Two and Three-Dimensional Magnetohydrodynamic Modeling in ALEGRA

An update on recent progress

August 6-7, 1998

Los Alamos Workshop on Radiation MHD

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy under contract DE-AC04-94AL85000.

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The Z Facility

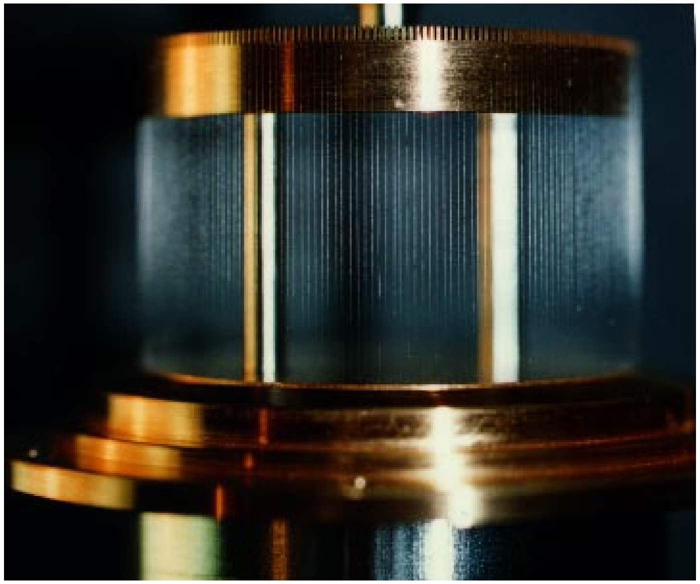
Performance Milestones Achieved on Z

Pulsed Power Milestones	required value	achieved value	date achieved
x-ray energy	1.5 MJ	1.8 MJ 2.0 MJ	Nov. 1996 March 1997
x-ray power	150 TW	200 TW 290 TW	Nov. 1996 Jan. 1998
radiation temperature for weapon physics	100 eV	100 eV 140 eV	April 1997 Oct. 1997
radiation temperature for capsule compression	150 eV	155 eV	March 1998

First shot on Z - October 2, 1996

Why Two-Dimensional, Massively Parallel, Coupled Radiation Magnetohydrodynamics?

- There is a large degree of azimuthal symmetry in the array that allows 2D cylindrical simulations.
- Wire merger modeling assumes axial symmetry that allows 2D Cartesian modeling.
- 2D simulations are faster and cheaper than 3D simulations.
- Many tools used today are 2D and predictive with tuned initial perturbations.
- Code comparisons in 2D.



The 240 wire array, 2 cm tall and 4 cm in diameter, from Z shot #26 that achieved 1.85 MJ x-ray energy in a 160 TW, 6.8 ns fwhm pulse.

Applications of 2D Magnetohydrodynamics at Sandia

Z pinch simulations

- Axisymmetric wire array and liner implosions and radiation production
- Magneto-Raleigh-Taylor simulation and mitigation
- End-on hohlraum simulations
- Static wall hohlraum simulations and capsule implosion
- Dynamic hohlraum simulations and capsule implosion

Power flow simulations

- Disk feed power flow under extremely high currents and magnetic fields

Magnetoquasistatics neglects terms from electromechanics.

$$\dot{\rho} + \rho \nabla \bullet \mathbf{u} = 0 \text{ (mass)} \tag{74}$$

$$\rho \dot{\mathbf{u}} = \nabla \bullet \underset{\sim}{\mathbf{T}} + \kappa_1 \rho_f \boldsymbol{E} + \kappa_2 \boldsymbol{J} \times \boldsymbol{B} \text{ (momentum)} \tag{75}$$

$$\rho \dot{e} = \underset{\sim}{\mathbf{T}} : \nabla \mathbf{u} + \kappa_1 \hat{J} \bullet \hat{\boldsymbol{E}} \text{ (energy)} \tag{76}$$

$$\nabla \times \boldsymbol{E} = -\kappa_3 \partial \boldsymbol{H} / \partial t \text{ (Faraday)} \tag{77}$$

$$\nabla \times \boldsymbol{H} = \kappa_5 \boldsymbol{J} + \kappa_4 \partial \boldsymbol{D} / \partial t \text{ (Ampere)} \tag{78}$$

$$\nabla \bullet \boldsymbol{B} = 0 \text{ (divergence)}, \mu_0 \boldsymbol{H} = \boldsymbol{B}, \nabla \bullet \boldsymbol{D} = \kappa_6 \rho_f \text{(Gauss)}, \varepsilon_0 \boldsymbol{E} = \boldsymbol{D} \tag{79}$$

$$\hat{J} = J - \rho_f \boldsymbol{u}, \hat{E} = E + \boldsymbol{u} \times \boldsymbol{B}, \hat{H} = H - \boldsymbol{u} \times \boldsymbol{D} \tag{80}$$

$$\text{Constitutive equations, e.g. : } \hat{J} = \sigma(\rho, \theta) \hat{E} \text{ (Ohm)}, \underset{\sim}{\mathbf{T}} = -p(\rho, e) \boldsymbol{I} \tag{81}$$

κ_1, κ_2, κ_3, κ_4, κ_5, and κ_6 are constants that allow multiple systems of units.

Summary of Approach

Operator split within ALEGRA framework.

Finite element formalism.

Solve for vector potential and magnetic field component orthogonal to mesh.

- A_z and B_z in cartesian geometry
- A_θ and B_θ in cylindrical geometry

Components solved for depend upon the boundary conditions.

All other magnetic quantities are derived from these.

We must approach the "ideal" MHD limit ($\sigma \to \infty$) as well as the highly diffusive limit ($\sigma \to 0$) with a scalable algorithm.

2D Cartesian Magnetohydrodynamics

Faraday's, Ohm's and Ampere's laws lead to

$$\frac{\partial A_z}{\partial t} + V_x \frac{\partial A_z}{\partial x} + V_y \frac{\partial A_z}{\partial y} = \frac{\eta}{\kappa_2 \kappa_5}\left[\frac{\partial}{\partial x}\left(\nu \frac{\partial A_z}{\partial x}\right) + \frac{\partial}{\partial y}\left(\nu \frac{\partial A_z}{\partial y}\right)\right] \tag{82}$$

and

$$\frac{\partial B_z}{\partial t} + V_x \frac{\partial B_z}{\partial x} + V_y \frac{\partial B_z}{\partial y} = \frac{1}{\kappa_2 \kappa_5}\left[\frac{\partial}{\partial x}\left(\eta \frac{\partial \nu B_z}{\partial x}\right) + \frac{\partial}{\partial y}\left(\eta \frac{\partial \nu B_z}{\partial y}\right)\right] - \left[\frac{\partial V_x}{\partial x} + \frac{\partial V_y}{\partial y}\right] B_z \tag{83}$$

The constants κ_2 and κ_5 allow for multiple systems of units.

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2D Cartesian Magnetohydrodynamics (cont.)

