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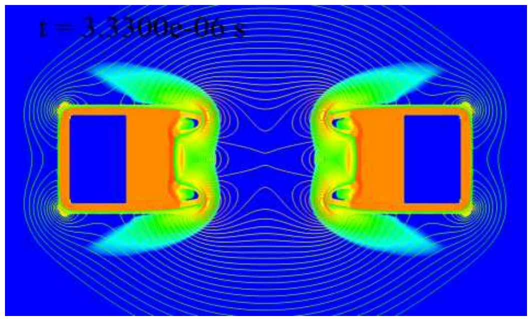


# Progress toward 3D Extended MHD modeling in an ALE Framework in Alegra

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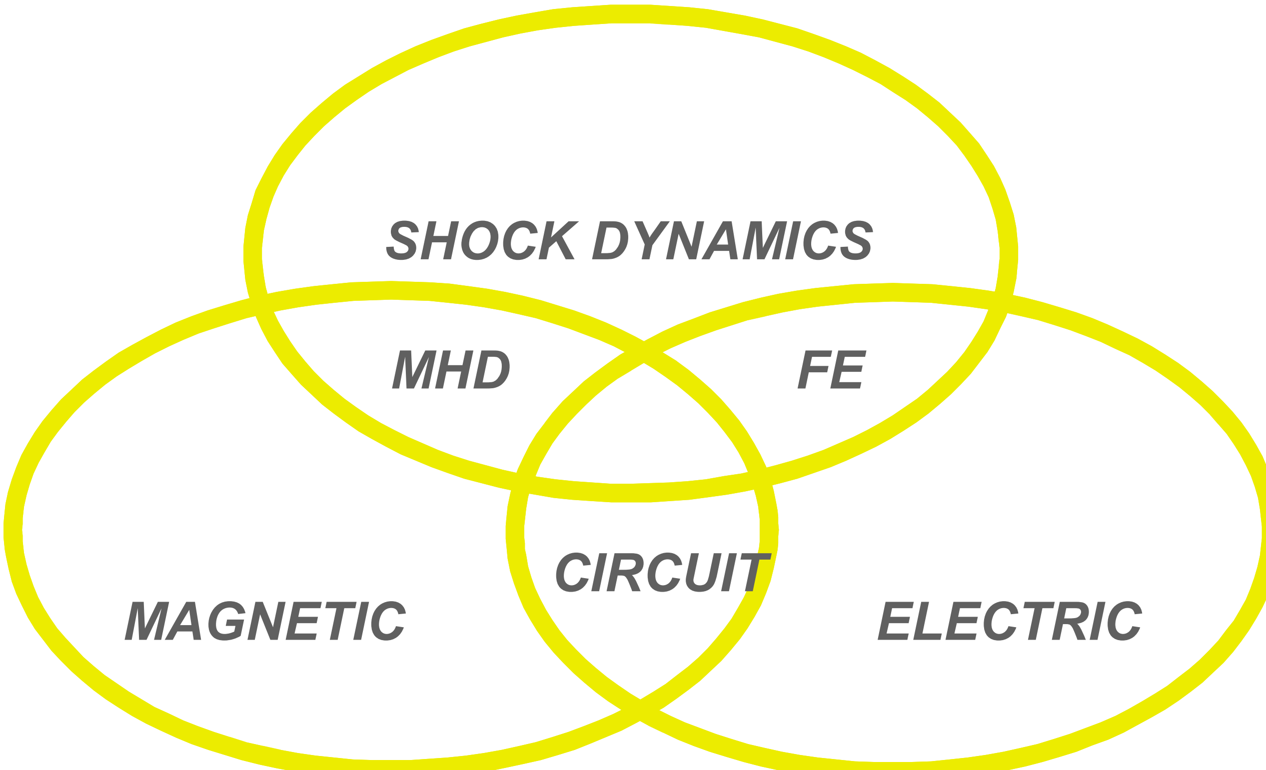
# Outline

- Basic ALE multiphysics approach in Alegra
- Z impact  and issues
- Two step plan for better low density modeling
- Theory
- Status on remap software component.

# ALEGRA SHOCK & MULTIPHYSICS



# Continuum shock algorithms ("hydrocode")

AlON panels.

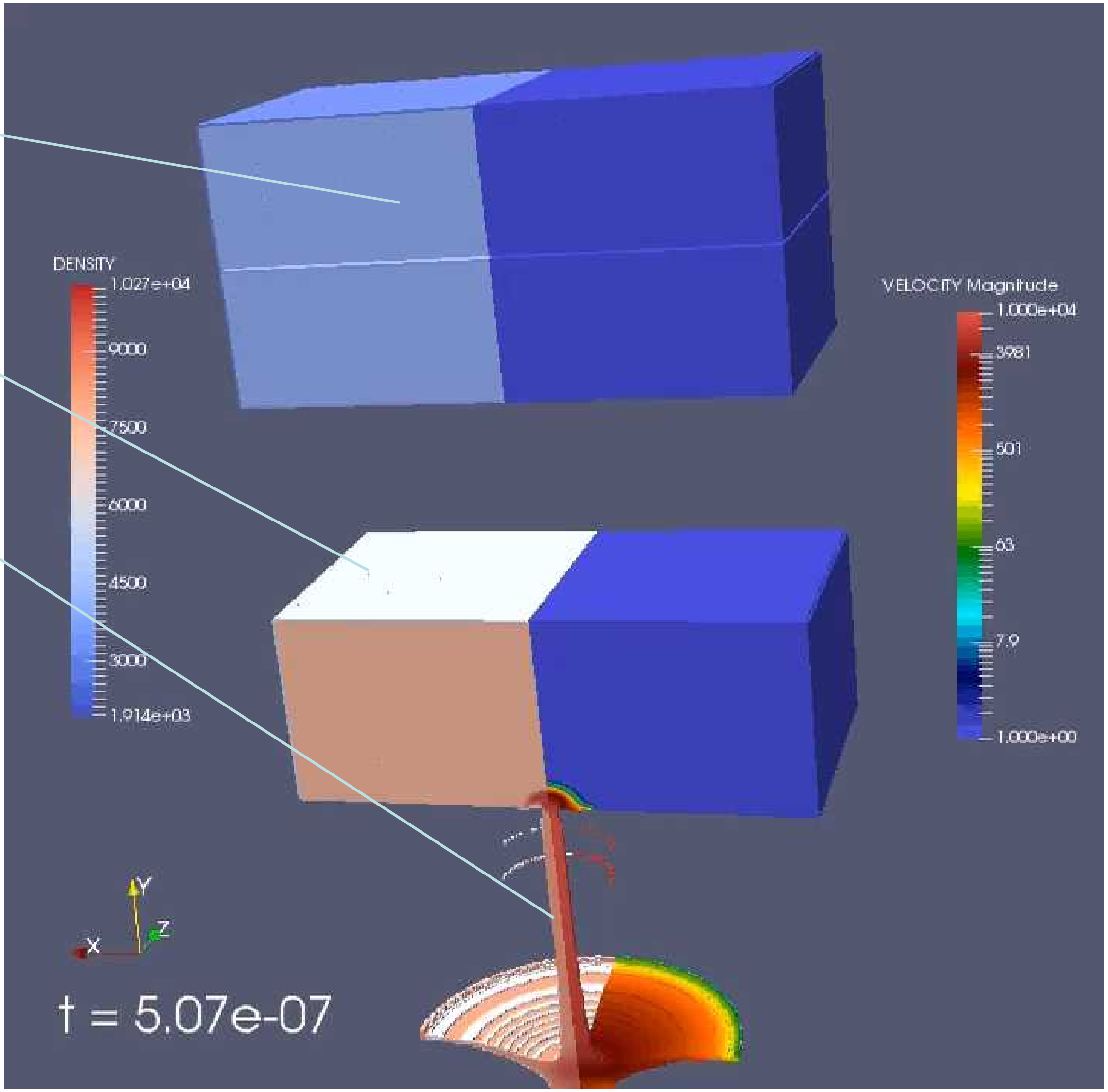
Steel plate.

