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Progress on Extended MHD Modeling in ALEGRA

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Acknowledgements

Many people have contributed to various aspects of ALEGRA over the years. The present work seeks to implement extended MHD modeling capabilities in ALEGRA that build upon those previous contributions.

Work on extended MHD modeling in ALEGRA began some years ago with contributions from Duncan McGregor and Allen Robinson. The present work is composed primarily of improvements and modifications of those algorithms.

ALEGRA Overview

- Multiphysics finite-element ALE shock hydro code.
- Many coupled physics modules: MHD (various), electromechanics, radiation transport, etc.

Refs:

- A. Robinson, T. Brunner, S. Carroll, R. Drake, C. Garasi, T. Gardiner, T. Haill, H. Hanshaw, D. Hensinger, D. Labreche, R. Lemke, E. Love, C. Luchini, S. Mosso, J. Niederhaus, C. Ober, S. Petney, W. Rider, G. Scovazzi, O. Strack, R. Summers, T. Trucano, V. Weirs, M. Wong, and T. Voth, *ALEGRA: An arbitrary Lagrangian-Eulerian multimaterial, multiphysics code*, in 46th AIAA Aerospace Sciences Meeting and Exhibit, Reno, Nevada, Jan. 2008, American Institute of Aeronautics and Astronautics, doi:10.2514/6.2008-1235.

- J. H. Niederhaus, S. W. Bova, J. B. Carleton, J. H. Carpenter, K. R. Cochrane, M. M. Crockatt, W. Dong, T. J. Fuller, B. N. Granzow, D. A. Ibanez, S. R. Kennon, C. B. Luchini, R. J. Moral, C. J. O'Brien, M. J. Powell, A. C. Robinson, A. E. Rodriguez, J. J. Sanchez, W. A. Scott, C. M. Siefert, A. K. Stagg, I. K. Tezaur, T. E. Voth, and J. R. Wilkes, *Alegra: Finite element modeling for shock hydrodynamics and multiphysics*, International Journal of Impact Engineering, 180 (2023), p. 104693, doi:10.1016/j.ijimpeng.2023.104693.

MHD Models

- Consider only full 3D implementations in this presentation.

RMHD: (Resistive MHD) Standard resistive MHD model.

FMHD: (Full-Maxwell MHD) Includes displacement current in Ampere's Law. Works for $\sigma = 0$.

Ref: D. A. McGregor and A. C. Robinson, *An indirect ALE discretization of single fluid plasma without a fast magnetosonic time step restriction*, Computers & Mathematics with Applications, 78 (2019), pp. 417–436, doi:10.1016/j.camwa.2018.10.012.

GMHD: (Generalized MHD) Use a generalized Ohm's law and include displacement current in Ampere's Law. Models the Hall effect.

$$\tau \dot{\mathbf{J}} + \frac{e\tau}{m_e}\mathbf{J} \times \mathbf{B} + \mathbf{J} = \sigma \mathbf{E} \qquad \text{(fluid frame)}$$

Electromagnetics discretization

- Implicit in time.
- Structure preserving (edge, face) discretization for $\mathbf{E}$ and $\mathbf{B}$.
- **Key question:** How to handle $\mathbf{J}$?

Maxwell's equations:

$$\epsilon \partial_t \mathbf{E} - \operatorname{curl}\left(\mu^{-1}\mathbf{B}\right) + \mathbf{J} = 0$$
$$\partial_t \mathbf{B} + \operatorname{curl} \mathbf{E} = 0$$

Semi-discrete system:

$$\int \left[\left(\frac{\epsilon}{\Delta t} \mathbf{E}^{n+1} + \mathbf{J}^{n+1} \right) \cdot \mathbf{\Psi} + \frac{\Delta t}{\mu} \operatorname{curl} \mathbf{E}^{n+1} \cdot \operatorname{curl} \mathbf{\Psi} \right] d\Omega = \int \left[\frac{\epsilon}{\Delta t} \mathbf{E}^{n} \cdot \mathbf{\Psi} + \mu^{-1} \mathbf{B}^{n} \cdot \operatorname{curl} \mathbf{\Psi} \right] d\Omega$$

