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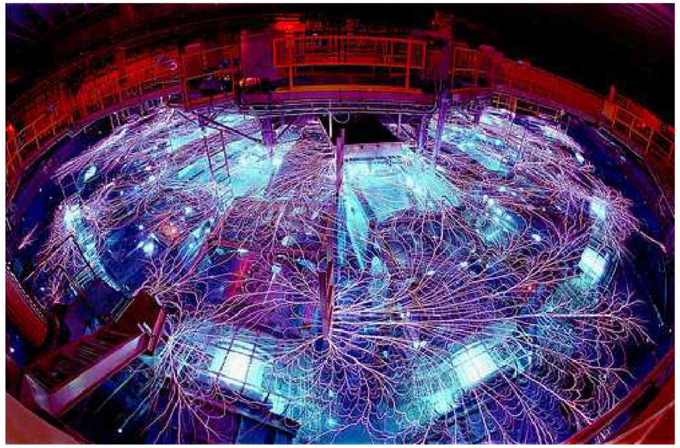
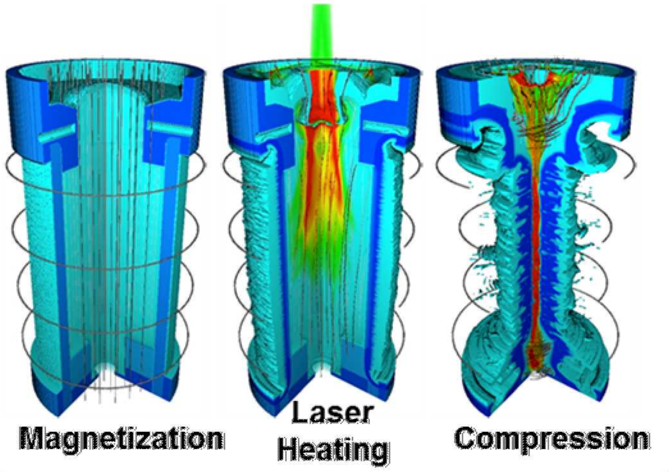


FLEXO: Development Activities for Z-Next Simulation

Presented by: Nat Hamlin

PERSEUS/FLEXO Team: Kristian Beckwith, Stephen Bond, Brian Granzow, Nat Hamlin, Glen Hansen, Heath Hanshaw, Chris Jennings, Matt Martin, Alan Stagg, Tom Voth



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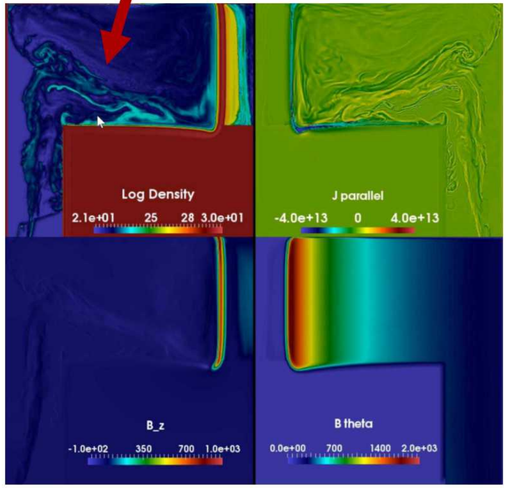
PERSEUS/FLEXO Overview

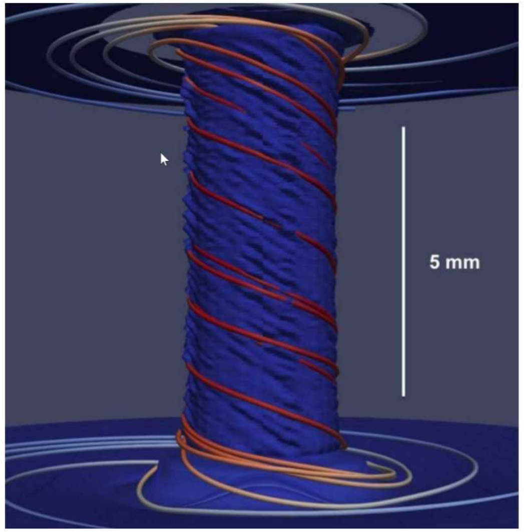
- **PERSEUS** – generalized Ohm's Law (XMHD), FORTRAN90, Discontinuous Galerkin (DG) code, originally developed at Cornell (Martin, Seyler) and licensed to SNL with numerous publications demonstrating the need for XMHD physics in the modeling of pulsed power systems.

- **FLEXO** – new C++ XMHD code (Flux Limited EXtended Ohm's law) based on PERSEUS, developed at SNL with new capabilities: multi-material equation of state (EOS), adaptive mesh refinement (AMR), and scalable DG radiation transport, all compatible with advanced architectures (GPU).

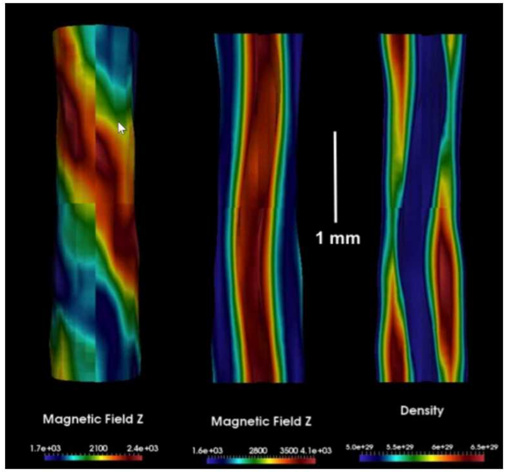
Enable a predictive simulation capability for design work on Z and future pulsed power facilities

