. Lagrangian currents
~~(Med Risk) Introduction of Electric field physics~~ ***Addressed by FMHD!***

(High Risk) Split EOS – hard physics problem.

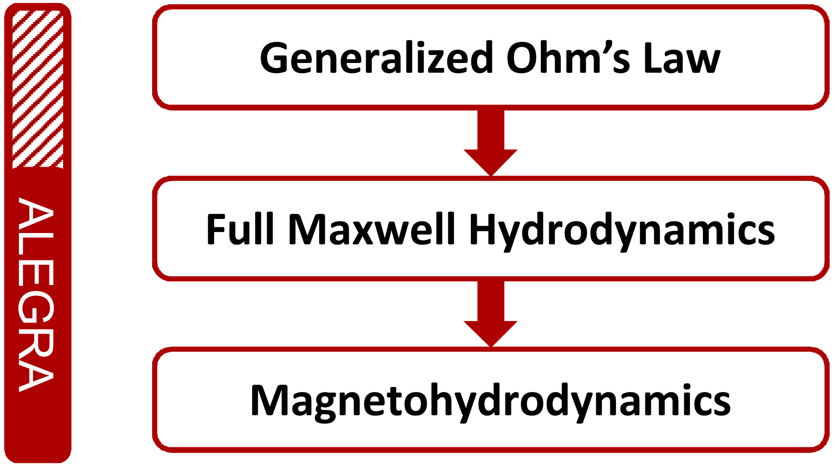
Milestones

EOFY 2018

1. 3D FMHD released to designers (Porwitzky) and validated against a library of pulse shapes
2. Circuit coupling and q boundary conditions
3. Begin implementing generalized Ohm's Law

EOFY 2019

1. 3D FMHD hardened and stood up as default ALEGRA option for DMP design
2. Generalized Ohm's Law prototyped and reproducing Perseus/Flexo results.



Technology Goals

1. Strongly stable weak remap
2. 2nd order IMEX time integration
3. Multimaterial permittivity
4. Investigate weak remap for momentum?
5. 2D mode
6. Weak Remap for Momentum (kinetic energy conservation)?

Questions?

Work Timeline

Stage 1: Initial Analysis (Fall 2016-Spring 2017)

- Read work of Martin and Seyler, etc.
- Formulated began formulating a Lagrangian frame model
- Analysis suggests displacement currents independent of GOL is beneficial

Stage 2: Hodge Star (Spring 2017 – Fall 2018)

- Implemented Maxwell solver
- Develop and prove stability of IMEX predictor corrector integrator
- Implemented Hodge-star Full Maxwell Hydro
  - Solved for E on edges and projected to D on faces and remapped D with constrained transport
- Demonstrate AP properties and speed up on prototype
- Demonstrate the Hodge star ***does <u>not</u> conserve charge***

Stage 3: Weak Lie Derivative (Fall 2018 – present)

- Develop the weak Lie derivative formalism
  - Never break mimetic interpretation
- Implement weak Lie derivative advection remap
- Demonstrate speed on AP with weak Lie FMHD
- Weak Lie strategy ***does conserve charge***

IMEX Predictor Corrector for FMHD

$$\frac{\partial}{\partial t}\begin{pmatrix}\mathbf{x}\\ \rho_0\mathbf{v}\\ \rho_0\varepsilon\\ \epsilon_0\mathcal{E}\\ \mathbf{B}\\ q\end{pmatrix} = \begin{pmatrix}\mathbf{v}\\ \operatorname{div}\mathbb{T}\\ \mathbb{T}:\nabla\mathbf{v}\\ 0\\ 0\\ 0\end{pmatrix} + \begin{pmatrix}0\\ q\mathcal{E}+\sigma\mathcal{E}\times\mathbf{B}\\ \sigma|\mathcal{E}|^2\\ -\sigma\mathcal{E}+\mathbf{curl}\,\mu^{-1}\mathbf{B}\\ -\,\mathbf{curl}\,\mathcal{E}\\ -\operatorname{div}\sigma\mathcal{E}\end{pmatrix}$$

Explicit

Implicit

$$\int \left(\tfrac{\epsilon_0}{\Delta t}+\sigma\right)\mathcal{E}^{n+1}_{(i+1)}\cdot\mathbf{\Psi}+\tfrac{\Delta t}{\mu}\,\mathbf{curl}\,\mathcal{E}^{n+1}_{(i+1)}\cdot\mathbf{curl}\,\mathbf{\Psi}\;dV=\int \tfrac{\epsilon_0}{\Delta t}\mathcal{E}^{n}\cdot\mathbf{\Psi}+\mu^{-1}\mathbf{B}^{n}\cdot\mathbf{curl}\,\mathbf{\Psi}\;dV$$

$$\int (q^{n+1}_{(i+1)}-q^{n})\varphi dV=\Delta t\int \sigma\mathcal{E}^{n+1}_{(i+1)}\cdot\nabla\varphi\;dV$$

$$\mathbf{B}^{n+1}_{(i+1)}=\mathbf{B}^{n}_{(i+1)}-\Delta t\,\mathbf{curl}\,\mathcal{E}^{n+1}_{(i+1)}$$