Electromagnetics discretization

$$\int \left[\left(\frac{\epsilon}{\Delta t} \mathbf{E}^{n+1} + \mathbf{J}^{n+1} \right) \cdot \mathbf{\Psi} + \frac{\Delta t}{\mu} \operatorname{curl} \mathbf{E}^{n+1} \cdot \operatorname{curl} \mathbf{\Psi} \right] d\Omega = \int \left[\frac{\epsilon}{\Delta t} \mathbf{E}^{n} \cdot \mathbf{\Psi} + \mu^{-1} \mathbf{B}^{n} \cdot \operatorname{curl} \mathbf{\Psi} \right] d\Omega$$

For RMHD and FMHD:

- $\mathbf{J}$ is stored as an element-averaged quantity.
- Substitution with Ohm's law is straightforward: $\mathbf{J}^{n+1} = \sigma^n \mathbf{E}^{n+1}$.
- Have the usual curl-curl linear system to solve for edge-centered $\mathbf{E}^{n+1}$.

Electromagnetics discretization

$$\int \left[\left(\frac{\epsilon}{\Delta t} \mathbf{E}^{n+1} + \mathbf{J}^{n+1} \right) \cdot \mathbf{\Psi} + \frac{\Delta t}{\mu} \operatorname{curl} \mathbf{E}^{n+1} \cdot \operatorname{curl} \mathbf{\Psi} \right] d\Omega = \int \left[\frac{\epsilon}{\Delta t} \mathbf{E}^{n} \cdot \mathbf{\Psi} + \mu^{-1} \mathbf{B}^{n} \cdot \operatorname{curl} \mathbf{\Psi} \right] d\Omega$$

For GMHD the semi-discrete Ohm's law has the form:

$$\left[\left(1 + \frac{\tau}{\Delta t} \right) \underline{\mathbf{I}} - \underline{\boldsymbol{\beta}}^{n} \right] \cdot \mathbf{J}^{n+1} = \sigma^{n} \mathbf{E}^{n+1} + \frac{\tau}{\Delta t} \mathbf{J}^{n} \qquad \text{where} \qquad \underline{\boldsymbol{\beta}}^{n} \cdot \mathbf{J} = \frac{e\tau}{m_e} \mathbf{B}^{n} \times \mathbf{J}$$

First attempt:

- ➤ Use element-centered projection of $\mathbf{B}$ to allow analytic solution of Ohm's law.
- ➤ Substitute into EM weak form as before.
- ➤ **Result:** Works in some cases but not others. Unstable for EM shock problems (Brio-Wu) unless cyclotron frequency is resolved.

Electromagnetics discretization

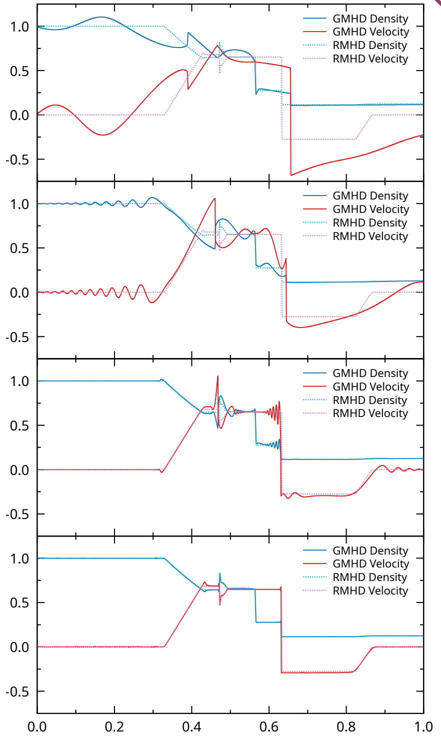
Instead, discretize $\mathbf{J}$ on edges:

$$\int \left[\frac{\epsilon}{\Delta t} \mathbf{E}^{n+1} \cdot \mathbf{\Psi} + \frac{\Delta t}{\mu} \operatorname{curl} \mathbf{E}^{n+1} \cdot \operatorname{curl} \mathbf{\Psi} \right] d\Omega + \int \mathbf{J}^{n+1} \cdot \mathbf{\Psi} \, d\Omega$$

$$= \int \left[\frac{\epsilon}{\Delta t} \mathbf{E}^{n} \cdot \mathbf{\Psi} + \mu^{-1} \mathbf{B}^{n} \cdot \operatorname{curl} \mathbf{\Psi} \right] d\Omega,$$

$$\int \left[\left(1 + \frac{\tau}{\Delta t}\right) \underline{\mathbf{I}} - \underline{\boldsymbol{\beta}}^{n} \right] \cdot \mathbf{J}^{n+1} \cdot \mathbf{\Psi} \, d\Omega - \int \sigma^{n} \mathbf{E}^{n+1} \cdot \mathbf{\Psi} \, d\Omega = \int \frac{\tau}{\Delta t} \mathbf{J}^{n} \cdot \mathbf{\Psi} \, d\Omega.$$

- ➤ Requires solving 2×2 block system for $\mathbf{E}$ and $\mathbf{J}$ simultaneously.
- ➤ Stable for EM shock problems (Brio-Wu) without resolving cyclotron frequency.
- ➤ Replace weak-form edge remap for $\mathbf{E}$ with strong-form edge remap for $\mathbf{E}$ and $\mathbf{J}$.
- ➤ Development of scalable preconditioners is ongoing.