1) Feed plasma transport requires XMHD due to low densities



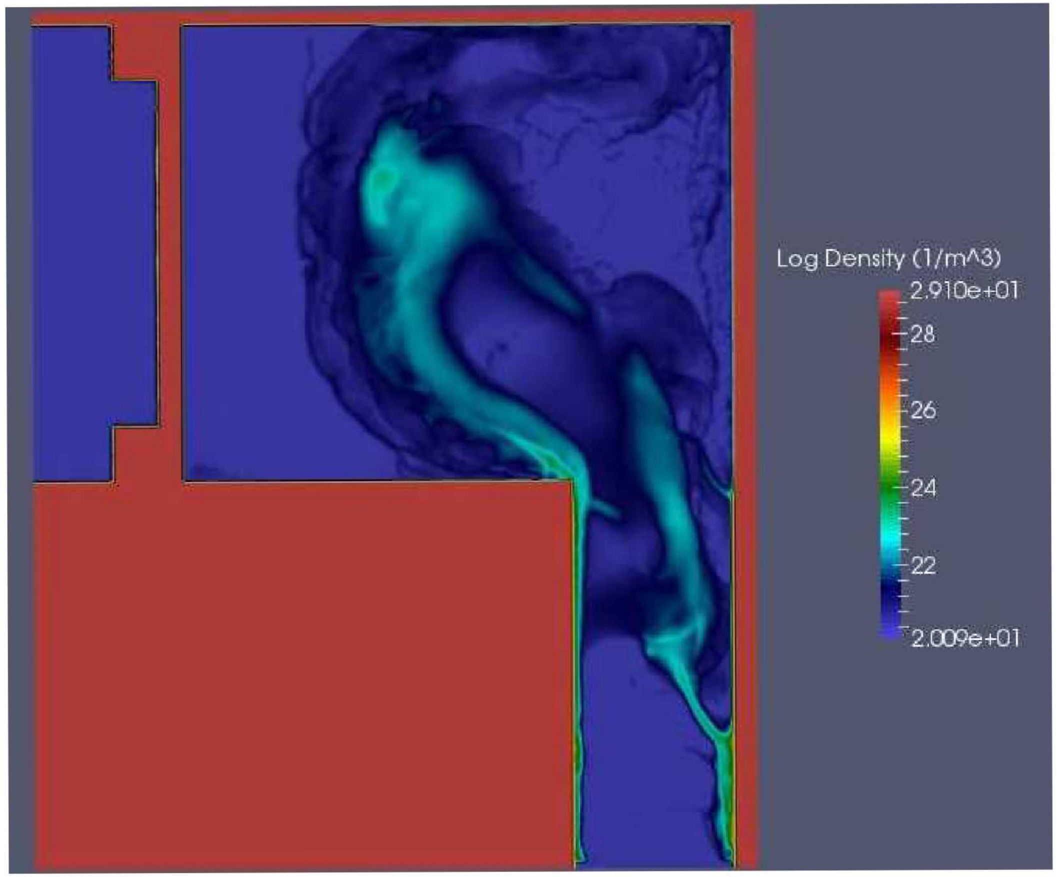


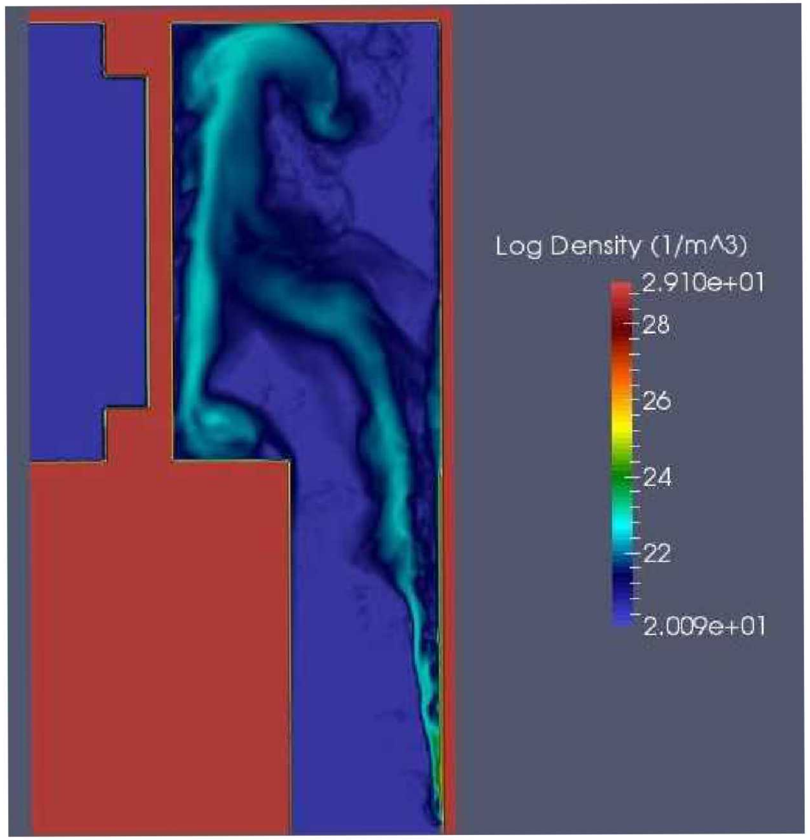
2) XMHD predicts helical instability in 3D calculations due to feed plasma driving flux compression in MagLIF



3) Low density feed plasma (~10^18/cc) changes morphology and stability of liner stagnation