Compute *B* components from curl of *A*

$$B_x = \frac{\partial A_z}{\partial y} \text{ and } B_y = -\frac{\partial A_z}{\partial x} \tag{84}$$

Compute *J* from Ampere's Law

$$J_x = \frac{1}{\kappa_5}\left(\frac{\partial \nu B_z}{\partial y}\right) \text{ and } J_y = \frac{-1}{\kappa_5}\left(\frac{\partial \nu B_z}{\partial x}\right) \tag{85}$$

$$J_z = \frac{1}{\kappa_5}\left[\frac{\partial \nu B_y}{\partial x} - \frac{\partial \nu B_x}{\partial y}\right] = \frac{-1}{\kappa_5}\left[\frac{\partial}{\partial x}\left(\nu\frac{\partial A_z}{\partial x}\right) + \frac{\partial}{\partial y}\left(\nu\frac{\partial A_z}{\partial y}\right)\right] \tag{86}$$

Compute *E* from Ohm's Law

$$\vec{E} = \frac{1}{\kappa_1}[\eta\vec{J} - \kappa_2(\vec{V} \times \vec{B})] \tag{87}$$

Faraday's, Ohm's and Ampere's laws lead to

$$\frac{\partial A_\theta}{\partial t} + V_r\left(\frac{1}{r}\frac{\partial r A_\theta}{\partial r}\right) + V_z\frac{\partial A_\theta}{\partial z} = \frac{\eta}{\kappa_2\kappa_5}\left[\frac{\partial}{\partial r}\left(\nu\frac{1}{r}\frac{\partial r A_\theta}{\partial r}\right) + \frac{\partial}{\partial z}\left(\nu\frac{\partial A_\theta}{\partial z}\right)\right] \quad (88)$$

$$\frac{\partial\psi}{\partial t} + V_r\frac{\partial\psi}{\partial r} + V_z\frac{\partial\psi}{\partial z} = \frac{\eta}{\kappa_2\kappa_5}\left[r\frac{\partial}{\partial r}\left(\nu\frac{1}{r}\frac{\partial\psi}{\partial r}\right) + \frac{\partial}{\partial z}\left(\nu\frac{\partial\psi}{\partial z}\right)\right] \text{ where } \psi = rA_\theta \quad (89)$$

and

$$\frac{\partial B_\theta}{\partial t} + V_r\frac{\partial B_\theta}{\partial r} + V_z\frac{\partial B_\theta}{\partial z} = \frac{1}{\kappa_2\kappa_5}\left[\frac{\partial}{\partial r}\left(\eta\frac{1}{r}\frac{\partial r\nu B_\theta}{\partial r}\right) + \frac{\partial}{\partial z}\left(\eta\frac{\partial \nu B_\theta}{\partial z}\right)\right] - \left[\left(\frac{\partial V_r}{\partial r} + \frac{\partial V_z}{\partial z}\right)B_\theta\right] \quad (90)$$

$$\frac{\partial\chi}{\partial t} + V_r\frac{\partial\chi}{\partial r} + V_z\frac{\partial\chi}{\partial z} = \frac{1}{\kappa_2\kappa_5}\left[r\frac{\partial}{\partial r}\left(\eta\frac{1}{r}\frac{\partial\nu\chi}{\partial r}\right) + \frac{\partial}{\partial z}\left(\eta\frac{\partial\nu\chi}{\partial z}\right)\right] - \left[\left(\frac{\partial V_r}{\partial r} + \frac{\partial V_z}{\partial z} - \frac{V_r}{r}\right)\chi\right] \text{ where}$$
$$\chi = rB_\theta \quad (91)$$

The constants κ_2 and κ_5 allow for multiple systems of units.

2D Cylindrical Magnetohydrodynamics (cont.)

Compute *B* components from curl of *A*

$$B_r = -\frac{\partial A_\theta}{\partial z} \text{ and } B_z = \frac{1}{r}\frac{\partial r A_\theta}{\partial r} \qquad (92)$$

Compute *J* from Ampere's Law

$$J_r = \frac{-1}{\kappa_5}\left(\frac{\partial \nu B_\theta}{\partial z}\right) \text{ and } J_z = \frac{1}{\kappa_5}\left(\frac{1}{r}\frac{\partial r \nu B_\theta}{\partial r}\right) \qquad (93)$$

$$J_\theta = \frac{-1}{\kappa_5}\left[\frac{\partial \nu B_z}{\partial r} - \frac{\partial \nu B_r}{\partial z}\right] = \frac{-1}{\kappa_5}\left[\frac{\partial}{\partial r}\left(\nu \frac{1}{r}\frac{\partial r A_\theta}{\partial r}\right) + \frac{\partial}{\partial z}\left(\nu \frac{\partial A_\theta}{\partial z}\right)\right] \qquad (94)$$

Compute *E* from Ohm's Law

$$\vec{E} = \frac{1}{\kappa_1}[\eta \vec{J} - \kappa_2(\vec{V} \times \vec{B})] \qquad (95)$$

Finite Element Formulation

Using a weak formulation of the equations, the symmetric, semi-discrete form of the equations in matrix form become

Cartesian:

$$M\frac{DA}{Dt} + KA = L_A \qquad (96)$$

$$M\frac{DB}{Dt} + KB + SB = L_B \qquad (97)$$

Cylindrical:

$$M\frac{D\psi}{Dt} + K\psi = L_\psi \qquad (88)$$

$$M\frac{D\chi}{Dt} + K\chi + S\chi = L_\chi \qquad (89)$$

where

M **= "mass" matrix involving conductivity for *A*, constants for *B***

K **= "diffusion" matrix involving permeability for *A* and *B* and conductivity for *B***

S **= stretch matrix involving velocity gradients**

L **= boundary integral column matrix for boundary conditions, (*H* on the boundary for *A*, *J* on the boundary for *B*)**

Time Integration

The time differencing is devised to support fully implicit, fully explicit, or hybrid methods.

For *A* (or ψ)

$$[M + \Delta t\theta K]\mathbf{A}^{n+1} = [M - \Delta t(1-\theta)K]\mathbf{A}^{n} + [\Delta t\theta L^{n+1} + \Delta t(1-\theta)L^{n}] \tag{98}$$

For *B* (or χ)

$$\begin{aligned}(M + \Delta t\theta K + \Delta t\theta_s S)B^{n+1} &= (M - \Delta t(1-\theta)K + \Delta t(1-\theta_s)S)B^{n} \\ &\quad + [\Delta t\theta L^{n+1} + \Delta t(1-\theta)L^{n}]\end{aligned} \tag{99}$$

with $0 < \theta \le 1$ **and** $0 < \theta_s \le 1$

2D Problems Tested

Magnetic Diffusion

Unperturbed and perturbed liner implosions

Single wire explosion

Multi-wire merger (shows need for Eulerian)