Midpoint predictor-corrector method

- Second order method for Lagrangian hydrodynamics.
- More expensive than central difference (but stable).
- Exactly conserves total energy during the Lagrangian step.
- Usually use two correction iterations.

Table 1
Outline of the predictor–multi-corrector algorithm

Retrieve loop parameters: n_{step}, $i_{\max}$
Initialize all variables with initial conditions
Form $[\mathbf{M}_L]$ and $\mathbf{M}_{\text{el}}$
For $n = 0, \ldots, n_{\text{step}}$ (*Time-step loop begins*)
    Set Δt (respecting the CFL condition)
    Predictor: $\mathbf{Y}^{(0)}_{n+1} = \mathbf{Y}_n$
    For $i = 0, \ldots, i_{\max} - 1$ (*Multi-corrector loop begins*)
        Assembly: $\mathbf{F}^{(i)}_{n+1/2}$
        Velocity update: $\mathbf{v}^{(i+1)}_{n+1} = \mathbf{v}_n - \Delta t[\mathbf{M}_L]^{-1}\mathbf{F}^{(i)}_{n+1/2}$
        Assembly: $\mathbf{W}^{(i,i+1)}_{n+1/2}$
        Internal energy update: $\boldsymbol{\epsilon}^{(i+1)}_{n+1} = \boldsymbol{\epsilon}_n - \Delta t\,[\mathbf{M}_{\text{el}}]^{-1}\mathbf{W}^{(i,i+1)}_{n+1/2}$
        Position update: $\mathbf{x}^{(i+1)}_{n+1} = \mathbf{x}_n + \Delta t\mathbf{v}^{(i+1)}_{n+1/2}$
        Volume update: $\mathbf{V}^{(i+1)}_{n+1} = \mathbf{V}(\mathbf{x}^{(i+1)}_{n+1})$
        Density update: $\boldsymbol{\rho}^{(i+1)}_{n+1} = [\mathbf{V}^{(i+1)}_{n+1}]^{-1}\mathbf{M}_{\text{el}}$
        Equation of state update: $\mathbf{p}^{(i+1)}_{n+1} = \hat{\mathbf{p}}(\boldsymbol{\rho}^{(i+1)}_{n+1}, \boldsymbol{\epsilon}^{(i+1)}_{n+1})$
    End (*Multi-corrector loop ends*)
    Time update: $\mathbf{Y}_{n+1} = \mathbf{Y}^{(i_{\max})}_{n+1}$
End (*Time-step loop ends*)
Exit

Ref: G. Scovazzi, E. Love, and M. Shashkov, *Multi-scale Lagrangian shock hydrodynamics on Q1/P0 finite elements: Theoretical framework and two-dimensional computations*, Computer Methods in Applied Mechanics and Engineering, 197 (2008), pp. 1056–1079, doi:10.1016/j.cma.2007.10.002

Midpoint predictor-corrector method for XMHD

Existing strategy for multiphysics in ALEGRA:

- First order operator splitting.
- Example (RMHD): Lagrangian step with ideal MHD –> Remap –> Magnetic diffusion.

New strategy for XMHD:

- No operator splitting: Solve EM equations on Lagrangian mesh.
- Use implicit Euler method for EM equations.
- Implicit Euler step taken at each correction iteration.
- Multiple implicit solves required for each time step.