PERSEUS predicts flux compression effects

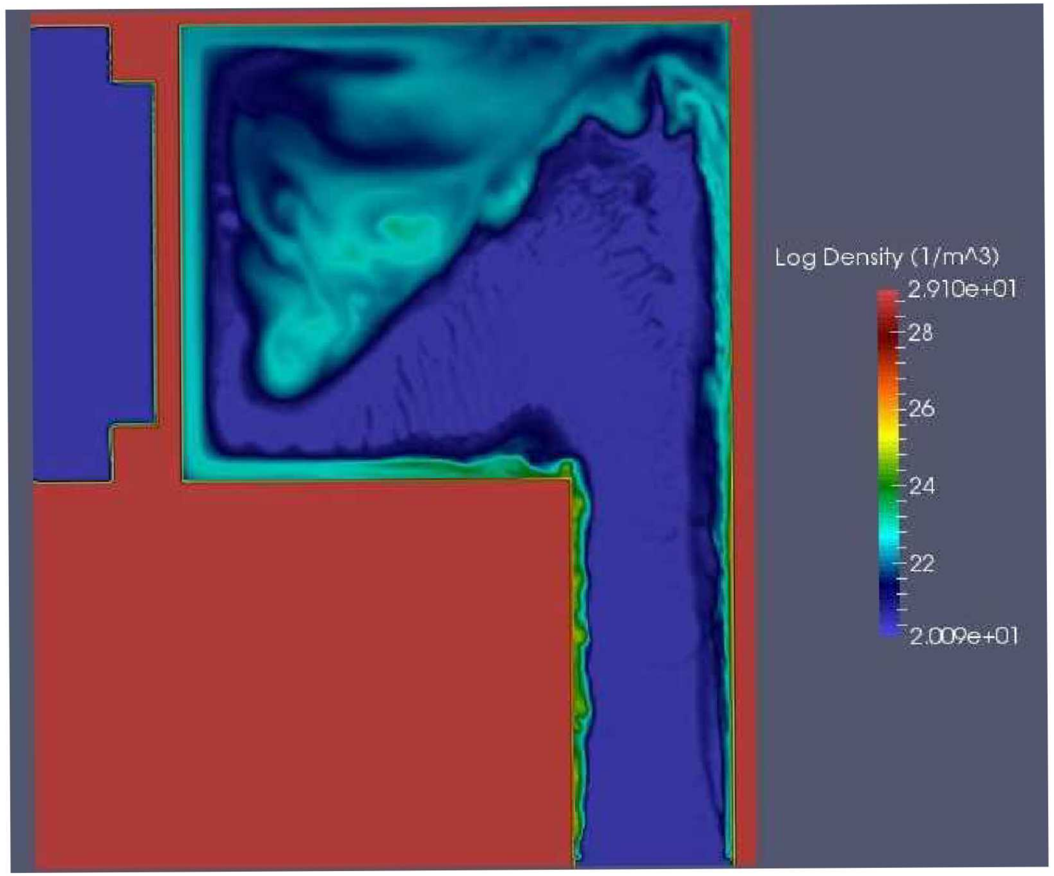


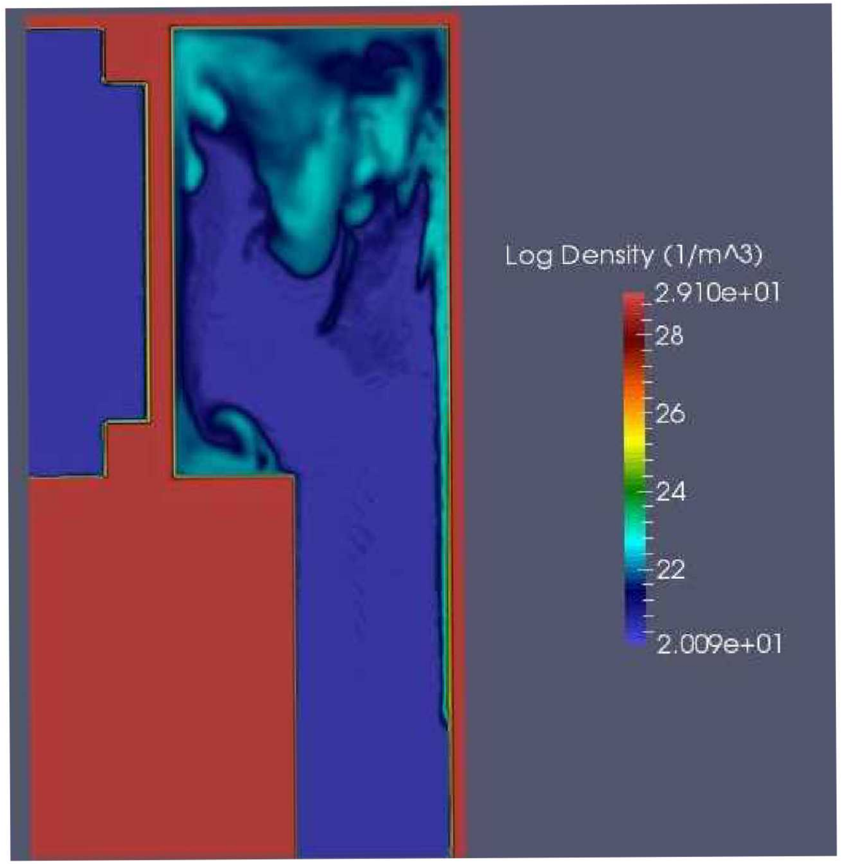


The plasma compresses the flux against the surface of the liner sooner for the small diameter return can (t = 25 ns)

Flux compression prediction (late time)

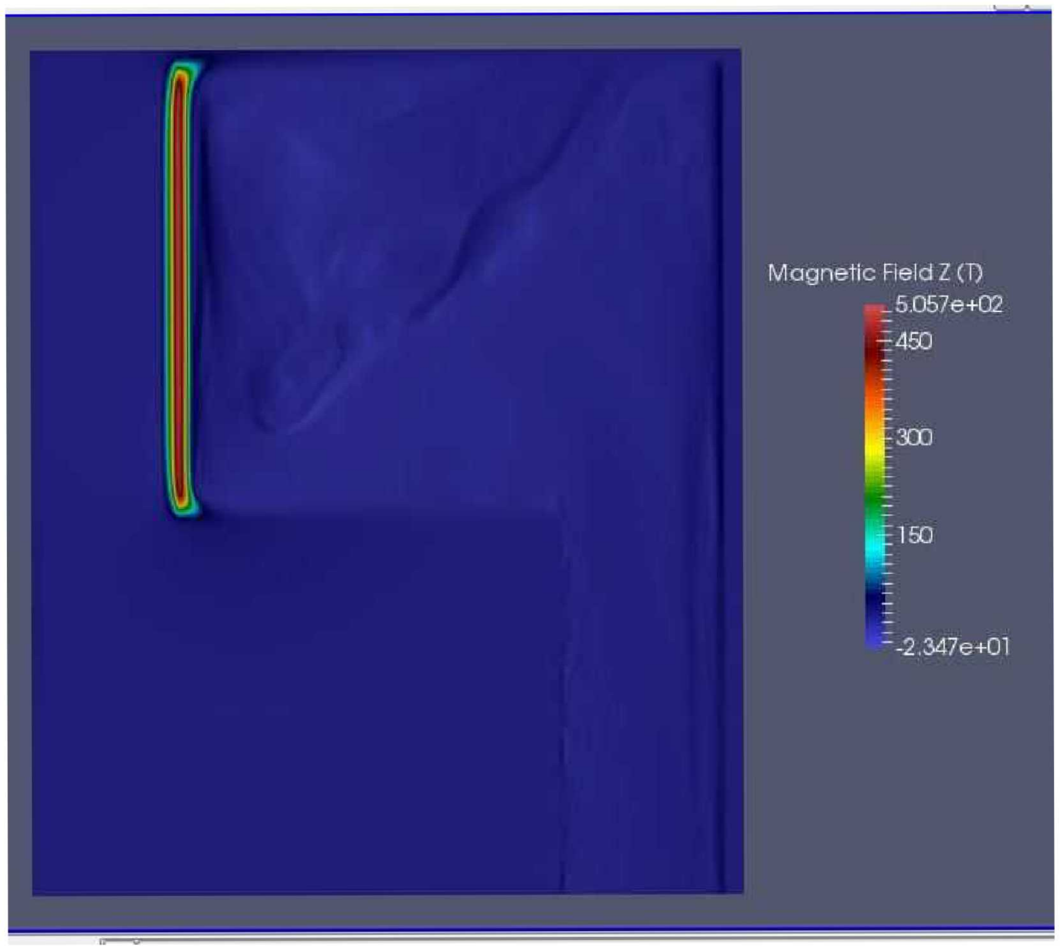
- By 50 ns both cases have swept the majority of the flux against the surface of the liner

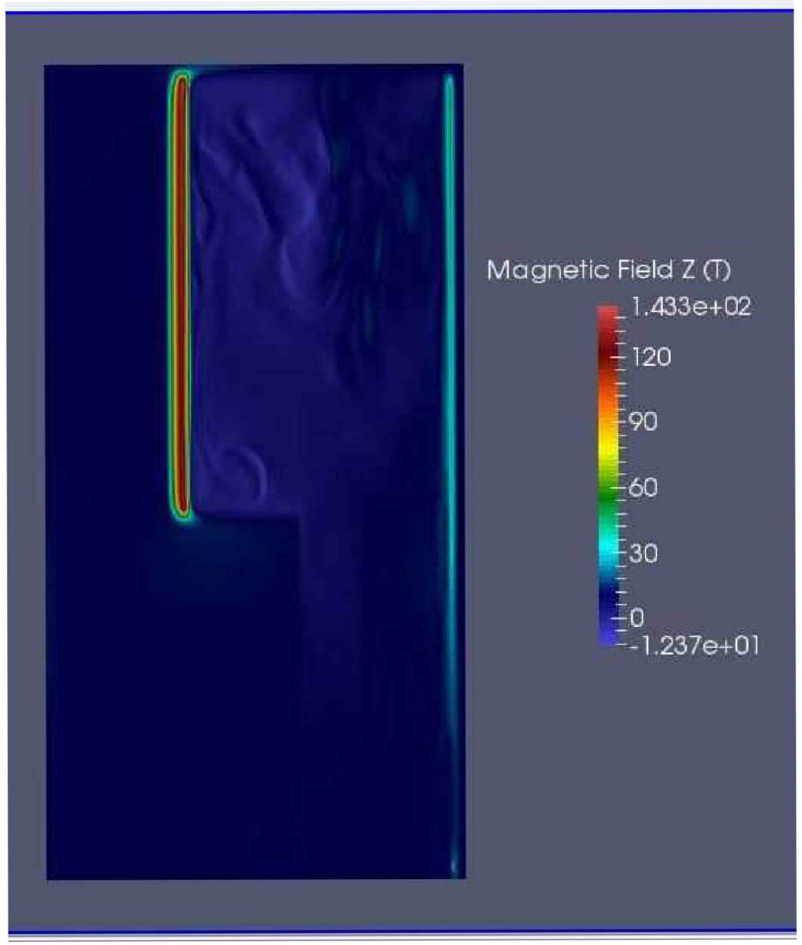




Flux compression prediction (late time)