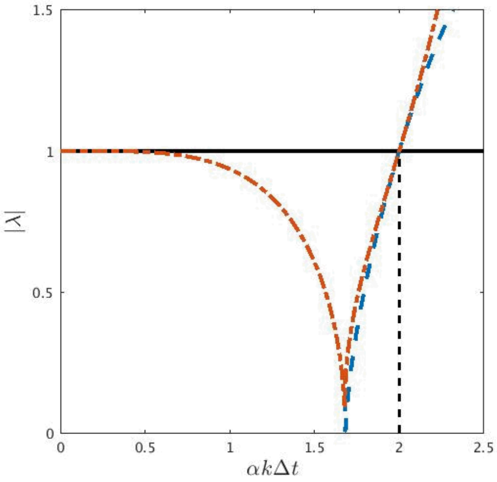
$$\int \rho_0(\mathbf{v}^{n+1}_{(i+1)}-\mathbf{v}^{n})\cdot\boldsymbol{\varphi}dV=-\Delta t\int \mathbb{T}^{n+1/2}_{(i)}:\nabla\boldsymbol{\varphi}-(q\mathcal{E}+\sigma\mathcal{E}\times\mathbf{B})^{n+1/2}_{(i+1)}\cdot\boldsymbol{\varphi}\;dV$$

$$\mathbf{x}^{n+1}_{(i+1)}=\mathbf{x}^{n}+\Delta t\mathbf{v}^{n+1/2}_{(i+1)}$$

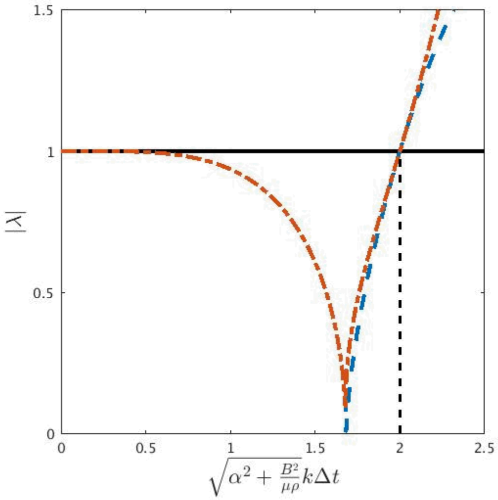
$$\int \rho_0(\varepsilon^{n+1}_{(i+1)}-\varepsilon^{n})\;dV=\Delta t\int (\mathbb{T}:\nabla\mathbf{v})^{n+1/2}_{(i+1)}+(\sigma|\mathcal{E}|^2)^{n+1/2}_{(i+1)}dV$$

Stability of IMEX Predictor Corrector

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



FMHD Stability Region



MHD Stability Region

- 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** (on faces) is the Galilean Invariant. Weak Lie derivatives!

Weak Remap Algorithm (no stabilization)

```
$\mathbf{R}_e^j = \int_{\Omega_h^j} \epsilon \mathbf{E}_j^n \cdot \mathbf{\Psi}_e \; dV, \quad \forall \mathbf{\Psi}_e \in \mathscr{E}_h^j$
$I = [t_j, t_{j+1}]$
for $nodes\ n \in \mathscr{N}^j$ do
    Find the upwind element $P \in \mathscr{P}^j : n(\mathbf{u}_h(t_j - t_{j+1})) \in P$
    for $edges\ e \in P$ do
        Compute the interior product on the swept edge
        $\int_I (\mathbf{u}_h \cdot \mathbf{\Psi}_e)_n \; dt = \int_{S^I_{\mathbf{u}_h}(n)} \mathbf{\Psi}_e \cdot d\mathbf{S}$
        for $elements\ \tilde{P} \in \mathscr{P}^j : n \in \tilde{P}$ do
            Increment the right hand side
            $\mathbf{R}_e^j \mathrel{+}= \int_{\tilde{P}} \epsilon \mathbf{E}_h^n \cdot \mathbf{grad} \int_I (\mathbf{u}_h \cdot \mathbf{\Psi}_e)_n dt \; dV$
        end
    end
end
for $edges\ e \in \mathscr{E}^j$ do
    Find find the upwind element $P \in \mathscr{P}$ such that $e(\mathbf{u}(-\Delta t)) \in P$
    for $edges\ \tilde{e} \in P^j$ do
        Compute the interior product on the swept face
        $\int_I (-\mathbf{u}_h \times \mathbf{curl} \mathbf{\Psi}_{\tilde{e}})_e \; dt = \int_{S^I_{\mathbf{u}_h}(e)} \mathbf{curl}\, \mathbf{\Psi}_{\tilde{e}} \cdot d\mathbf{A}$
        for $elements\ \tilde{P} \in \mathscr{P}^j : e \in \tilde{P}$ do
            $\mathbf{R}_{\tilde{e}}^j \mathrel{+}= \int_{\tilde{P}} \epsilon \mathbf{E}_h^n \cdot \int_I (-\mathbf{u}_h \times \mathbf{curl} \mathbf{\Psi}_{\tilde{e}})_e dt \; dV$
        end
    end
end
```