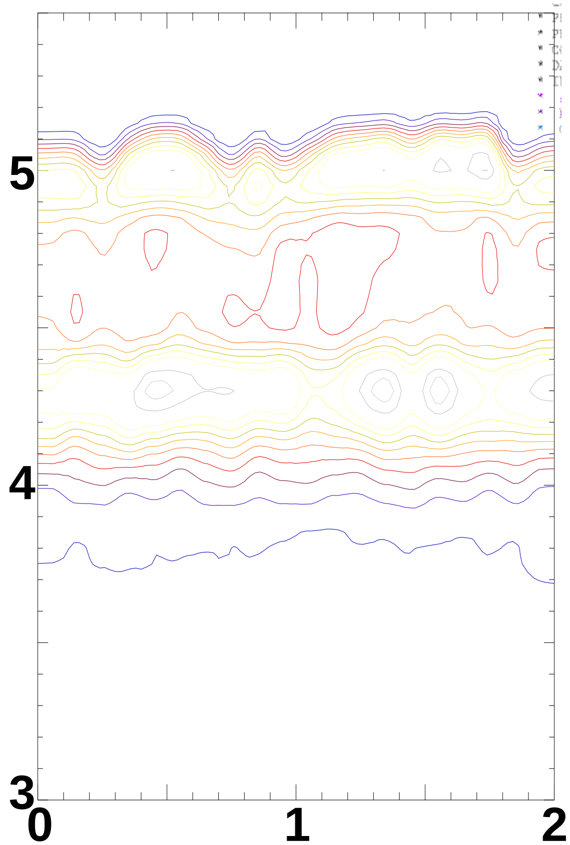
Magneto-RT (shows need for Eulerian)

Simulations with radiation (problems in different treatments of energy deposition)

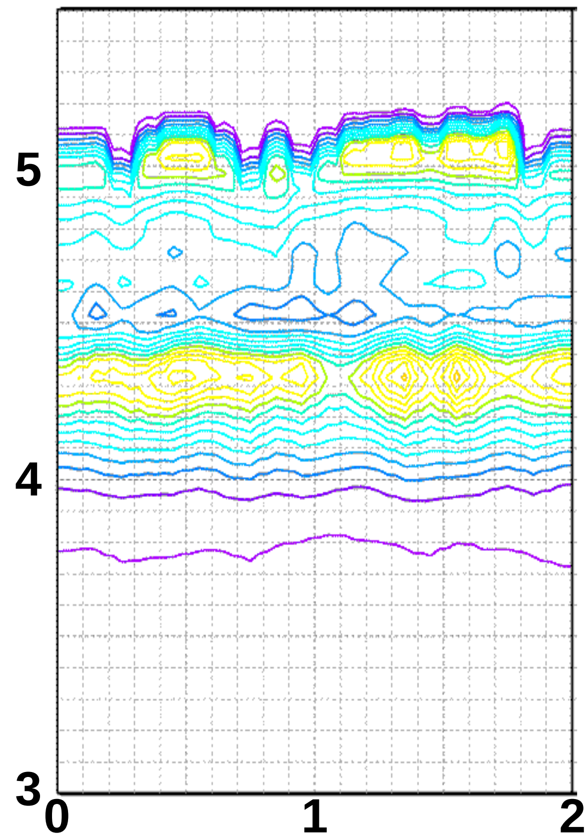
Pegasus Aluminum Liner - Code Comparison

Density Contours
time = 80 ns

Alegra



Peterson

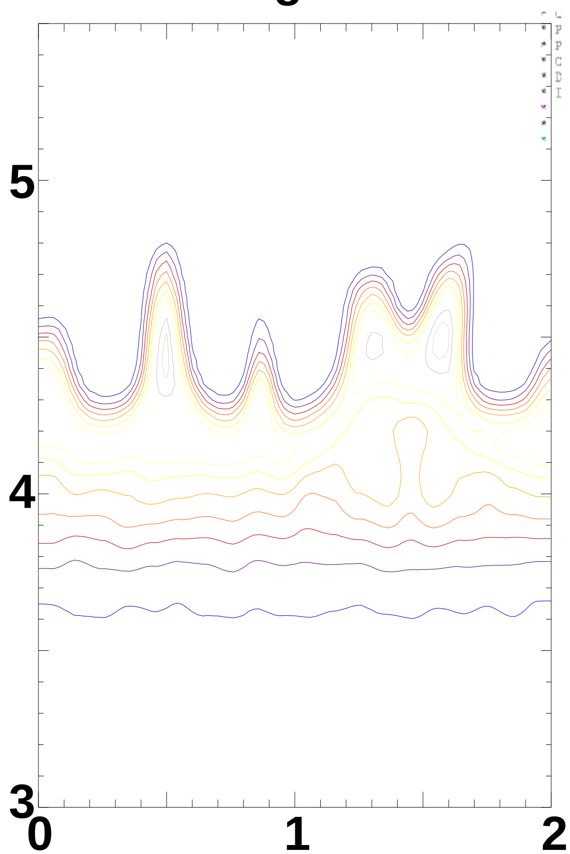


Peterson, et al., Phys. Plasmas 3 (1) 368, Jan 1996

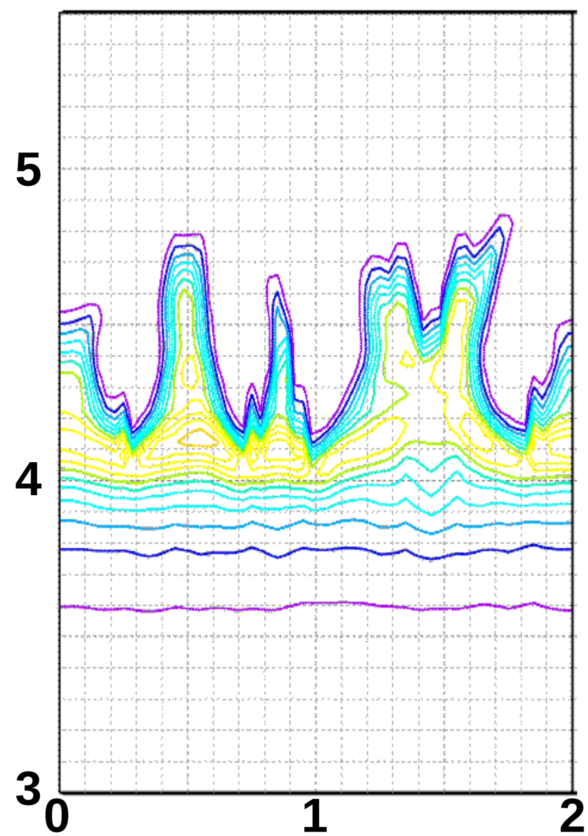
Pegasus Aluminum Liner - Code Comparison