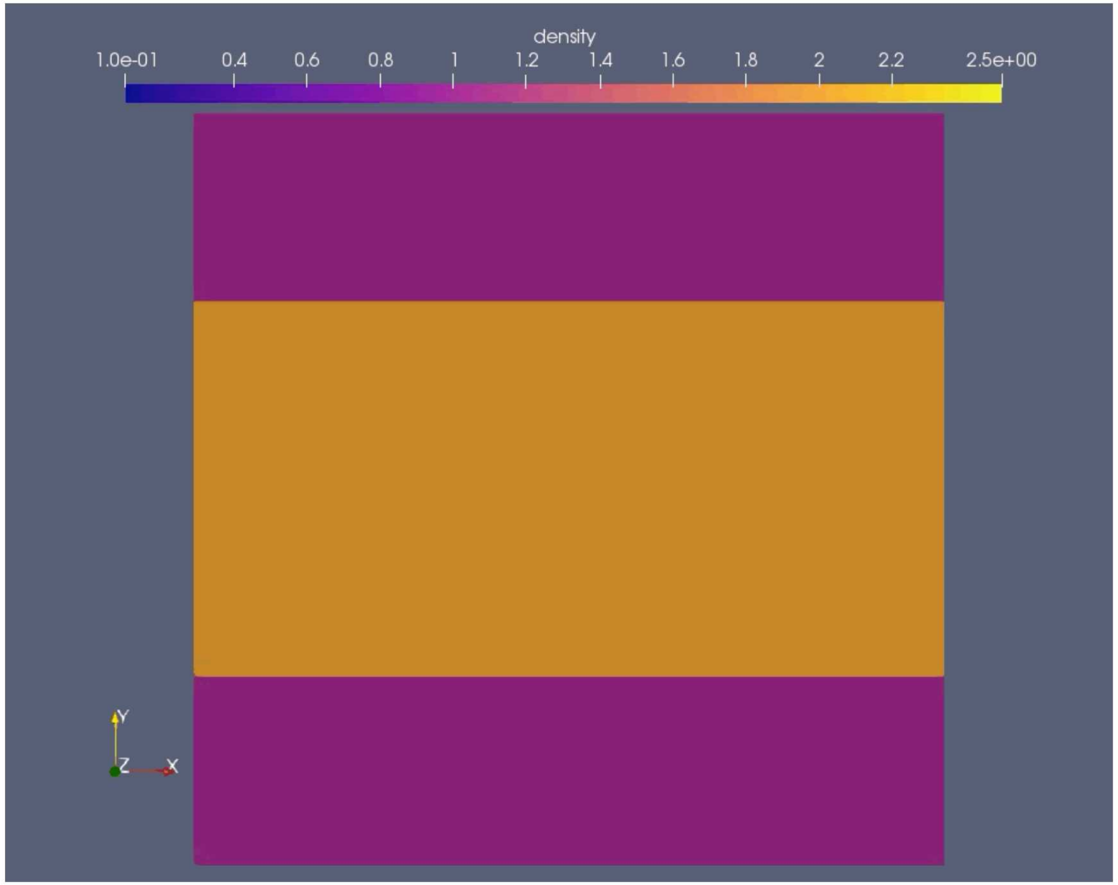
- By 50 ns , a larger volume allows greater axial flux compression onto the liner surface.





PERSEUS/FLEXO – is rapidly gaining capabilities and is contributing to design efforts on Z

- PERSEUS is the design code for experiments to investigate the origins of the helical instability in MagLIF
- PERSEUS/FLEXO validation tests on Z experimental results are bringing new insights into previously unexplained data:
  - MagLIF simulations show steeper helical pitch on liner surface for larger flux compression volume.
  - PERSEUS shows close qualitative agreement for influence of Hall physics on B-field diffusion into low-density plasma.
- Present capabilities:
  - Initial implementations of static mesh AMR and multi-material tabular EOS
  - A wide range of verification and validation tests for these new capabilities
  - Born on MPI-X (distributed memory + GPU/OpenMP/…)
- Work remains on:
  - Multi-material, tabular EOS and AMR
  - More extensive set of boundary conditions
  - Radiation transport