Fully-formed shaped charge jet imported from 2D axisymmetric Alegra simulation.

Alegra is an MPI distributed memory parallel code.

The code is fundamentally an "indirect" Arbitrary Lagrangian-Eulerian (ALE) technology.

Multiphysics is included as a first order operator split in the indirect ALE approach.




Courtesy of J. Niederhaus (SNL) and B. Leavy (ARL)

# We want to give users effective control over Electromagnetic Continuum Mechanics

$$\dot{\rho} + \rho \nabla \cdot \mathbf{v} = 0$$

Mass

$$\rho \dot{\mathbf{g}} = \nabla \cdot T + \rho \mathbf{b}$$

Momentum

$$\rho \dot{\epsilon} = \nabla \cdot T^T \mathbf{v} + \rho \mathbf{v} \cdot \mathbf{b} + \rho h - \mathrm{div}(\mathbf{q} + \mathcal{E} \times \mathcal{H})$$

Energy

$$\begin{aligned}
\nabla \times \mathcal{H} &= \mathcal{J} + \overset{*}{\mathbf{D}}, \\
\nabla \cdot \mathbf{D} &= q, \\
\nabla \times \mathcal{E} &= -\overset{*}{\mathbf{B}}, \\
\nabla \cdot \mathbf{B} &= 0, \\
\mathbf{D} &= \epsilon_0 \mathbf{E} + \mathbf{P}, \\
\mathbf{H} &= \mathbf{B}/\mu_0 - \mathbf{M}
\end{aligned}$$

Maxwell Equations

$$\mathcal{E} = \mathbf{E} + \mathbf{v} \times \mathbf{B}$$

$$\mathcal{H} = \mathbf{H} - \mathbf{v} \times \mathbf{D}$$

$$\mathcal{J} = \mathbf{J} - q\mathbf{v}$$

closure relationships for $\mathbf{g}, T, \epsilon, \mathbf{q}, s, \mathcal{M}$, $\mathbf{P}$ and $\mathcal{J}$

# Alegra Indirect ALE Splitting Today

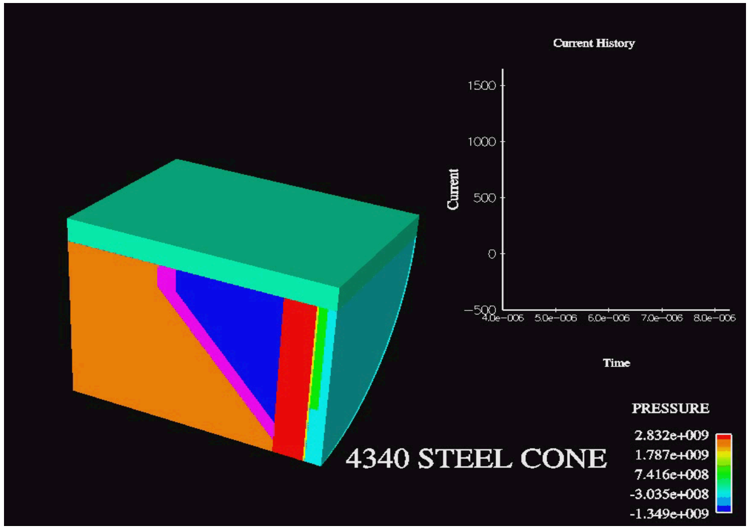
- Lagrangian Frame
  - Mesh moves with material
  - No discretization for advection necessary
  - Useful for solid mechanics constitutive models
  - Mesh deteriorates over time
  - Careful attention to Lagrangian integral invariants
- Remesh/Remap
  - Create a new mesh, nicer mesh (or choose your new mesh as your last mesh)
  - Local remap can be thought of as an advection operator which places new data on old mesh
- Static Frame (everything else assuming u=0)
  - Magnetic Diffusion
  - Circuit Coupling
  - Joule Heating
  - Heat Conduction

# *Alegra (FE) - Quasi-static electric field approximation to Maxwell Equations*

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

$$\rho \dot{\mathbf{v}} = \nabla \cdot \mathbf{T} + \mathbf{f}$$

$$\rho \dot{e} = \rho s + \mathbf{T} : \mathbf{L} - \nabla \cdot \mathbf{q}$$




Movie shows an example simulation of a shock actuated power supply.

$$\nabla \cdot \mathbf{D} = 0 \qquad \nabla \times \mathbf{E} = 0 \Rightarrow \mathbf{E} = -\nabla \phi$$

$$\nabla \cdot \mathbf{D} = 0 \Rightarrow \nabla \cdot (\epsilon \nabla \phi) = \nabla \cdot \mathbf{p}$$

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P} = \epsilon \mathbf{E} + \mathbf{p}$$

**material polarization** ($\mathbf{P}$) — **permittivity** ($\epsilon$) — **remnant, permanent or spontaneous polarization** ($\mathbf{p}$)

$$\begin{aligned} \mathbf{T} &= \mathbf{T}(\mathbf{S}, \mathbf{E}) \\ \mathbf{D} &= \mathbf{p}(\mathbf{S}) + \epsilon(\mathbf{S})\mathbf{E} \end{aligned}$$

# Resistive Magnetohydrodynamic (MHD) Equations

(Neglect displacement current =quasi-static magnetic field approximation)

$$\dot{\rho} + \rho \nabla \cdot \mathbf{v} = 0$$

$$\rho \dot{\mathbf{v}} = \nabla \cdot \left( \mathbf{T} + \mathbf{T}^{M} \right) + \mathbf{f}$$