Density Contours
time = 160 ns

Alegra



Peterson



Peterson, et al., Phys. Plasmas 3 (1) 368, Jan 1996

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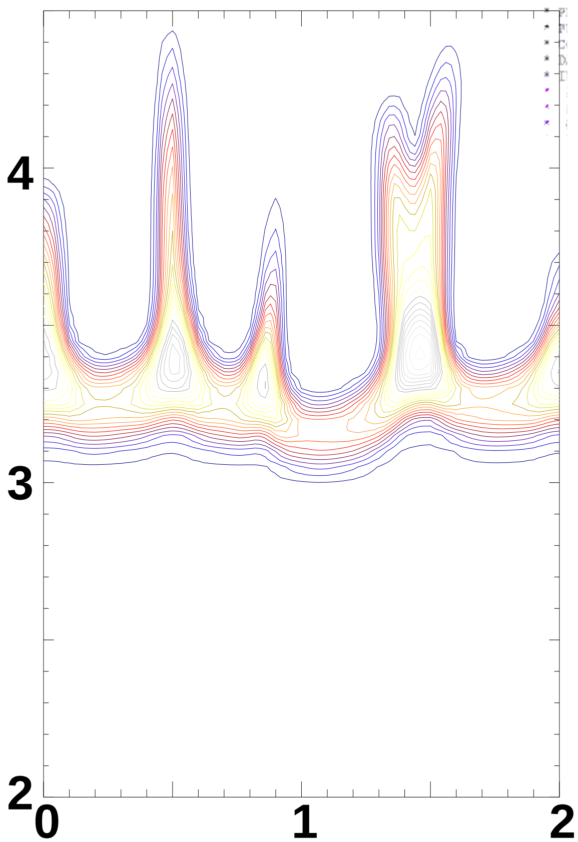
Pegasus Aluminum Liner - Code Comparison

Computational Physics R&D Department — *Pulsed Power Sciences Center*

Density Contours
time = 240 ns

Alegra



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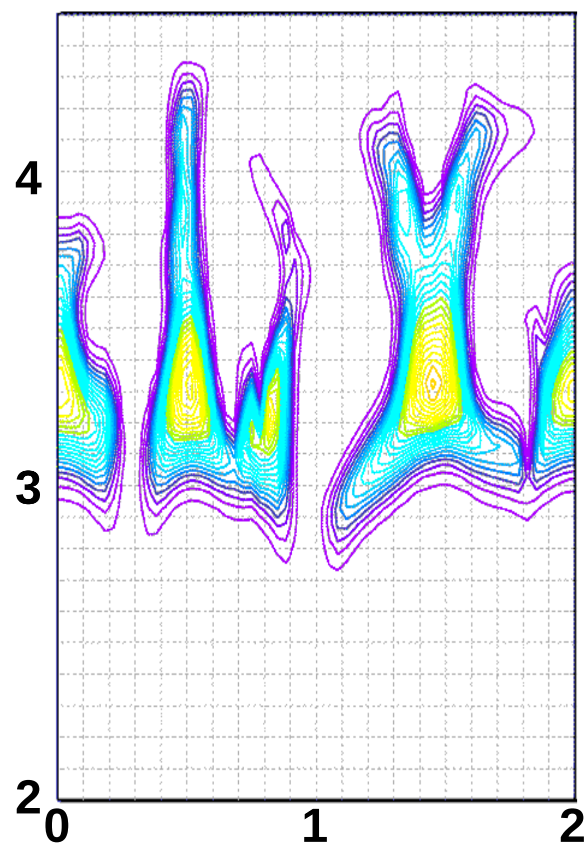


Peterson, et al., Phys. Plasmas 3 (1) 368, Jan 1996

Current and Future Work

Detailed verification efforts to gain confidence and understanding of both ALEGRA hydro, MHD and radiation.

ALE/Eulerian modeling with instabilities (advection)

More accurate calculation of J from A and B (Use BC info)

Circuit equation coupling

Combined MHD and radiation simulations (synergy)

Periodic boundary conditions to reduce mesh requirements

General production robustness

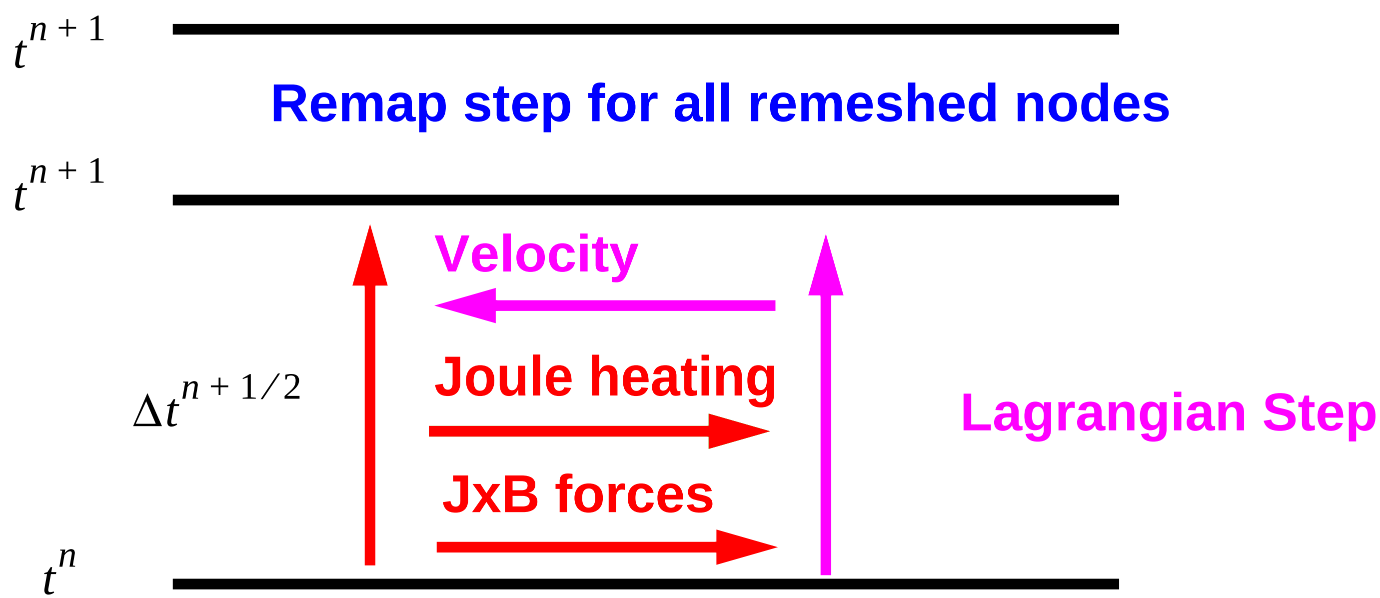
Summary of Approach

Galerkin finite element approach. Vector potential in 3D.

$$\nabla\times\left(\frac{1}{\mu_0}\nabla\times\boldsymbol{A}\right)+\sigma\left(\frac{\partial\boldsymbol{A}}{\partial t}+\nabla\phi-\boldsymbol{u}\times(\nabla\times\boldsymbol{A})\right) = 0$$

In 2D, use the vector potential component and/or magnetic field component orthogonal to mesh (cartesian or cylindrical)

Operator split within the ALEGRA framework



Formulations for 3D Magnetics

Several formulations of the magnetics are possible. We have been working with the:

"Lorentz" vector potential formulation (preferred).

(Bryant, Emson and Trowbridge).

"Modified" vector potential formulation (deficient).

Other possible future options of interest to pursue:

A-ϕ vector potential formulations.