Table 1
Outline of the predictor–multi-corrector algorithm

Retrieve loop parameters: n_{step}, $i_{\max}$
Initialize all variables with initial conditions
Form $[\mathbf{M}_L]$ and $\mathbf{M}_{\text{el}}$
For $n = 0, \ldots, n_{\text{step}}$ (*Time-step loop begins*)
  Set Δt (respecting the CFL condition)
  Predictor: $\mathbf{Y}_{n+1}^{(0)} = \mathbf{Y}_n$
  For $i = 0, \ldots, i_{\max} - 1$ (*Multi-corrector loop begins*)
    Assembly: $\mathbf{F}_{n+1/2}^{(i)}$
    Velocity update: $\mathbf{v}_{n+1}^{(i+1)} = \mathbf{v}_n - \Delta t [\mathbf{M}_L]^{-1} \mathbf{F}_{n+1/2}^{(i)}$
    Assembly: $\mathbf{W}_{n+1/2}^{(i,i+1)}$
    Internal energy update: $\boldsymbol{\epsilon}_{n+1}^{(i+1)} = \boldsymbol{\epsilon}_n - \Delta t \, [\mathbf{M}_{\text{el}}]^{-1} \mathbf{W}_{n+1/2}^{(i,i+1)}$
    Position update: $\mathbf{x}_{n+1}^{(i+1)} = \mathbf{x}_n + \Delta t \mathbf{v}_{n+1/2}^{(i+1)}$
    Volume update: $\mathbf{V}_{n+1}^{(i+1)} = \mathbf{V}(\mathbf{x}_{n+1}^{(i+1)})$
    Density update: $\boldsymbol{\rho}_{n+1}^{(i+1)} = [\mathbf{V}_{n+1}^{(i+1)}]^{-1} \mathbf{M}_{\text{el}}$
    Equation of state update: $\mathbf{p}_{n+1}^{(i+1)} = \hat{\mathbf{p}}(\boldsymbol{\rho}_{n+1}^{(i+1)}, \boldsymbol{\epsilon}_{n+1}^{(i+1)})$
  End (*Multi-corrector loop ends*)
  Time update: $\mathbf{Y}_{n+1} = \mathbf{Y}_{n+1}^{(i_{\max})}$
End (*Time-step loop ends*)
Exit

Ref: G. Scovazzi, E. Love, and M. Shashkov, *Multi-scale Lagrangian shock hydrodynamics on Q1/P0 finite elements: Theoretical framework and two-dimensional computations*, Computer Methods in Applied Mechanics and Engineering, 197 (2008), pp. 1056–1079, doi:10.1016/j.cma.2007.10.002

IMEX Runge-Kutta (RK) methods

Initial value problem:

$$\dot{y} = f(y, t) + g(y, t),$$

Discrete stages:

$$y^{(i)} = y^n + \Delta t \sum_{j=1}^{i-1} \hat{A}_{ij} f\left(t^n + \hat{c}_j \Delta t, y^{(i)}\right) + \Delta t \sum_{j=1}^{i} A_{ij} g\left(t^n + c_j \Delta t, y^{(i)}\right),$$

$$y^{n+1} = y^n + \Delta t \sum_{i=1}^{s} \hat{b}_i f\left(t^n + \hat{c}_j \Delta t, y^{(i)}\right) + \Delta t \sum_{i=1}^{s} b_i g\left(t^n + c_j \Delta t, y^{(i)}\right).$$

Coefficient tableaux:

$$\begin{array}{c|c} \hat{c} & \hat{A} \\ \hline & \hat{b}^T \end{array} \qquad \begin{array}{c|c} c & A \\ \hline & b^T \end{array}$$

Reformulate as midpoint Runge-Kutta method

$$
\begin{aligned}
\dot{\mathbf{x}} &= \mathbf{v} \\
\rho \dot{\mathbf{v}} &= \nabla_{\mathbf{x}} \cdot \underline{\boldsymbol{\sigma}} \\
\rho \dot{e} &= \underline{\boldsymbol{\sigma}} : \nabla_{\mathbf{x}} \mathbf{v}
\end{aligned}
$$

- Use two-stage IMEX midpoint method:

$$
\begin{array}{c|cc}
0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & 0 \\
\hline
 & 0 & 1
\end{array}
\qquad
\begin{array}{c|cc}
\frac{1}{2} & \frac{1}{2} & 0 \\
\frac{1}{2} & 0 & \frac{1}{2} \\
\hline
 & 0 & 1
\end{array}
$$

- Velocity advanced “implicitly”.
- Other hydrodynamics variables advanced explicitly.
- Only re-interpreting existing algorithm.

Initial XMHD method as RK

- Extend hydro IMEX method to incorporate additional physics (MHD) using the generalized-structure additively partitioned RK (GARK) approach.

  Ref: A. SANDU AND M. GÜNTHER, *A generalized-structure approach to additive Runge–Kutta methods*, SIAM Journal on Numerical Analysis, 53 (2015), pp. 17–42, doi:10.1137/130943224.