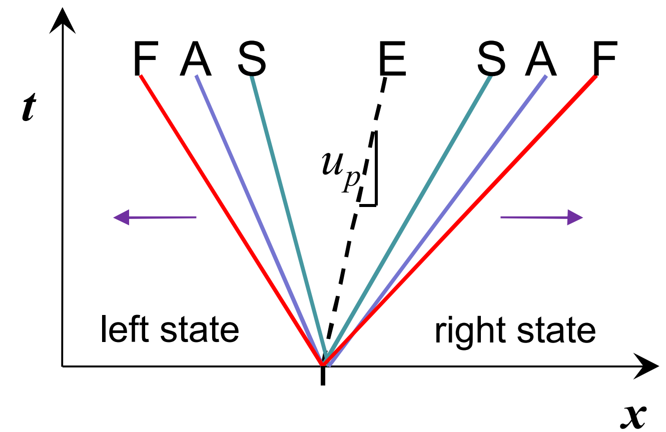
$$\rho \dot{e} = \rho s + \mathbf{T} : \mathbf{L} - \nabla \cdot \mathbf{q} + \frac{1}{\sigma} \mathbf{J} \cdot \mathbf{J}$$

$$\overset{*}{\mathrm{B}} = \frac{\partial \mathrm{B}}{\partial t} + \nabla \times (\mathrm{B} \times \mathbf{v}) + \mathbf{v}(\nabla \cdot \mathrm{B}) = -\nabla \times \frac{1}{\mu_0 \sigma} (\nabla \times \mathrm{B})$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \frac{\mathrm{B}}{\mu_0} = \mathrm{J}$$

$$\mathbf{T}^{M} = \frac{1}{\mu_0} \left( \mathbf{B}\mathbf{B}^{T} - \frac{1}{2} \mathbf{B}^2 \mathbf{I} \right)$$



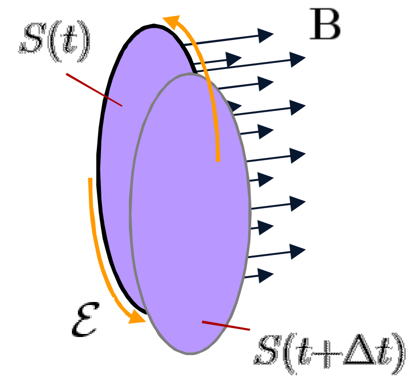

Ideal MHD wave speeds

**Closure relations for the stress, $\mathrm{T} = -p(\rho, e)I$, electrical conductivity, J = $\sigma(\rho, \theta)\, E$, and heat flux, $q = -k(\rho, \theta) \nabla \theta$ , are required to solve the equations.**

# Faraday's Law (Natural operator splitting)

A straightforward **B**-field update is possible using Faraday's law.

$$\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0 \qquad \mathcal{E} = \mathbf{E} + \mathbf{v} \times \mathbf{B}$$




Integrate over time-dependent surface $S(t)$, apply Stokes theorem, and discretize in time:

$$\frac{d}{dt}\int_{S(t)} \mathbf{B}\cdot d\mathbf{a} + \oint_{\partial S(t)} \mathcal{E}\cdot d\mathbf{x} = 0$$

$$\frac{1}{\Delta t}\int_{S(t+\Delta t)} (\mathbf{B}^{n+1} - \tilde{\mathbf{B}}^{n+1})\cdot d\mathbf{a}^{n+1} + \oint_{\partial S(t+\Delta t)} \mathcal{E}^{n+1}\cdot d\mathbf{x}^{n+1}$$

$$+ \frac{1}{\Delta t}\left[\int_{S(t+\Delta t)} \tilde{\mathbf{B}}^{n+1}\cdot d\mathbf{a}^{n+1} - \int_{S(t)} \mathbf{B}^{n}\cdot d\mathbf{a}^{n}\right] = 0$$

Zero **for ideal MHD** by frozen-in flux theorem:

$$\frac{d}{dt}\int_{S_t} \mathbf{B}\cdot d\mathbf{a} = \int_{S_t} \overset{*}{\mathbf{B}}\cdot d\mathbf{a} = 0$$

Terms in red are zero for ideal MHD so nothing needs to be done if fluxes are degrees of freedom.

# Solve magnetic diffusion using edge/face elements which preserve discrete divergence free property

weakly enforced

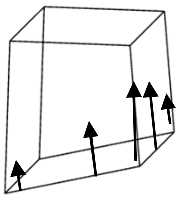
$$\nabla \times \mathbf{H} = \mathbf{J} \qquad \frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$$

Exact relationship

$$\nabla \bullet \mathbf{J} = 0 \qquad \nabla \bullet \mathbf{B} = 0$$

$$\mathbf{B} = \mu \mathbf{H} \qquad \mathbf{J} = \sigma \mathbf{E}$$

$$\text{boundary conditions} \begin{cases} \mathbf{E} \times \mathbf{n} = \mathbf{E}_b \times \mathbf{n} \text{ on } \Gamma_1 (Dirichlet), \\ \mathbf{H} \times \mathbf{n} = \mathbf{H}_b \times \mathbf{n} \text{ on } \Gamma_2 (Neumann) \end{cases}.$$



Edge element

$$\int \sigma \mathbf{E}^{n+1} \bullet \hat{\mathbf{E}} dV + \Delta t \int \frac{\text{curl}\, \mathbf{E}^{n+1} \bullet \text{curl}\, \hat{\mathbf{E}}}{\mu} dV = \int \frac{\mathbf{B}^{n} \bullet \mathbf{curl}\, \hat{\mathbf{E}}}{\mu} dV - \int \mathbf{H}_b \times \mathbf{n} \bullet \hat{\mathbf{E}} dA$$