Direct magnetic field and/or electric field formulations.

Special formulations to deal with void regions.

We must approach the "ideal" MHD limit ($\sigma \to \infty$) as well as the highly diffusive limit ($\sigma \to 0$) with a scalable algorithm.

Vector Potential Formulations

$$\nabla \bullet B = 0 \text{ implies } \boldsymbol{B} = \nabla \times \boldsymbol{A}$$

$$\nabla \times \left(\boldsymbol{E} + \frac{\partial \boldsymbol{A}}{\partial t} \right) = 0 \text{ (Faraday)}$$

$$\text{In general, } \boldsymbol{E} = -\nabla\phi - \frac{\partial \boldsymbol{A}}{\partial t}\text{, to obtain}$$

$$\nabla \times \left(\frac{1}{\mu_0} \nabla \times \boldsymbol{A} \right) + \sigma \left(\frac{\partial \boldsymbol{A}}{\partial t} + \nabla\phi - \boldsymbol{u} \times (\nabla \times \boldsymbol{A}) \right) = 0$$

An additional “gauge” condition must be imposed in order to specify the system due to the arbitrary scalar potential.

The Coulomb gauge is $\nabla \bullet \boldsymbol{A} = 0$ in which case one must impose conservation of current for an equation for ϕ.

Alternatively, we can choose ϕ as a convenient scalar function of A and u.

Formulations with a Specified Scalar Potential

Eulerian Form

$$\nabla\times\left(\frac{1}{\mu_0}\nabla\times\boldsymbol{A}\right) = \sigma\left(-\frac{\partial\boldsymbol{A}}{\partial t} + \boldsymbol{u}\times\nabla\times\boldsymbol{A} - \nabla\phi\right)$$

Lagrangian form ($\boldsymbol{u}\times\nabla\times\boldsymbol{A} = \boldsymbol{u}\bullet(\nabla\boldsymbol{A})^T - \boldsymbol{u}\bullet\nabla\boldsymbol{A}$)

$$\nabla\times\left(\frac{1}{\mu_0}\nabla\times\boldsymbol{A}\right) = \sigma\left(-\frac{D\boldsymbol{A}}{Dt} + \boldsymbol{u}\bullet(\nabla\boldsymbol{A})^T - \nabla\phi\right)$$

Can modify electric field definition by arbitrary $\nabla\phi$

$$\nabla\times\left(\frac{1}{\mu_0}\nabla\times\boldsymbol{A}\right) = \sigma\left(-\frac{D\boldsymbol{A}}{Dt} + \boldsymbol{u}\bullet(\nabla\boldsymbol{A})^T - \nabla(\boldsymbol{u}\cdot A)\right) = \sigma\left(-\frac{D\boldsymbol{A}}{Dt} - A\bullet(\nabla\boldsymbol{u})^T\right)$$

$$\nabla\times\left(\frac{1}{\mu_0}\nabla\times\boldsymbol{A}\right) = \sigma\left(-\frac{D\boldsymbol{A}}{Dt} - A\bullet(\nabla\boldsymbol{u})^T + \nabla\left(\frac{\nabla\bullet A}{\mu_0\sigma}\right)\right)$$

“Lorentz” Finite Element Formulation

The weak form for the “Lorentz” formulation is

$$\int_{\Omega} (\nabla \times N) \bullet \nu \nabla \times \boldsymbol{A}\, d\Omega + \int_{\Omega} \nabla \bullet (\sigma N) \cdot \nu \frac{\nabla \bullet A}{\sigma} d\Omega$$

$$+ \int_{\Omega} \sigma N \bullet \frac{D\boldsymbol{A}}{Dt} d\Omega + \int_{\Omega} \sigma N \bullet (A \bullet (\nabla u)^{T}) d\Omega = \int_{\Gamma} N \times H_{b} \bullet n\, d\Gamma + \int_{\Gamma} \nu (\nabla \bullet A)_{b} N \bullet n\, d\Gamma$$

Natural tangential magnetic field boundary conditions.

$(\nabla \bullet A)_{b} = \dfrac{-A_{b} \cdot n}{L\beta}$ **gives scalability for small σ.**

More work needed on tangential electric field BCs.

"Modified" Finite Element Formulation

The weak form for the "modified" formulation is

$$\int_{\Omega} (\nabla \times N) \bullet \nu \nabla \times \boldsymbol{A} \, d\Omega$$

$$+ \int_{\Omega} \sigma N \bullet \frac{D\boldsymbol{A}}{Dt} d\Omega + \int_{\Omega} \sigma N \bullet (A \bullet (\nabla u)^T) d\Omega = \int_{\Gamma} N \times H_b \bullet n \, d\Gamma$$

Natural tangential magnetic field boundary conditions.

Should not work well for small conductivities but for problems with large conductivities everywhere in the mesh should give the same results as the "Lorentz" formulation.

Time Integration

The discrete transient magnetic equations are

$$[M + \Delta t\theta K + \Delta t\theta_s S]\boldsymbol{A}^{n+1} =$$

$$[M - \Delta t(1-\theta)K + \Delta t(1-\theta_s)S]\boldsymbol{A}^{n} + \Delta t(1-\theta)\underset{\sim}{F}{}_A^{n} + \Delta t\theta\underset{\sim}{F}{}_A^{n+1}$$

where

- M **is the magnetic mass matrix**
- K **is the discrete curl-curl operator**
- S **is the contribution from the** $\boldsymbol{u} \bullet (\nabla \boldsymbol{A})^T$ **or** $A \bullet (\nabla u)^T$ **term.**
- F_A **is the contribution from the natural boundary conditions.**
- θ, θ_s **are time weights for K and S operator, resp.**

Fully integrated elements.

Solve using the Aztec parallel iterative solver package.

Algorithm Overview

- Lagrangian Step
  - Calculate $u^{n+1/2}$ using $\underset{\sim}{\mathbf{T}}^n, B^n, J^n$ and x^n (Explicit)
  - $x^{n+1} = x^n + u^{n+1/2}\Delta t^{n+1/2}$ (update current coordinates)
  - Calculate A^{n+1} using $u^{n+1/2}$ at x^n coordinates (Implicit)
  - Calculate B^{n+1}, J^{n+1} and deposit Joule heat
  - Calculate new material state at t^{n+1}
- Eulerian Step (Optional by blocks and ALE triggers)
  - Define new x^{n+1}.
  - Flux A^{n+1}
  - Recalculate material state and B^{n+1}, J^{n+1} at t^{n+1}
- Calculate new time step based on properties at t^{n+1}.