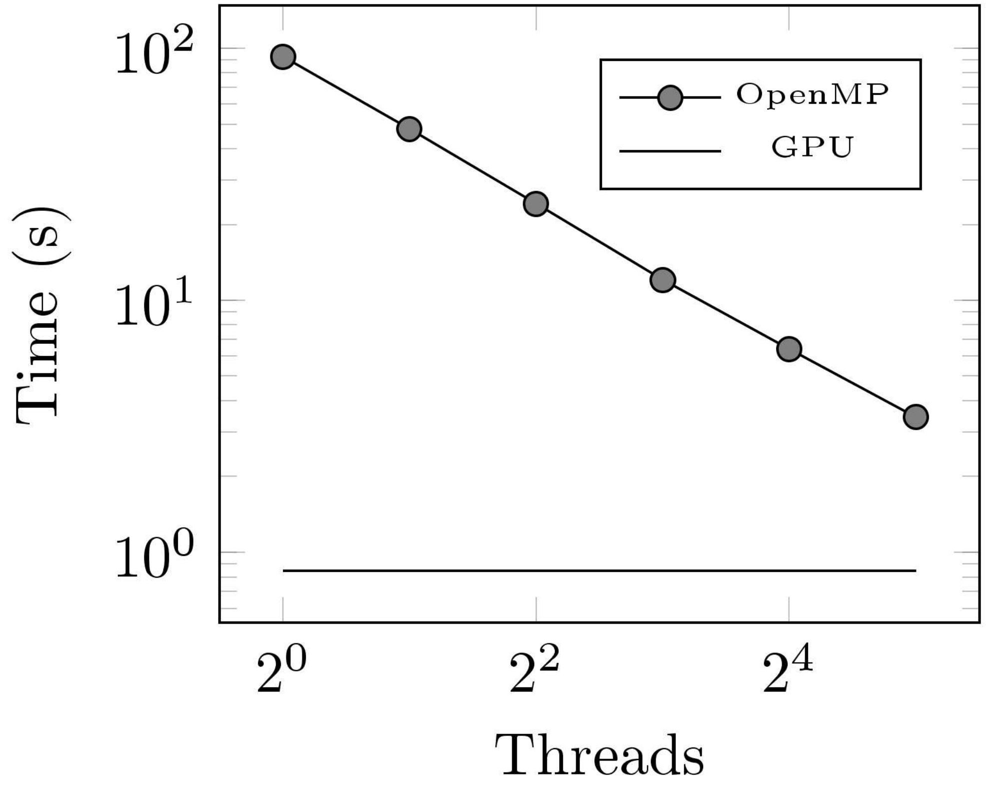


FLEXO DG Kelvin-Helmholtz Validation test on a 750x750 Grid

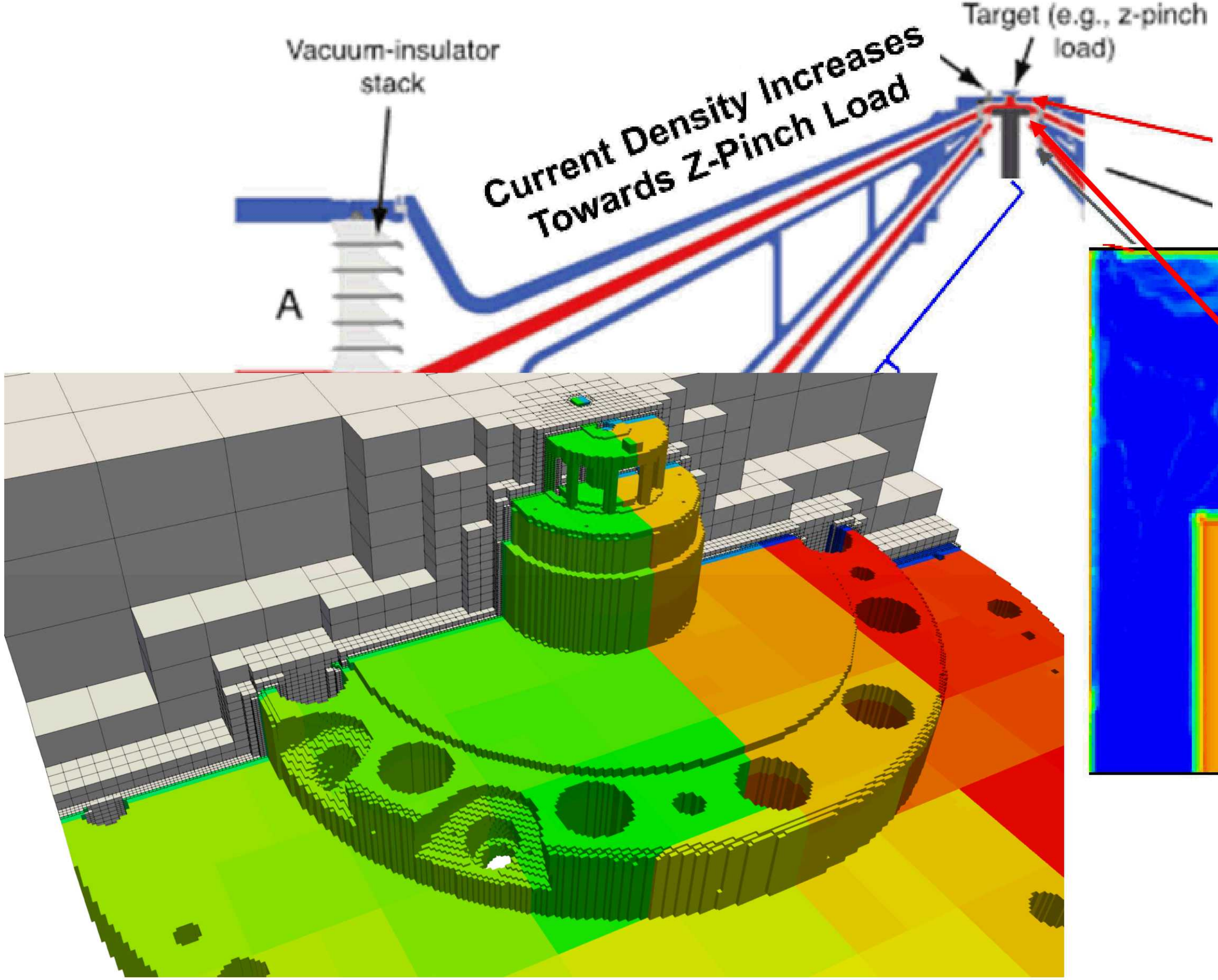
FLEXO designed from birth for GPU acceleration (MPI-X)

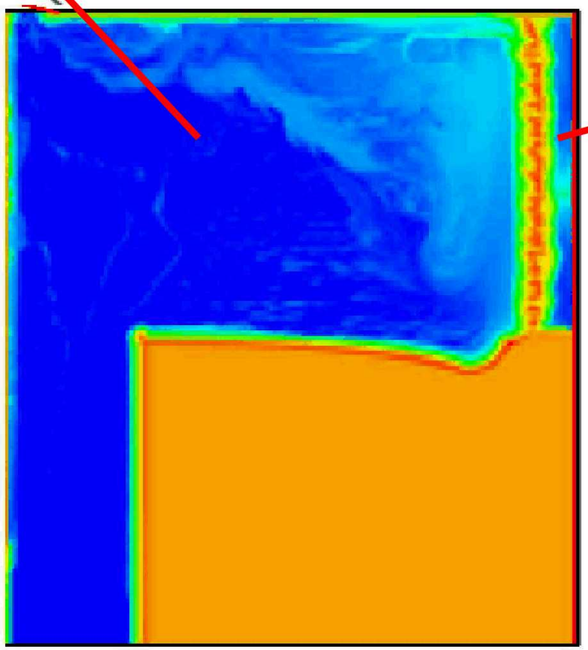
- Kokkos library for portably performant threading.
- Demonstrated on-rank (threaded) performance / scaling on GPU and traditional (OpenMP) threading.
- Redesigned code framework for improved MPI performance:
  - Initial weak scaling studies indicated significant cost for boundary updates.
  - Redesigned data storage on GPU resulted in **2X** speed-up.
  - Redesigned communication framework provided **300X** boundary comm. speed-up.
  - Implement overlapping communication and computation.

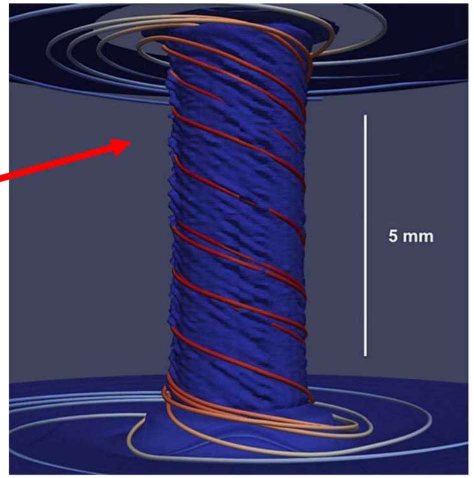
Timings for KH example (10 steps, 400x400x1 elems)