B = magnetic flux density   E = electric field   H = magnetic field

$\mu$ = permeability   $\sigma$ = conductivity   J = current density

$\mu$ and $\sigma$ positive and finite everywhere in W

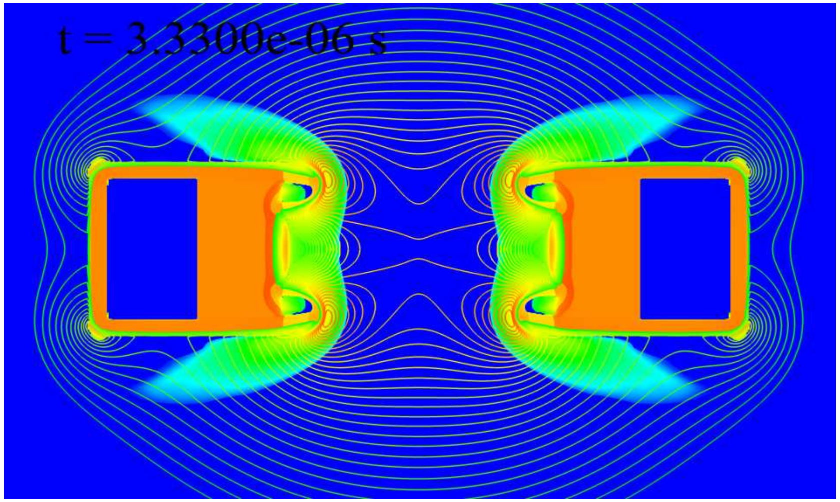
# Z Science with Alegra

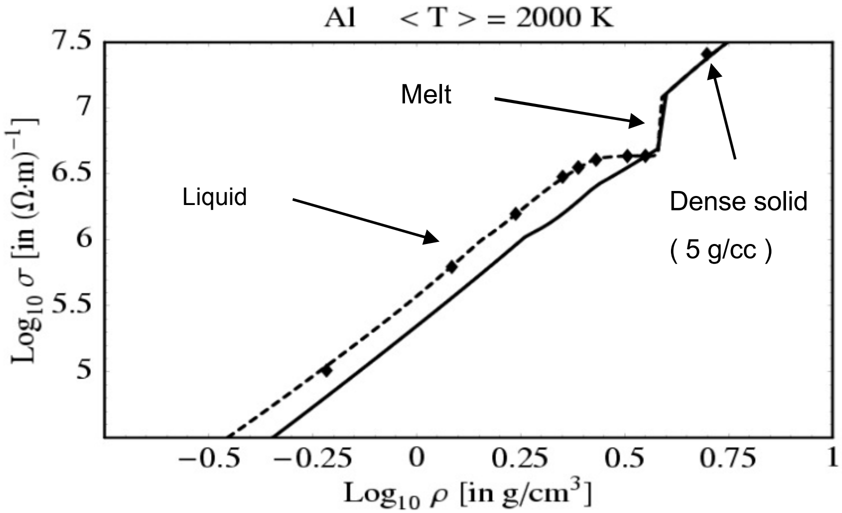
1. Using DFT models to produce material properties for Alegra in conjunction with appropriate circuit coupled magnetohydrodynamic (MHD) models, predictive design of Z dynamic materials experiments was enabled.

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

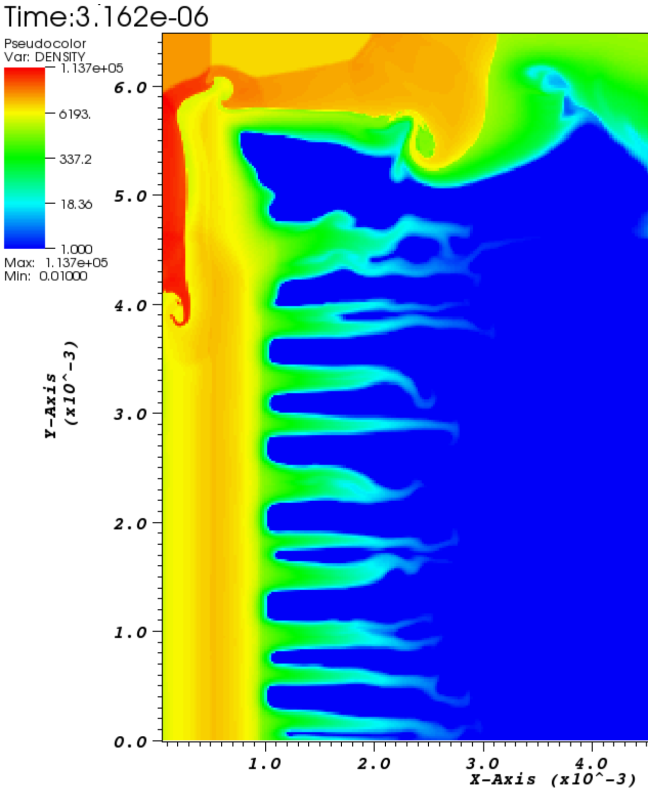
3. In the warm dense matter regime Alegra is a powerful tool for simulatir MHD physics

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



# However, Low Density Regions Matter



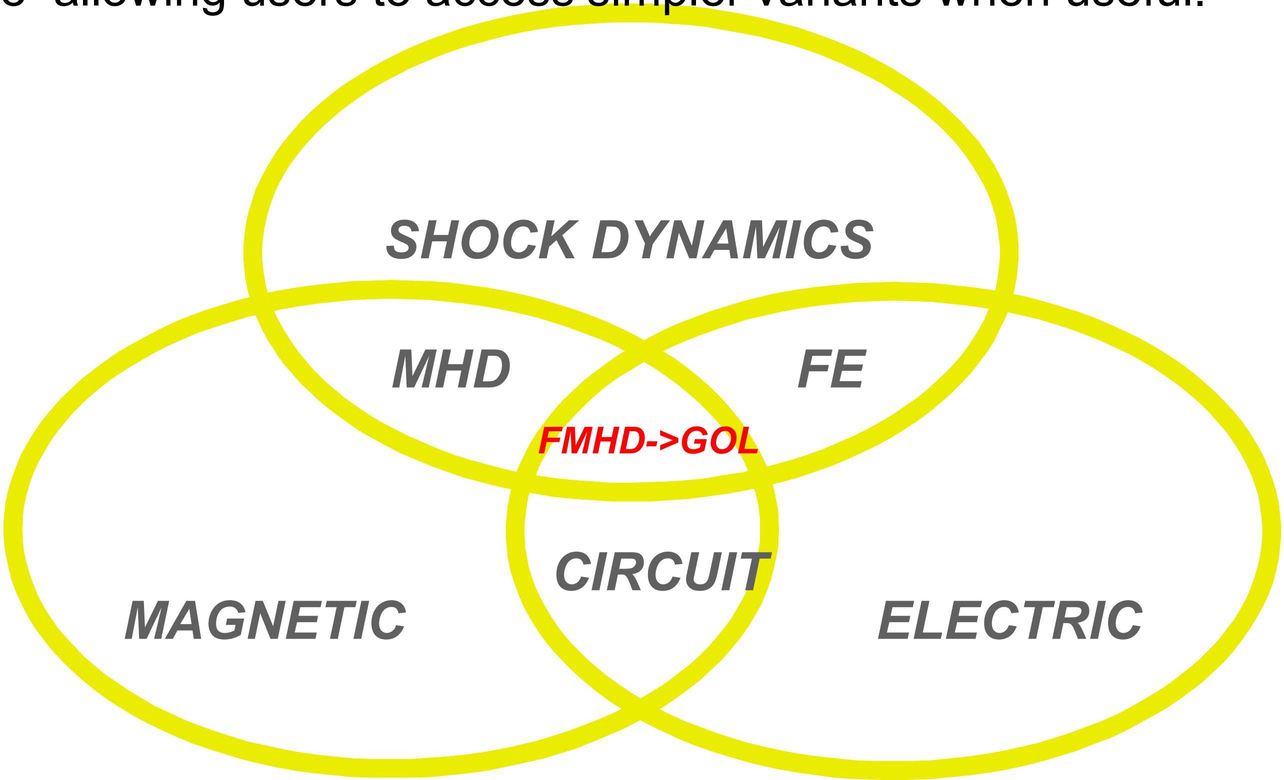

"Eddy" experiment on stagnation: the current flow in low density regions affects the dynamics