Consistent Formulation for Current Density

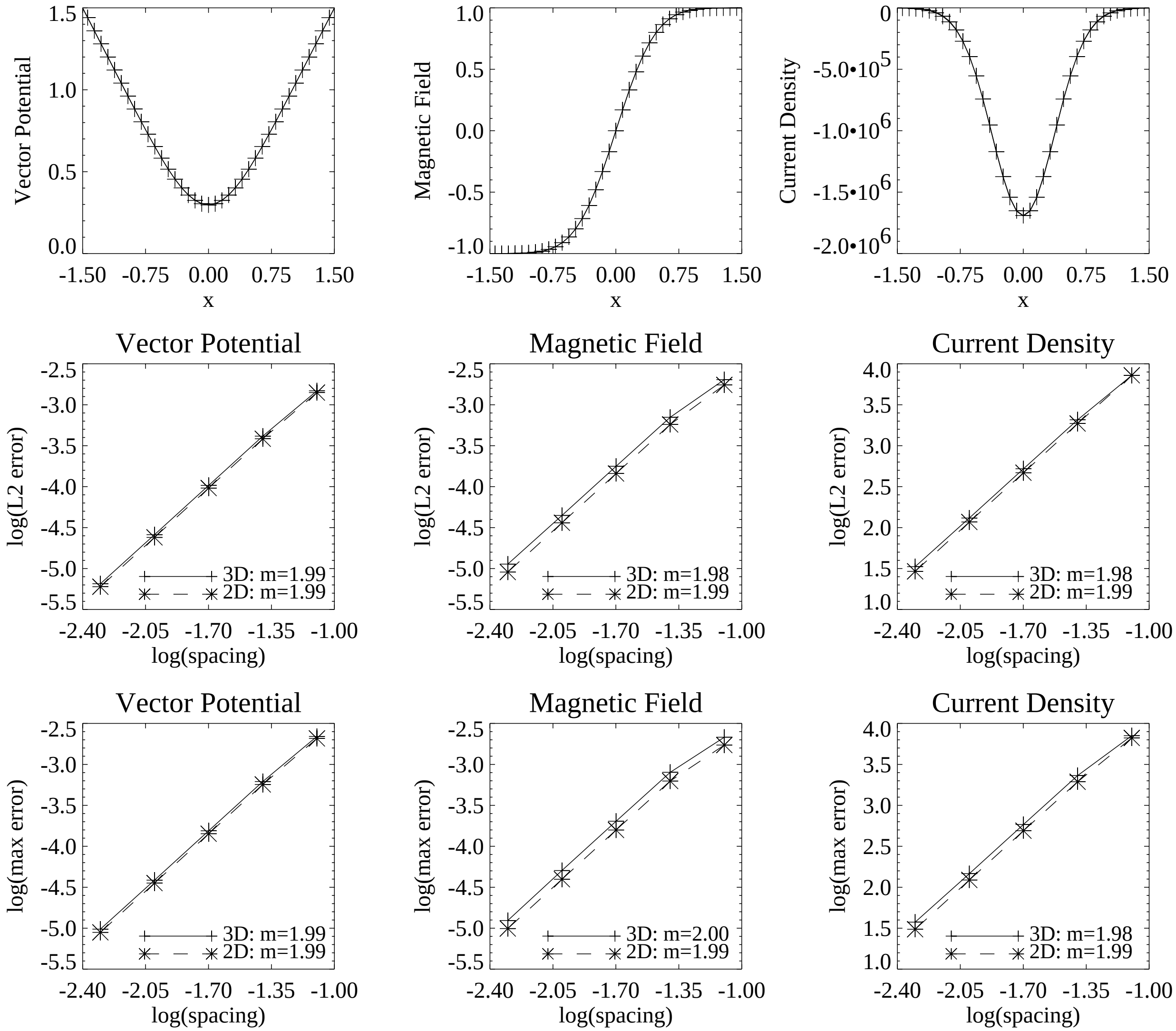
A consistent approach to calculating the current density, J, from the vector potential, A, is to use the weak form:

$$\int_{\Omega} (\nabla \times N) \bullet \nu \nabla \times \boldsymbol{A} \, d\Omega - \int_{\Omega} N \bullet J \, d\Omega = \int_{\Gamma} N \times H_b \bullet n \, d\Gamma$$

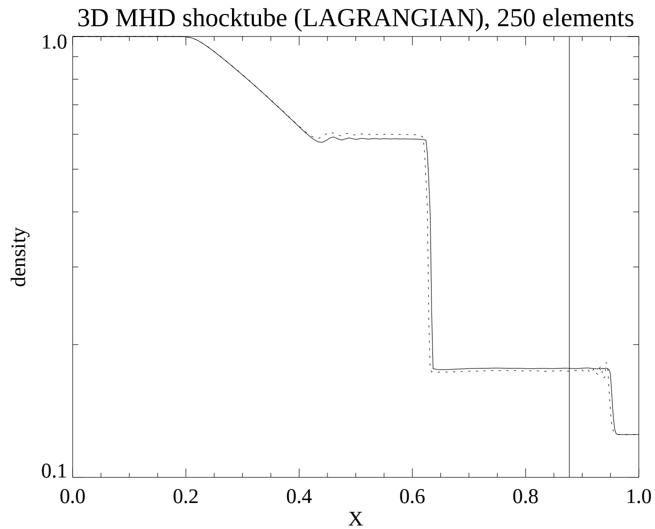
If H_b is known from boundary conditions, then the known value is applied in the boundary term. Otherwise the calculated value of $H_b = \nu \nabla \times \boldsymbol{A}$ is used to form the boundary term.

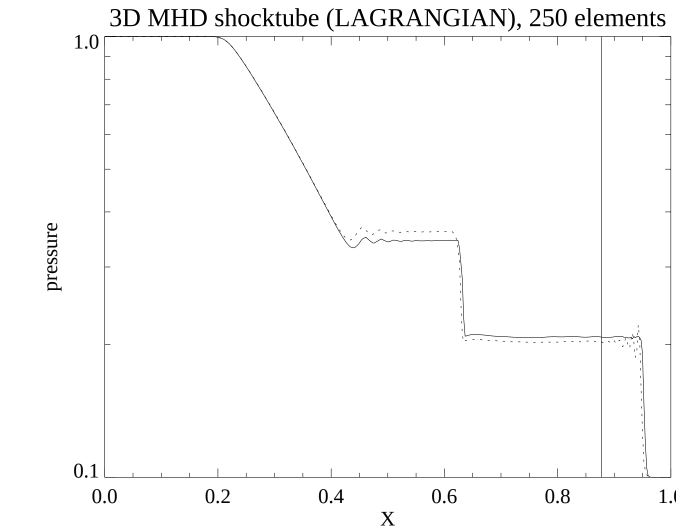
B is calculated from $\nabla \times A$ and and projected back to the nodes. Known BCs are applied.