Wide range of spatial scales suggests need for AMR

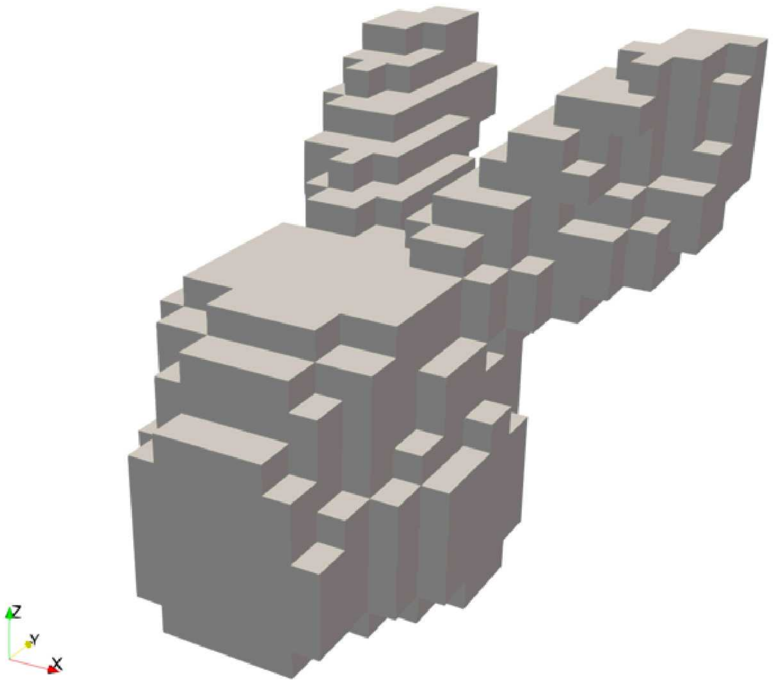


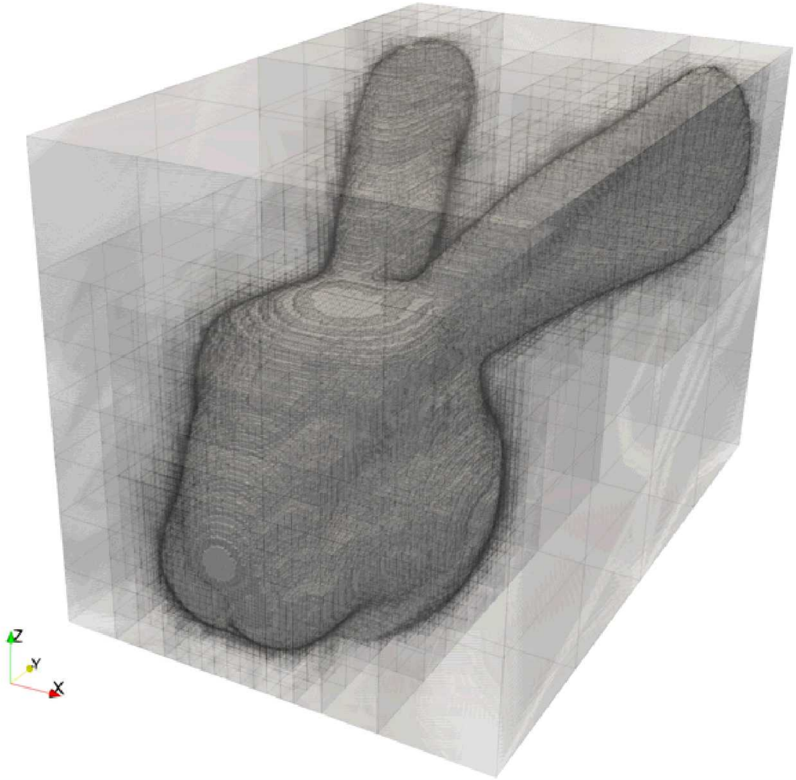




Threading greatly enhances mesh refinement performance

- Demonstrated ability to refine to CAD geometry
- Demonstrated utility of accelerators
  - i7 Mac laptop: 5 min. 55s time to solution
  - Ride GPU test-bed: 2s time to solution
- GPU and MPI initial scaling tests have been completed

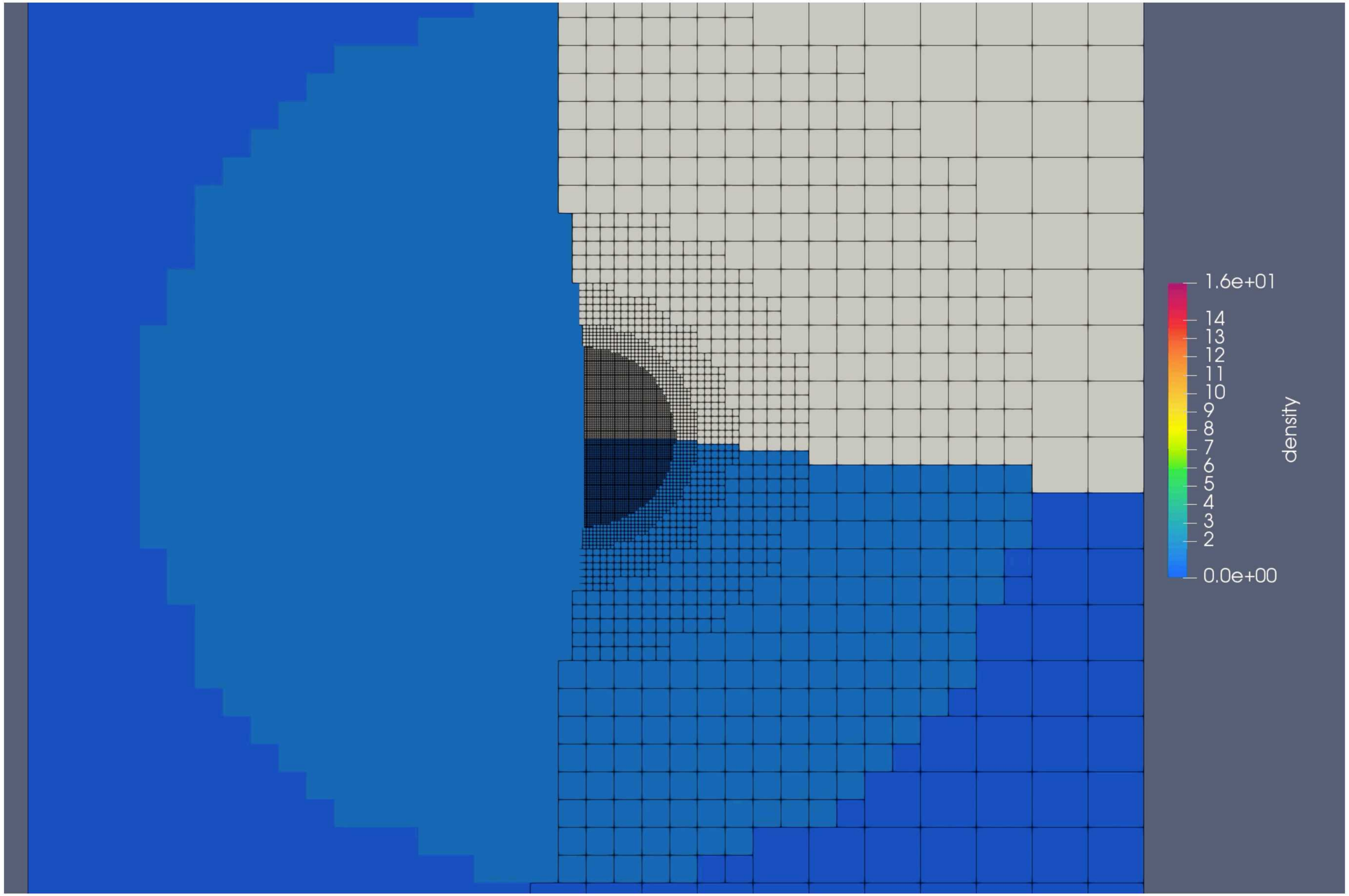




Static mesh refinement on path to full AMR (1)

- 2D Noh problem:

$$\gamma = 5/3$$
$$\rho_{inner} = 1$$
$$\rho_{outer} = 10^{-6}$$
$$e^{int} = 10^{-6}$$



Static refinement (2)

- Ideal MHD, Magnetized blast:

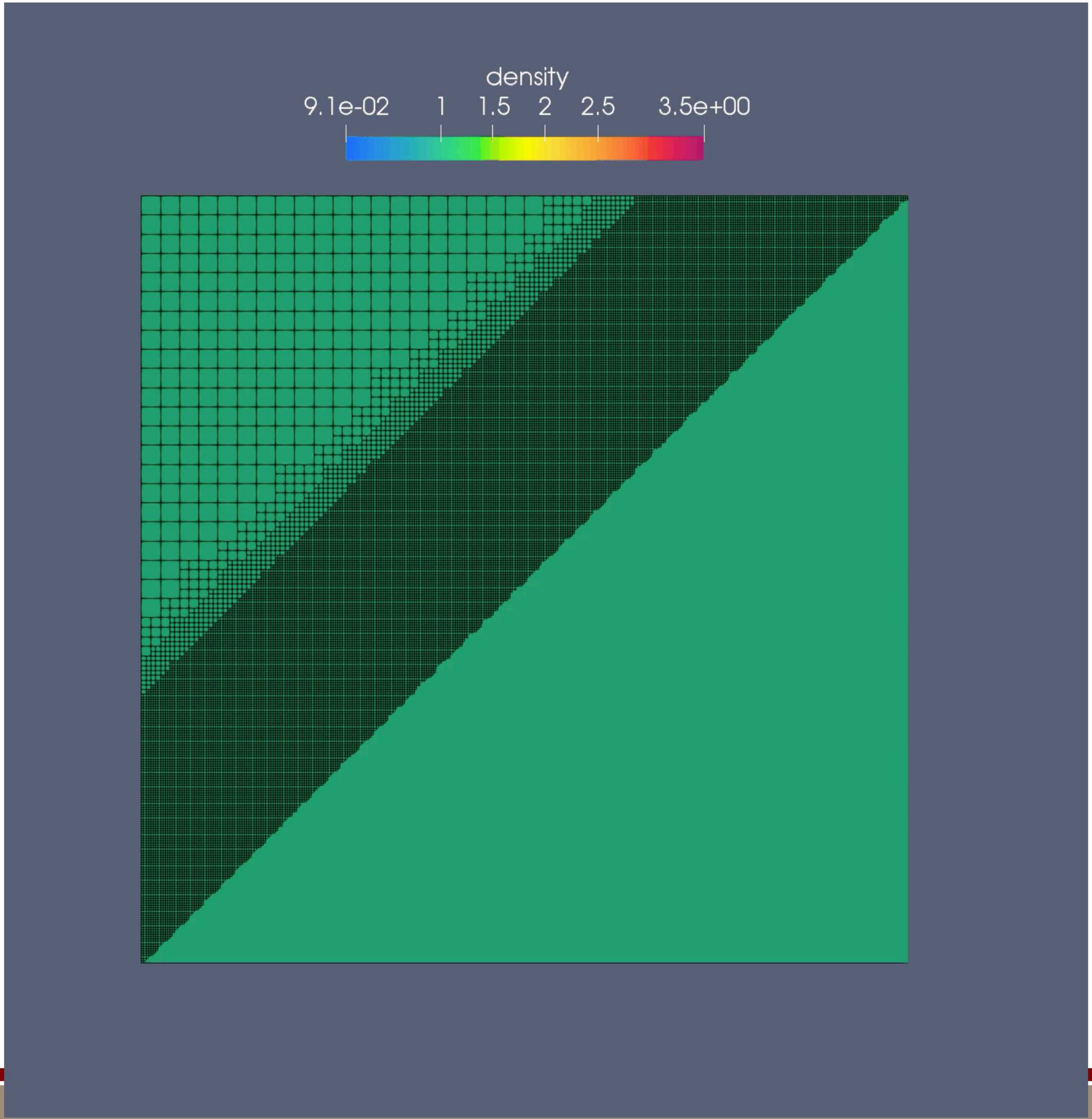
$$\gamma = 5/3$$

$$\rho = 1$$

$$p = \begin{cases} 10 \text{ for } r <= .1 \\ 0.1 \text{ for } r > .1 \end{cases}$$

$$B_x = B_y = \sqrt{2\pi}$$

Problem specs from:
https://www.astro.princeton.edu/~jstone/
Athena/tests/blast/blast.html



Exploring 5-Equation multi-material model

Uniform strain assumption

$$\frac{\partial \alpha_i}{\partial t} + \nabla \cdot (\alpha_i \mathbf{v}) = \begin{cases} \alpha_i \nabla \cdot \mathbf{v} \\ \text{or} \\ \frac{\alpha_i K_i}{\overline{K}} \nabla \cdot \mathbf{v} \end{cases}$$

Miller and Pucket (1996)
Murrone and Guillard (2005)

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

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

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

$$\rho = \sum_i \alpha_i \rho_i$$

$$\rho e = \sum_i \alpha_i \rho_i e_i$$

$$P_i = \rho_i e_i^{int} (\gamma_i - 1)$$

$$P = \sum_i \alpha_i P_i$$

… with pressure equilibration to close internal energy partition.

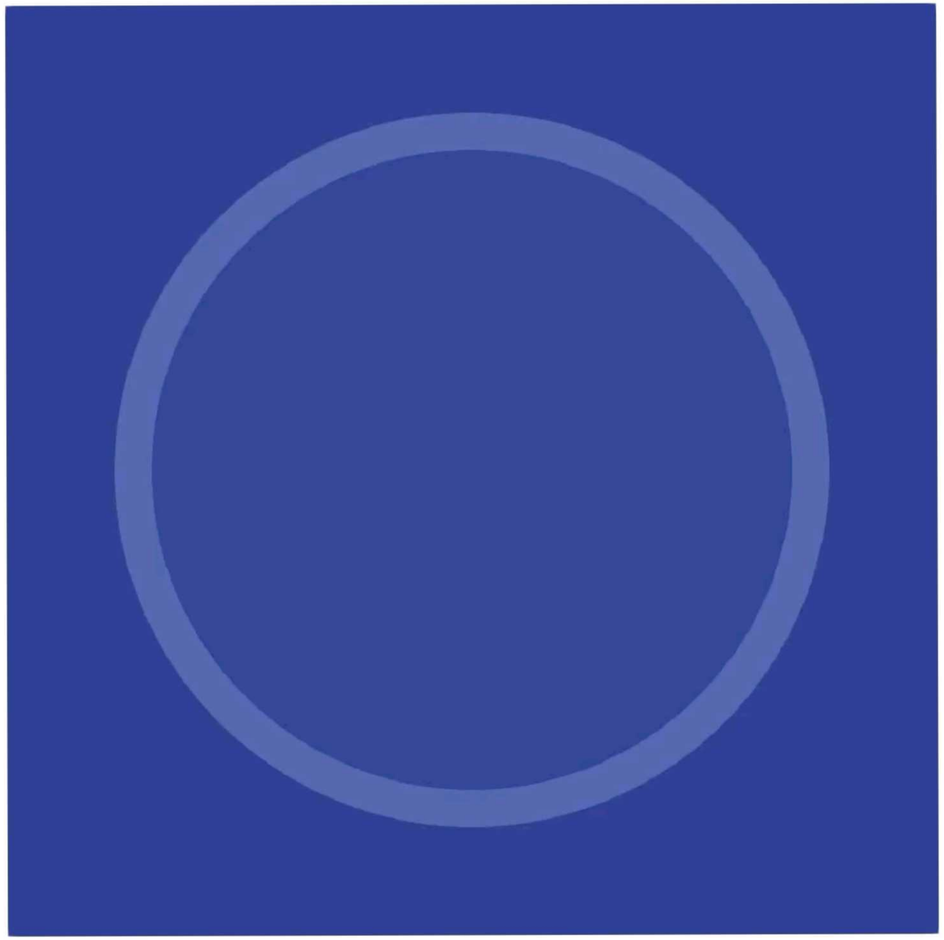
Diffusion suggests interface sharpening algorithms.