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 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?*
- *The standard MHD model has issues…*
- We have MHD and EM propagation behavior. We need a better set of equation options.

ALEGRA SHOCK & MULTIPHYSICS

We desire to move forward toward a more complete coverage of physics modeling space while  allowing users to access simpler variants when useful.




Development Strategy

1. FMHD = Full Maxwell Hydrodynamics
2. GOL = FMHD + current density equation derived from a 2-fluid model

# FMHD and Generalized Ohm's Law Equations

$$
\begin{cases}
\dfrac{\partial \rho}{\partial t} + \mathscr{L}_{\mathbf{u}}\rho = 0 & \text{Conservation of Mass} \\
\dfrac{\partial}{\partial t}(\rho \mathbf{u}) + \mathscr{L}_{\mathbf{u}}(\rho \mathbf{u}) = \operatorname{div} \mathbb{T} + q\mathcal{E} + \mathcal{J} \times \mathbf{B} & \text{Conservation of Momentum} \\
\overset{\star}{\mathbf{B}} = -\,\mathbf{curl}\,\mathcal{E} & \text{Faraday's Law} \\
\overset{\star}{\mathbf{D}} + \mathcal{J} = \mathbf{curl}\,\mathcal{H} & \text{Ampére's Law} \\
\dfrac{\partial \mathbf{J}}{\partial t} + \mathscr{L}_{\mathbf{u}}\mathbf{J} + \mathscr{L}_{\mathcal{J}}\mathbf{u} - \dfrac{1}{e n_e}\mathscr{L}_{\mathcal{J}}\mathcal{J} = \operatorname{div}\mathbb{T}_{\mathbf{j}} + \dfrac{n_e e^2}{m_e}\left(\mathcal{E} - \dfrac{1}{n_e e}\mathcal{J} \times \mathbf{B} - \eta \mathcal{J}\right) & \text{Generalized Ohm's Law} \\
\dfrac{\partial}{\partial t}q + \operatorname{div}\mathbf{J} = 0 & \text{Conservation of Charge} \\
\operatorname{div}\mathbf{D} = q & \text{Gauss' Law} \\
\operatorname{div}\mathbf{B} = 0 & \text{Involution Condition}
\end{cases}
$$

Ohm's Law

Hall Correction

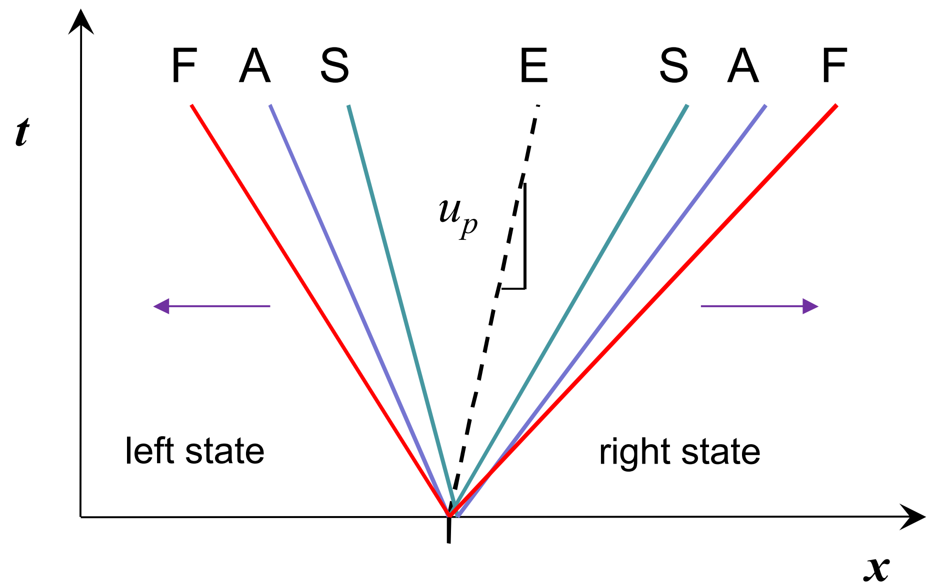
- Features:
  - Full Maxwell equation modeling (EM waves)
  - GOL includes additional equation for current density with stiff right hand side.
  - Need closures for permittivity, conductivity, electron pressure, and electron number density.

# Issues with MHD

- 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!
- Alegra has "maxfast" option which allows for user fudging to get problems to complete.




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

# Alegra's Time integration

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

Hydro

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

Ideal MHD

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

Magnetic Diffusion

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

- 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

$$\begin{cases} u_{(i+1)}^{n+1} = u^n - \frac{\Delta t}{2\rho} ik(p_{(i)}^{n+1} + p^n) \\ x_{(i+1)}^{n+1} = x^n + \frac{\Delta t}{2}(u_{(i+1)}^{n+1} + u^n) \\ p_{(i+1)}^{n+1} = p^n - \frac{\Delta t}{2} ik\rho\alpha^2(u_{(i+1)}^{n+1} + u^n) \end{cases}$$

Ideal MHD

$$\begin{cases} u_{(i+1)}^{n+1} = u^n - \frac{\Delta t}{2\rho} ik((p_{(i)}^{n+1} + p^n) + \mu^{-1}B_0(B_{(i)}^{n+1} + B^n)) \\ x_{(i+1)}^{n+1} = x^n + \frac{\Delta t}{2}(u_{(i+1)}^{n+1} + u^n) \\ p_{(i+1)}^{n+1} = p^n - \frac{\Delta t}{2} ik\rho\alpha^2(u_{(i+1)}^{n+1} + u^n) \\ B_{(i+1)}^{n+1} = B^n - \frac{\Delta t}{2} ikB_0(u_{(i+1)}^{n+1} + u^n) \end{cases}$$