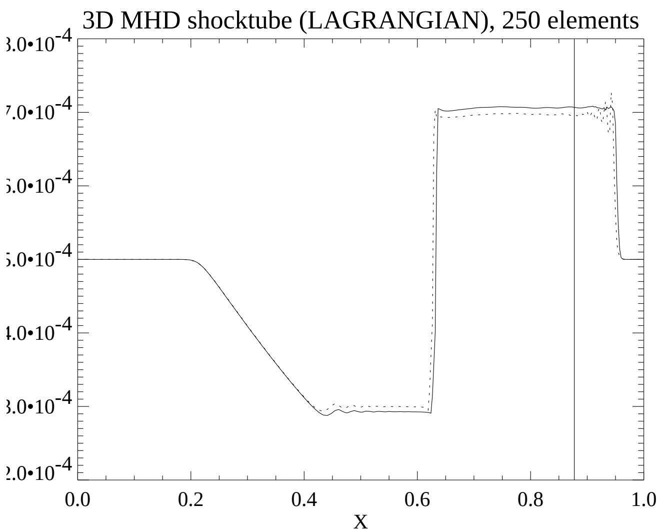
Diffusion Test Problem

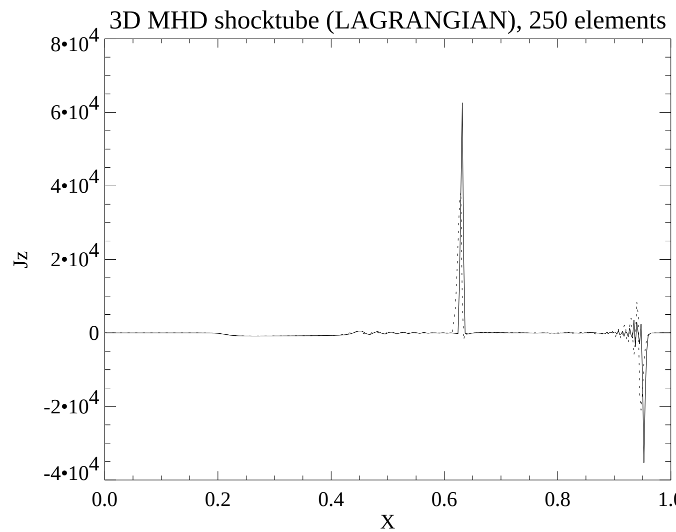


Consistent J (dotted) vs. Projected J (solid)









shock vel.= 2.36160 2.35833 2.35578 2.36161 , Avg= 2.37749 sigma= 0.00516765

Body Force and Energy Deposition

JxB body force (Laplace force or Lorentz force)

$$F_M^n = J^n \times B^n$$

Mixed cell energy deposition is treated using volume fraction average conductivity. (Void has a finite conductivity)

$$\sigma = \sum \phi_m \sigma_m$$

The energy deposited is given by

$$e_m^{n+1} - e_m^n = \frac{\sigma_m}{\sigma} \dot{Q} \frac{\Delta t^{n+1/2}}{\rho_m}$$

with $\dot{Q} = \sigma \left(\frac{J_{mid}}{\sigma_{max}} \right)^2$**. Work needed on time centering.**

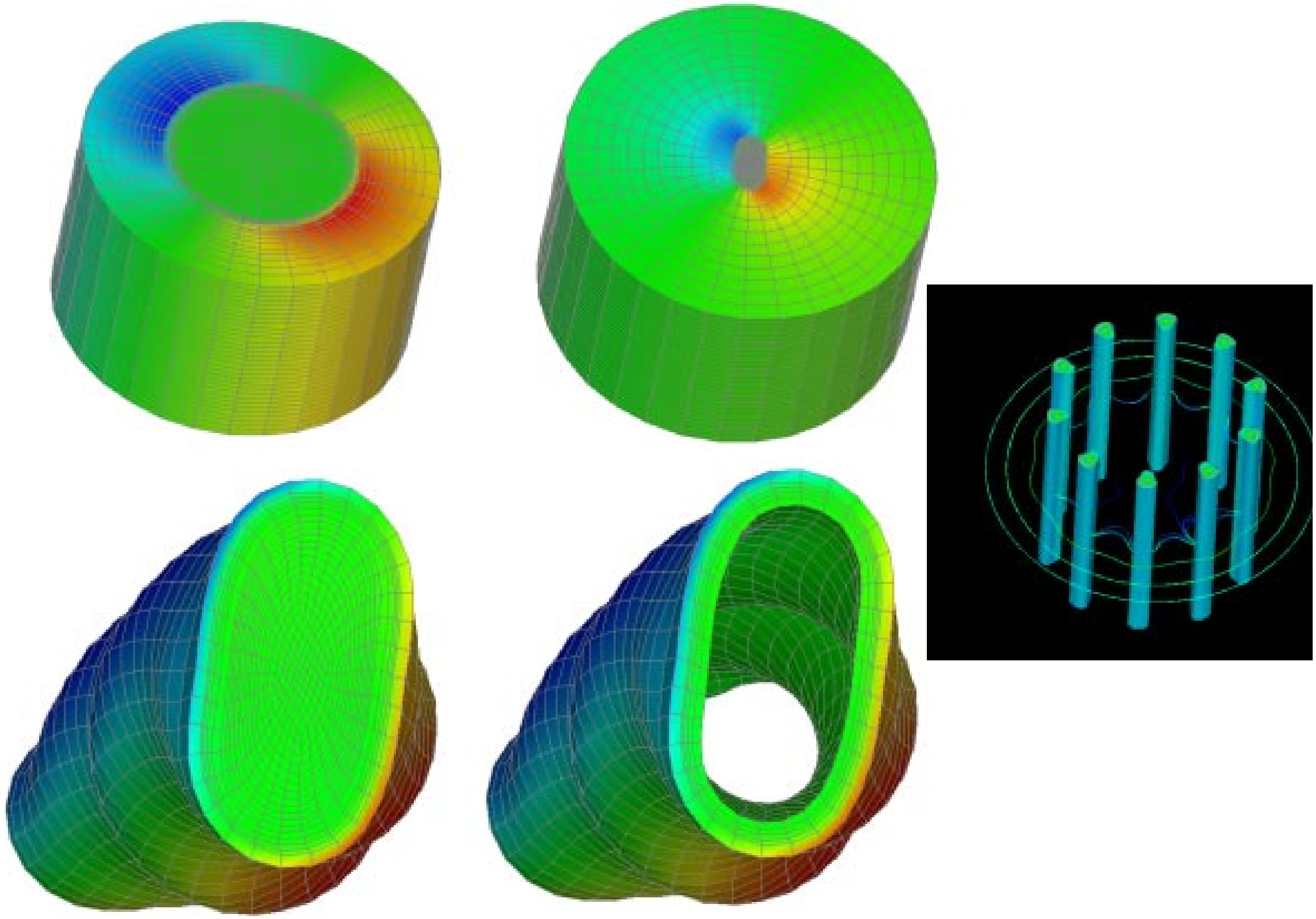
Time Step Control

The time step is determined using the standard ALEGRA time step scheme with the wavespeed w given by the mechanical wavespeed plus a term to give the fast Alfven wave speed.

$$w = \sqrt{c_{mech}^2 + \frac{B^2}{\rho\mu}}$$

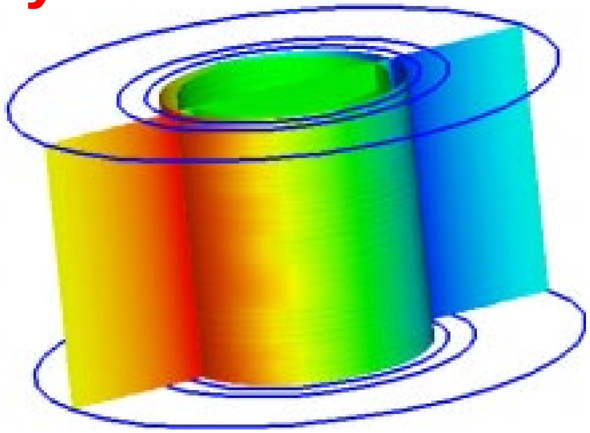
We tend to compute with pure void rather than using a low density gas in void regions.