- IMEX separates the IVP into two parts and treats them with different methods (implicit + explicit).
- GARK approach is a generalization from 2 coupled RK methods to N coupled RK methods.
- XMHD midpoint-corrector algorithm can be written into this framework by adding a two-stage implicit Euler tableau for the electromagnetics:

$$
\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \hline & 0 & 1 \end{array}
\qquad
\begin{array}{c|cc} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \hline & 0 & 1 \end{array}
\qquad + \qquad
\begin{array}{c|cc} 1 & 1 & 0 \\ 1 & 0 & 1 \\ \hline & 0 & 1 \end{array}
$$

- Again: Only re-interpreting existing algorithm.

Improving the XMHD time discretization

- Two-stage implicit Euler method is inefficient, but GARK perspective gives us insight into how to make improvements.
- Leverage different methods to balance properties (cost, accuracy, stability).

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 0 & 1 \\ \hline & 0 & 1 \end{array}$$

Euler1:

- 1 implicit solve
- L-stable
- First order

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \hline & 0 & 1 \end{array}$$

Midpoint1:

- 1 implicit solve
- A-stable
- Second order
- Symplectic

$$\begin{array}{c|cc} \gamma & \gamma & 0 \\ 1 & 1-\gamma & \gamma \\ \hline & 1-\gamma & \gamma \end{array}$$

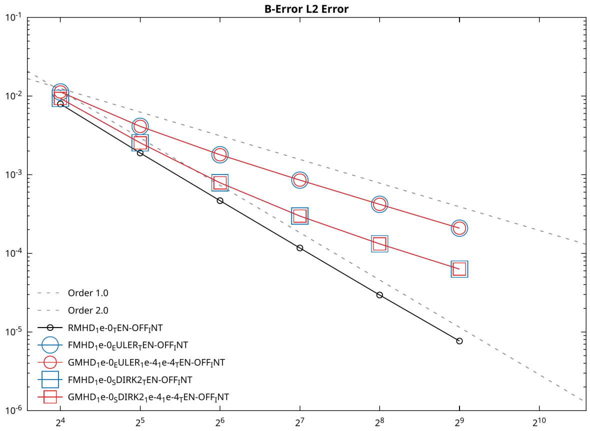
SDIRK2:

- 2 implicit solves
- L-stable
- Second order
- $\gamma = 1 - 1/\sqrt{2}$

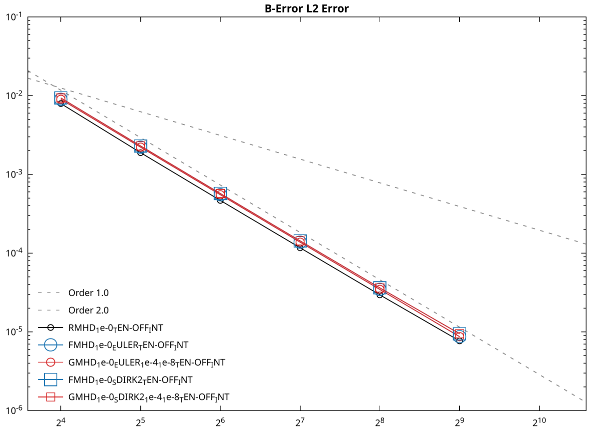
Improving the XMHD time discretization

- GARK perspective requires coupling conditions to be satisfied to ensure higher order.
- Result is that source terms in hydro equations need to use implicit midpoint for 2nd order.