4. Rewrite as matrix equations

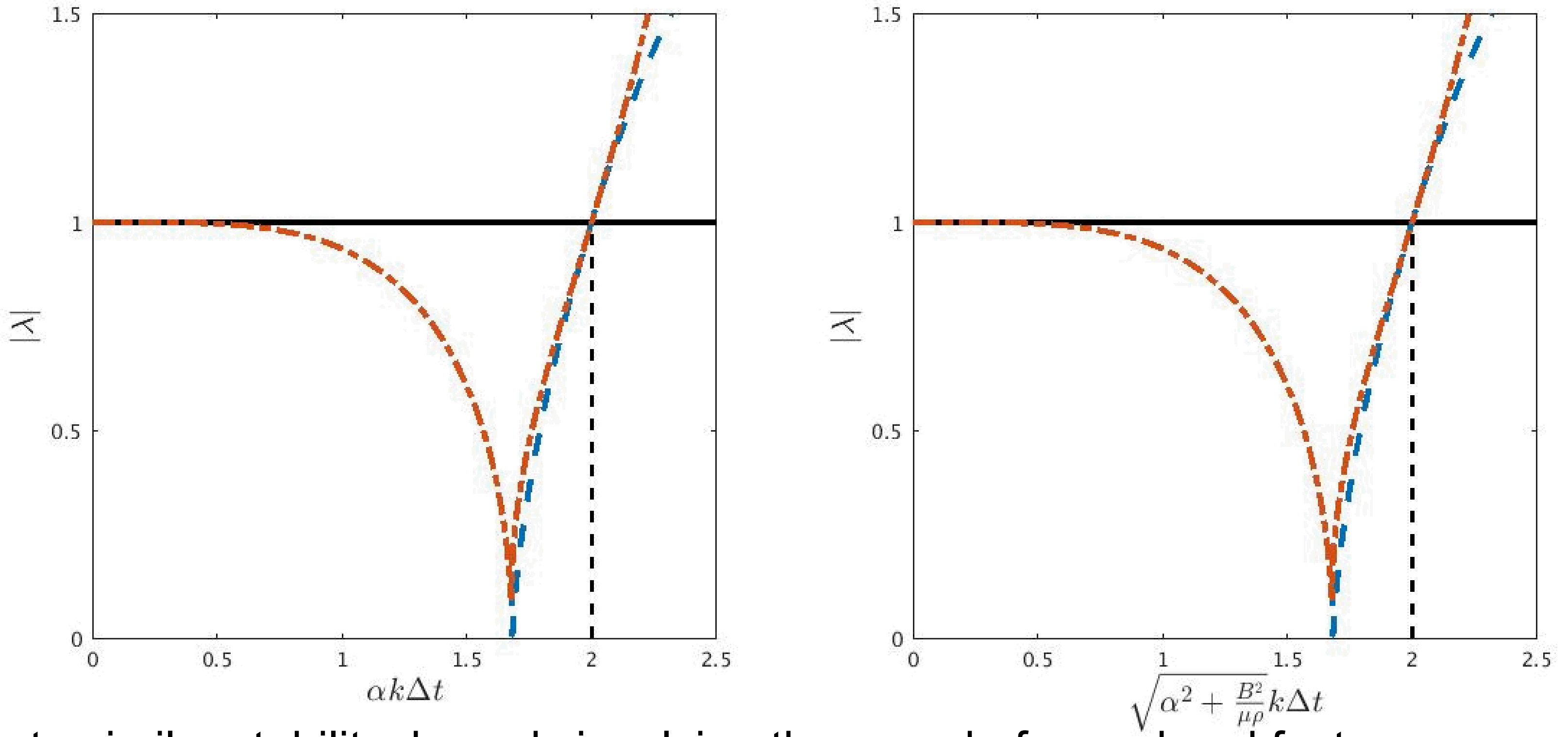
$$\xi_{(i+1)}^{n+1} = \mathbb{A}_1 \xi_{(i)}^{n+1} + \mathbb{A}_0 \xi^n \qquad \xi_{(2)}^{n+1} = \mathbb{A}\xi^n, \quad \mathbb{A} = \mathbb{A}_0 + \mathbb{A}_1(\mathbb{A}_0 + \mathbb{A}_1)$$

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

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

# Stability of Predictor Corrector

Time discrete analysis requires eigenvalues of an amplification matrix less than 1




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!

# Full Maxwell Hydrodynamics

$$
\begin{cases}
\dfrac{\partial}{\partial t}\rho + \mathrm{div}(\rho \mathbf{u}) = 0 \\
\dfrac{\partial}{\partial t}\mathbf{u} + \mathrm{div}(\mathbf{u} \otimes \mathbf{u} + \mathbb{I}p) = \sigma \mathbf{E} \times \mathbf{B} \\
\dfrac{\partial}{\partial t}\mathrm{U} + \mathrm{div}((\mathrm{U} + p)\mathbf{u}) = \sigma \mathbf{E} \cdot \mathbf{E} \\
\dfrac{\partial}{\partial t}\mathbf{E} + \dfrac{\sigma}{\epsilon_0}\mathbf{E} - \mathrm{c}_0^2 \, \mathbf{curl}\, \mathbf{B} = 0 \\
\dfrac{\partial}{\partial t}\mathbf{B} + \mathbf{curl}\, \mathbf{E} = 0
\end{cases}
$$

- Single Fluid Representation
- Classical Ohm's Law
- Do not neglect electric displacement
- Neglect Coulomb force for the moment (neutral plasma)

$$
\frac{\partial}{\partial t}\begin{bmatrix}\rho\\ u\\ p\\ E\\ B\end{bmatrix} + \frac{\partial}{\partial x}\begin{pmatrix} u & \rho & & & \\ & u & \frac{1}{\rho} & & \\ & \rho\alpha^2 & u & & \\ & & & & \mathrm{c}_0^2 \\ & & & 1 & \end{pmatrix}\begin{bmatrix}\rho\\ u\\ p\\ E\\ B\end{bmatrix} - \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sigma}{\rho}B & \frac{\sigma}{\rho}E \\ 0 & 0 & 0 & \sigma(\gamma-1)(2E-B) & -\sigma(\gamma-1)E \\ 0 & 0 & 0 & -\sigma & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}\begin{bmatrix}\rho\\ u\\ p\\ E\\ B\end{bmatrix} = \mathbf{0}
$$