SMALE

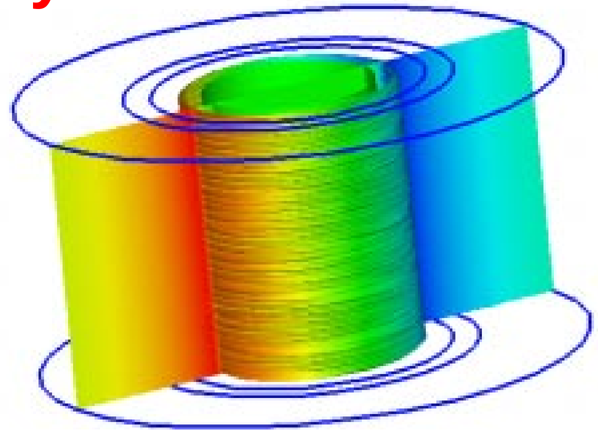


294400 Element Eulerian Calculation

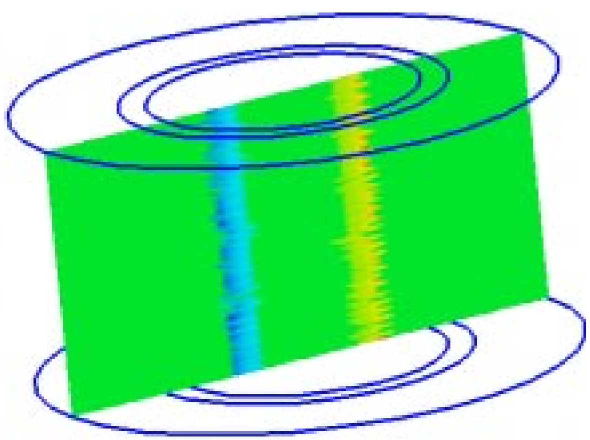
by-27ns



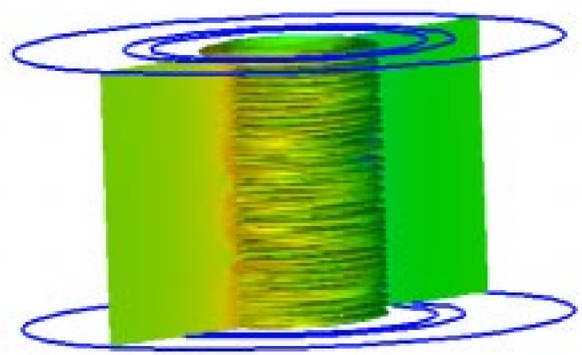
by-30ns



velx-33ns



by-33ns

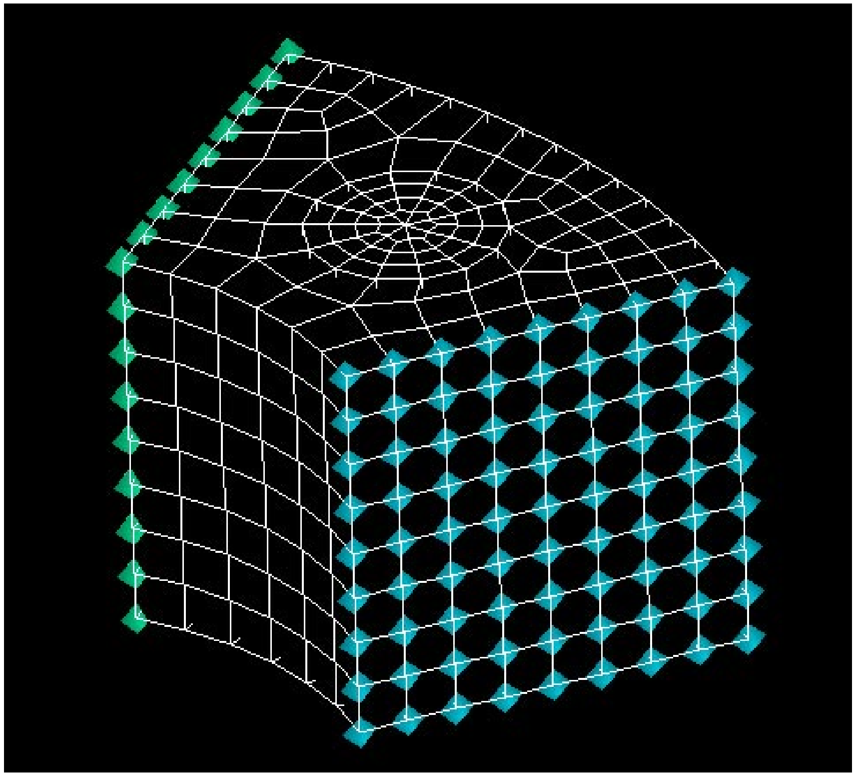


Why Periodic Boundary Conditions in ALEGRA?

Useful for test problems. In particular, one-dimensional test problems have transverse components.

Natural for meso-scale modeling.

Reduce mesh requirements and run times for 2D and 3D.



Periodic Boundary Conditions - User interface

PERIODIC BC, {ns1}, TRANSLATE {u}, {ns2}

$$x^2 = x^1 + u$$

PERIODIC BC, {ns1}, ROTATE {θ} ABOUT {p} {ns2}
PERIODIC BC, {ns1}, ROTATE {θ} ABOUT {p} AXIS {a}, {ns2}

$$x^2 - p = R(x^1 - p) = V\begin{bmatrix} \cos(\theta) & -\sin(\theta) & 0 \\ \sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{bmatrix} V^T(x^1 - p)$$

$$v^2 = Rv^1$$

$$T^2 = RT^1R^T$$

Periodic Boundary Conditions - Status

Approach: Use the "ghost element" technology inherent in ALEGRA for parallel computing as a means of implementing periodic boundary conditions. In principle, all physics will come up and work in parallel with minimal intrusion.

Parallel nodeset "matching" scheme implemented.

The PMeshIPC class has been derived from the MeshIPC class for special periodic boundary communications.

An initial parallel framework exists but work is still in progress.

Challenges

Run times for large calculations will be a problem. The Courant limit and iterative solver scaling will work against us. Will need multi-level solution technology.

Advection of A can lead to anomalous currents. We will want to improve numerics.

ALEGRA ALE capability should permit optimal, robust, automatic mesh smoothing. Mesh smoothing and optimization for accuracy and robustness must be smarter.

Improved formulations of magnetic force and joule heating may be required.

Continuous improvement through V and V activities.