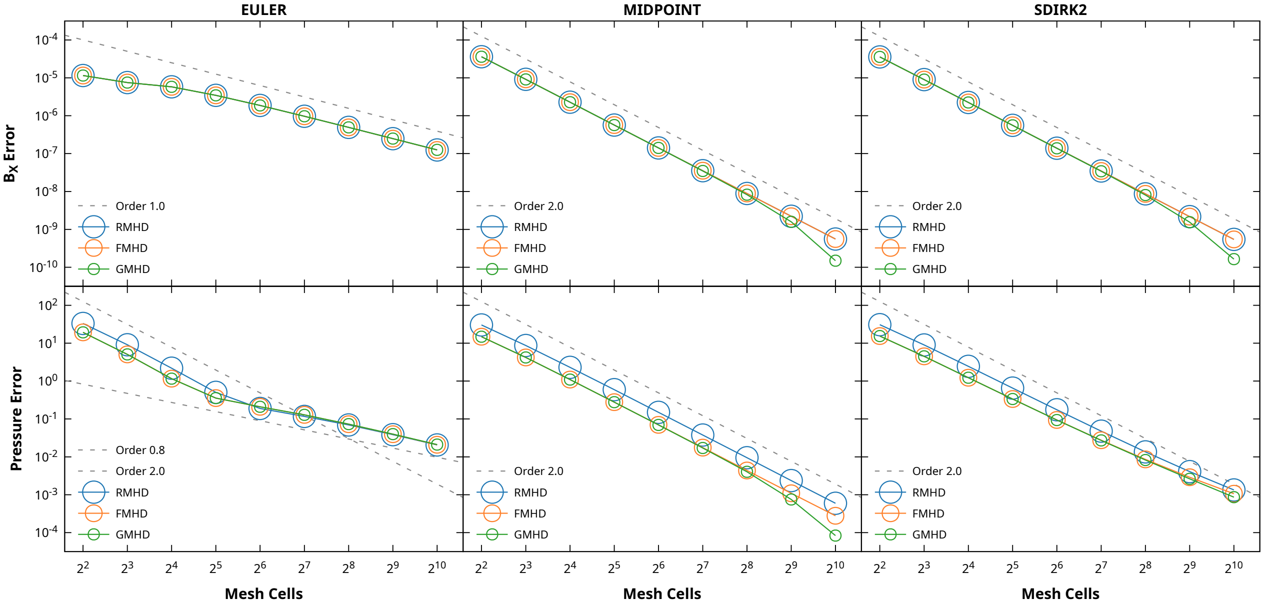
Lorentz force with EM integrator:



Lorentz force with midpoint:



VROD verification problem

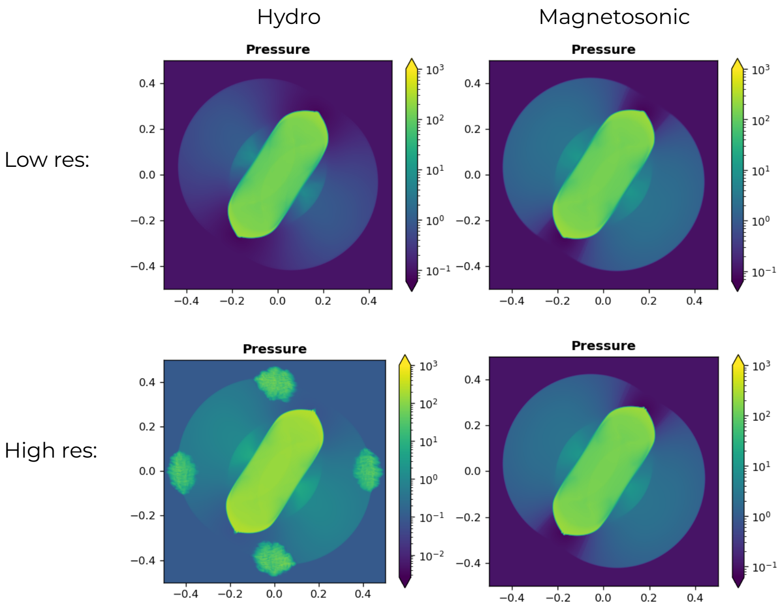


Ref: C. C. Ashcraft, J. H. Niederhaus, and A. C. Robinson, *Verification and validation of a coordinate transformation method in axisymmetric transient magnetics*, Tech. Report SAND2016-0804, Sandia National Laboratories, United States, Jan. 2016, doi:10.2172/1237004

Artificial viscosity

- FMHD designed to avoid time step restriction based on fast magnetosonic wave speed.
- Implications for artificial viscosity less clear.

- Existing approach uses only hydro wave speed for artificial viscosity, but is unstable.
- Using the fast magnetosonic wave speed is stable, but reintroduces explicit time step restriction.
- No indication that whistler wave needs special handling for GMHD.



Summary and ongoing work

Summary:

- Recast spatial discretization for stability.
- Recast time discretization for accuracy and efficiency.
- New IMEX time discretization opens opportunities for all multiphysics in ALEGRA.
- Initial results for common tests problems are good (Brio-Wu, magnetic blast, GEM challenge).

Ongoing work:

- Continued verification of IMEX coupled multiphysics implementation.
- Scalable solvers required for GMHD block system (Ray Tuminaro).
- Alternative solutions for handling of artificial viscosity.