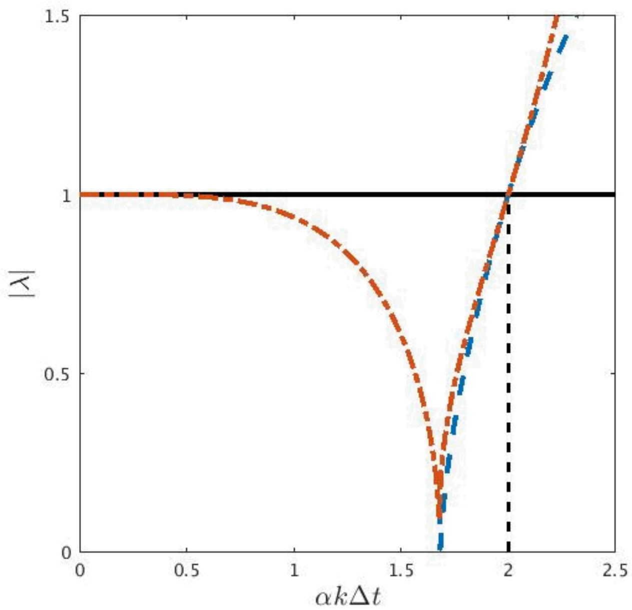
Characteristic Speeds $(\pm c, u, u \pm \alpha)$

Dispersion Relation $(\omega - ku)(\omega - k(u+\alpha))(\omega - k(u+\alpha))(\omega^2 + \mathrm{i}\frac{\sigma}{\epsilon_0}\omega - \mathrm{c}_0^2 k^2) = 0$

System has energy decay for every linear perturbation.
No Fast Alvén Speed
Result generalizes to 3D.

# Predictor Corrector for FMHD

$$\begin{cases} \rho_{(i)}^{n+1/2}\mathbf{u}_{(i+1)}^{n+1} = \mathbf{u}^n - \Delta t\left(\nabla p_{(i)}^{n+1/2} - \frac{\sigma}{\epsilon}\mathbf{D}_{(i)}^{n+1/2}\times\mathbf{B}_{(i)}^{n+1/2}\right) \\ \mathbf{x}_{(i+1)}^{n+1} = \mathbf{x}^n + \Delta t\,\mathbf{u}_{(i+1)}^{n+1/2} \\ \rho_{(i+1)}^{n+1} = \rho^n - \Delta t\,\rho_{(i+1)}^{n+1/2}\,\mathrm{div}\,\mathbf{u}_{(i+1)}^{n+1/2} \\ p_{(i+1)}^{n+1} = p^n - \Delta t\,\rho_{(i+1)}^{n+1/2}(\alpha_{(i+1)}^{n+1/2})^2\,\mathrm{div}\,\mathbf{u}_{(i+1)}^{n+1/2} + (\gamma-1)\frac{\sigma}{\epsilon^2}|\mathbf{D}_{(i+1)}^{n+1/2}|^2 \\ (1+\frac{\Delta t\sigma}{\epsilon})\mathbf{E}_{(i+1)}^{n+1} - \Delta t c^2\,\mathbf{curl}\,\mathbf{B}_{(i+1)}^{n+1} = \frac{1}{\epsilon}\mathbf{D}^n \\ \mathbf{B}_{(i+1)}^{n+1} + \Delta t\,\mathbf{curl}\,\mathbf{E}_{(i+1)}^{n+1} = \mathbf{B}^n \\ \mathbf{D}_{(i+1)}^{n+1} = \epsilon\mathbf{E}_{(i+1)}^{n+1} \end{cases}$$




- 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 Star.

Seems very similar to ALE-IMEX
2D von Neumann analysis seems prudent

# Field Solves and Time Step Control

1. We know how to precondition the Eddy Current Schur Complement system

$$\left(\mathbb{M}_{\mathscr{E}}^{\epsilon+\Delta t\sigma} + \mathbf{curl}_h^T \mathbb{M}_{\mathscr{F}}^{\mu^{-1}} \mathbf{curl}_h\right)\mathbf{E}^{n+1} = \epsilon^{-1}\mathbf{D}^n + \mathbf{curl}_h^T \mathbb{M}_{\mathscr{F}}^{\mu^{-1}} \mathbf{B}^n$$

$$\left(\left(\frac{h^2}{c^2\Delta t^2} + \frac{\sigma\mu h^2}{\Delta t}\right)\mathbb{I} + \mathbf{curl}_h^T \mathbf{curl}_h\right)\mathbf{E}^{n+1} = \frac{hZ}{\Delta t}\mathbf{D}^n + \mathbf{curl}_h^T \mathbf{B}^n$$

2. This system can be poorly conditioned. Use time step control to control ratio of material parameters. Experience with MHD K ~ 10^6 to 10^9 suffices

$$\frac{\frac{h_{\max}^2}{\Delta t^2 c^2} + \frac{\sigma_{\max}\mu h_{\max}^2}{\Delta t}}{\frac{h_{\min}^2}{\Delta t^2 c^2} + \frac{\sigma_{\min}\mu h_{\min}^2}{\Delta t}} < K \implies \Delta t < \frac{\epsilon(h_{\max}^2 - K h_{\min}^2)}{K h_{\min}^2 \sigma_{\min} - h_{\max}^2 \sigma_{\max}}$$

3. We can guess the EM dof from the predictor step for the correction step. Will this reduce # iterations for the second step? Set up for ML will probably make this improvement marginal.

# Remap Operators

1. Nodal Advection for velocities
2. Mesh intersection for cell centered quantities
3. Constrained Transport for Maxwell fields

## Constrained transport (CT)

1. Discrete Lie Derivative on 2-forms
2. Exterior derivative commutes with Lie Derivative so it preserves the involution condition on **B**
3. Essentially a finite volume technique on faces

# Remap Algorithms Extensions – Reynolds transport notation.

- **0-Form**

$$\frac{d}{dt}f = \frac{\partial f}{\partial t} + v \cdot \nabla f$$

- **1-Form**

$$\frac{\boldsymbol{d}}{\boldsymbol{dt}}\int_{M_t^1} \boldsymbol{A}\cdot \boldsymbol{dx} = \int_{M_t^1}\left[\frac{\boldsymbol{\partial A}}{\boldsymbol{\partial t}} - \boldsymbol{v}\times(\boldsymbol{\nabla}\times \boldsymbol{A}) + \boldsymbol{\nabla}(\boldsymbol{v}\cdot \boldsymbol{A})\right]\cdot \boldsymbol{dx}$$

- **2-Form**

$$\frac{\boldsymbol{d}}{\boldsymbol{dt}}\int_{M_t^2} \boldsymbol{B}\cdot \boldsymbol{da} = \int_{M_t^2}\left[\frac{\boldsymbol{\partial B}}{\boldsymbol{\partial t}} + \boldsymbol{v}(\boldsymbol{\nabla}\cdot \boldsymbol{B}) - \boldsymbol{\nabla}\times(\boldsymbol{v}\times \boldsymbol{B})\right]\cdot \boldsymbol{da}$$

- **3-Form**

$$\frac{d}{dt}\int_{M_t^3} \rho\, dV = \int_{M_t^3}\left[\frac{\partial \rho}{\partial t} + \nabla\cdot(v\rho)\right] dV$$

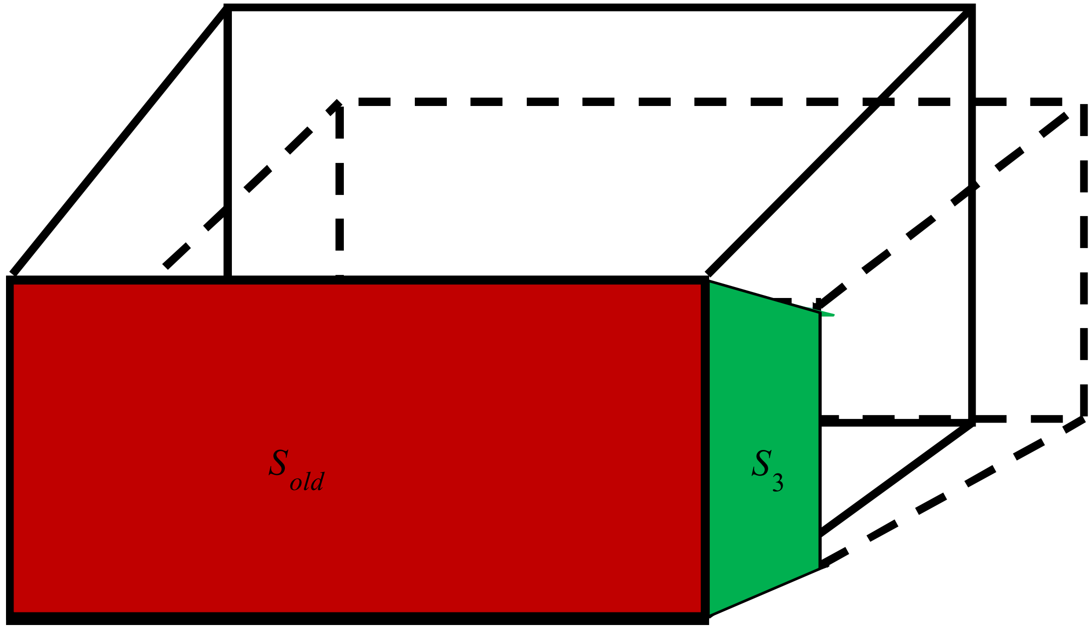
Previously implemented for curl free and div free fields

Need to add this contribution in for arbitrary fields

For FMHD we only need an extended 2-Form remap.

# Visual Representation of 2-Form remap

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




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).

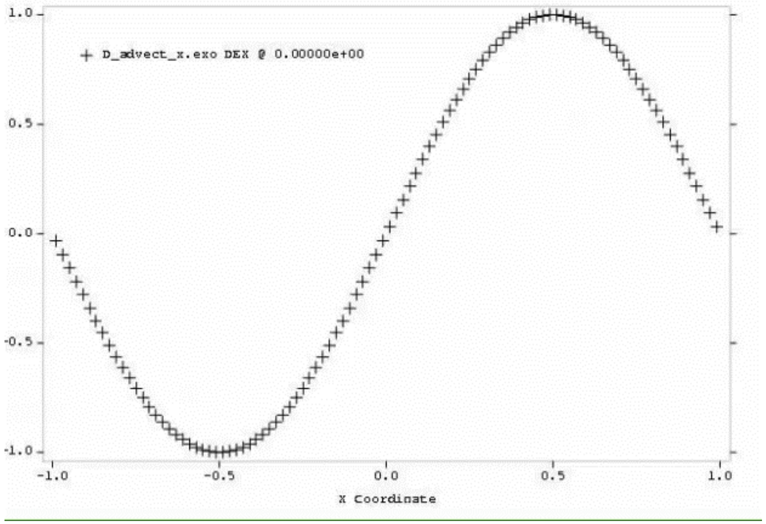
# General 2-Form Implementation

- We have extended the divergence free remap code to accommodate the volumetric contribution.
- This volumetric contribution must NOT be a spatially split remap operator since we are doing constrained transport which is fundamental unsplit.
- This operation is not exactly the same as a volume based remap since it is the swept volume contribution rather than final intersected cell volumes that are desired.
- We are using a toolkit in a third party library (r3d) to compute the signed swept volume.

# Initial General Face Element Remap Results

- A low order volume remap contribution is in testing and refinement phase.
- An initial test problem has the electric displacement field pointed in the direction of the periodic domain.
- 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.
- High order volume remap contribution algorithms are possible.

X component of electric displacement in periodic x domain



# ALE Splitting for GOL

GOL is not generally formulated in Galilean invariants. Starting from GOL not assuming quasi-neutrality we have derived a frame invariant formulation.

$$\mathcal{J} = \mathbf{J} - q\mathbf{u} \qquad \dot{q} = -\operatorname{div}\mathcal{J}$$

Galilean Current Density — Conservation of Charge

$$\dot{\mathbf{J}} = -\operatorname{div}(\mathcal{J}\otimes\mathbf{u} - \tfrac{1}{q_e}\mathcal{J}\otimes\mathcal{J}) - \tfrac{e}{m_e}(\nabla p_e - \mathcal{J}\times\mathbf{B}) + \epsilon\omega_p^2\mathcal{E} - \omega_i\mathcal{J}$$

Material Derivative — Stress Tensor — "Lorentz Force" + "friction"

**GOL → Current Density is a Compressible Fluid!** $\mathbf{J} \approx \mathbf{J}_h \in [\mathscr{V}_h]^3$

**Lagrangian Frame:** Incorporate J, into midpoint time integrator

**Remap:** Nodal Remap of **J.** Constrained transport of **D** implies cell centered remap of q.

**Charge Density:**

Discrete weak Galilean Invariant Ampere-Maxwell implies weak Galilean invariant Continuity Equation (on nodes)

***Do Edge -> Face projection operators (i.e. Discrete Hodge Star) create/destroy charge? Do we need to enforce charge conservation as an additional equation?***

# Summary

- We believe that there is a clear path forward to implementation of a Full Maxwell hydrodynamic option in Alegra.
- This option has promise to significantly improve the required explicit time step control at the cost of another diffusion solve but should allow for major elimination of knobs.
- Two Solves v. Fast Alven speed: Will it be possible to achieve better physics AND improvement in overall performance AND robustness?
- The approach extends naturally and conveniently to an extended Ohm's law model in the same ALE modeling framework which will allow a new extended MHD option for impact on Z modeling efforts.
- We are pushing forward to obtain a full integrated capability for continuum electrodynamic models of various types and getting them to work well together with full user control over options.