Consider Eddy experiment

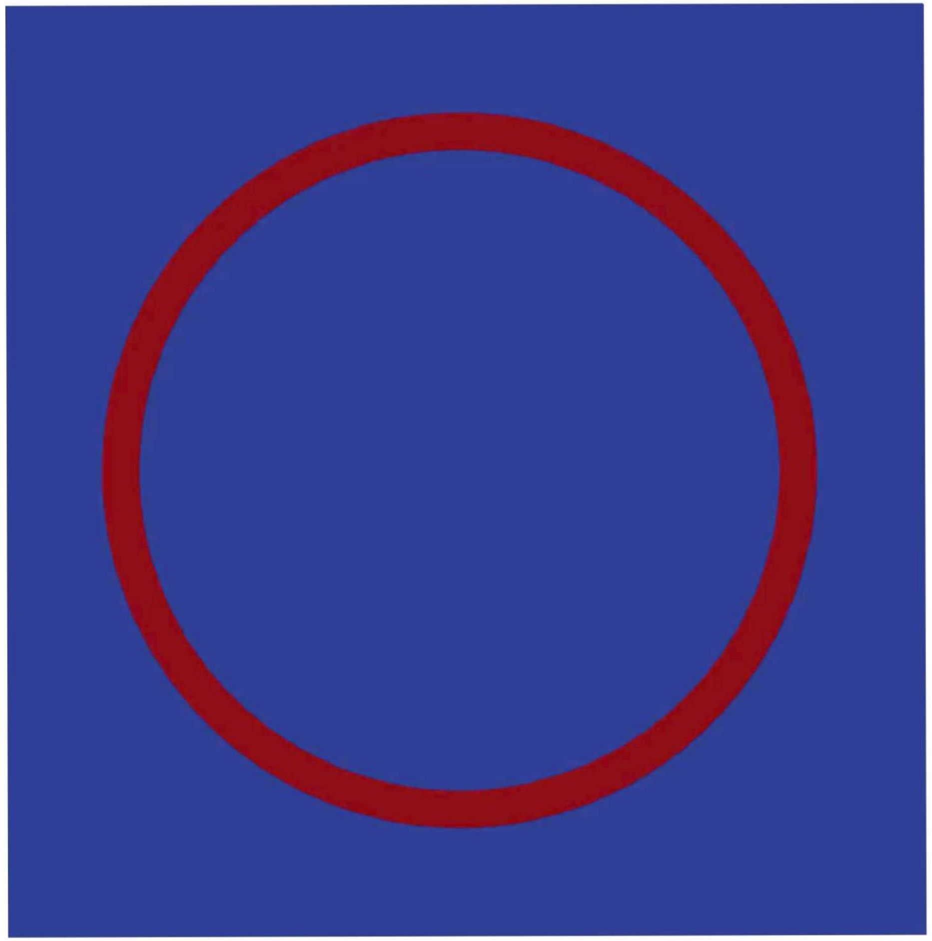
Some directions:
- Gorgon approach
- Interface reconstruction
- Flux Corrected Trans.

Multi-material demonstration in 2D

1M cell, GPU simulation of Eddy mock-up.



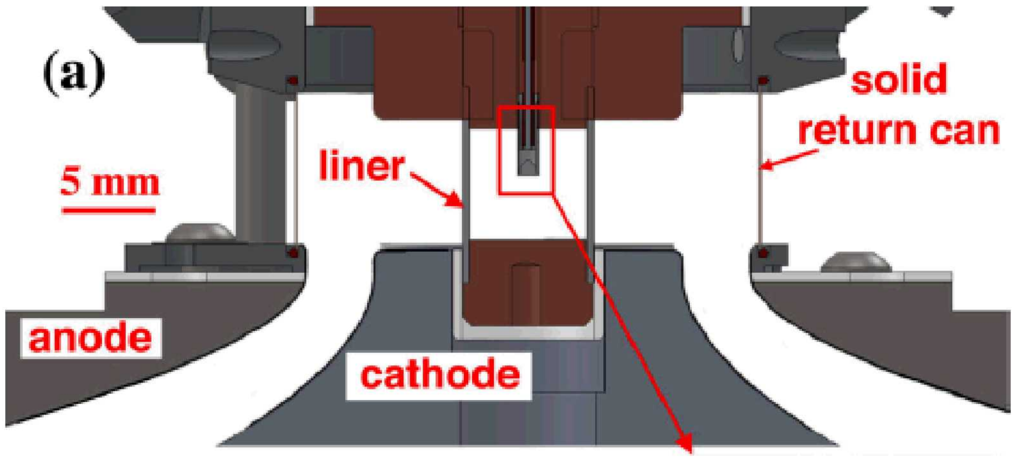
Mixed density

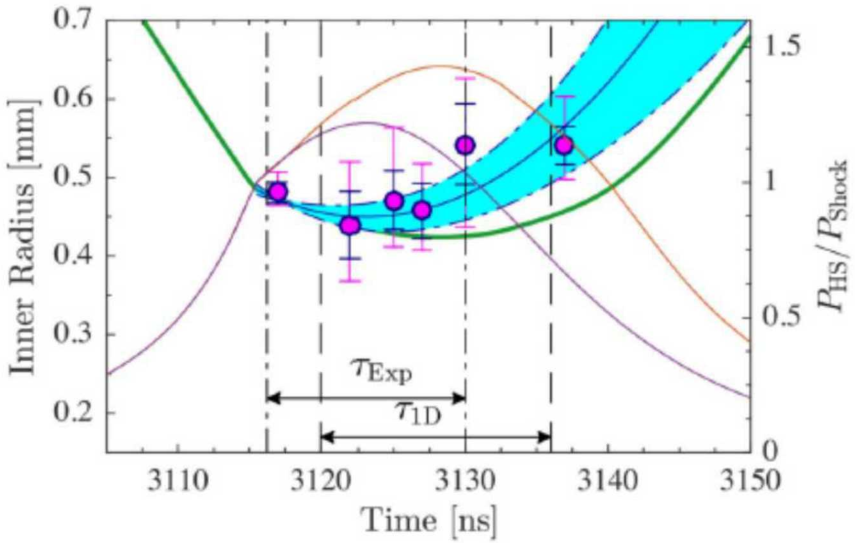


Cylinder volume fraction

Testing is an integral part of development efforts

- Nightly regression tests on a range of platforms including:
  - NVIDIA GPU (CUDA)
  - Traditional threaded architectures (e.g. Xeon; OpenMP)
- Ever increasing set of hydro/MHD verification tests.
- Development aimed at simulation of (div. 1600) Eddy experiment for validation purposes.





Conclusions

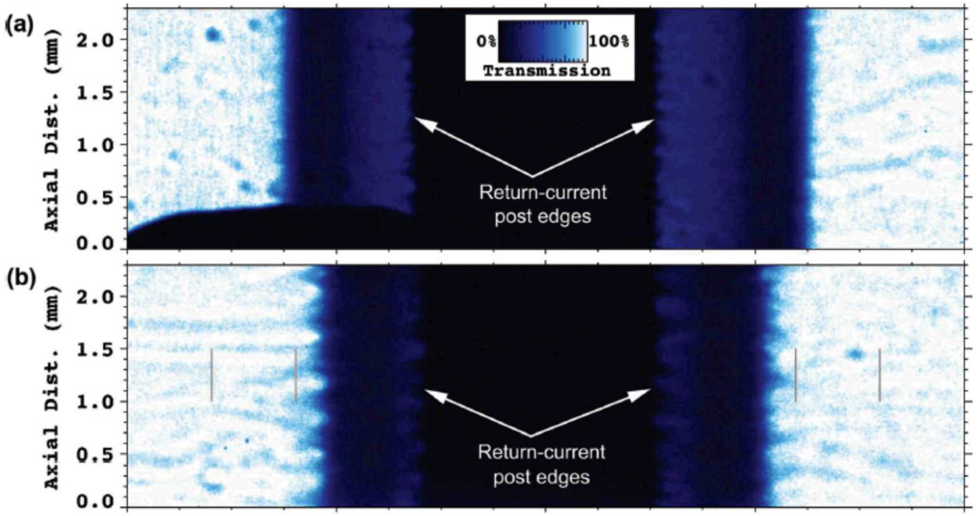
- Developing performant target design code for Z-Next
- Code is designed from birth to support MPI-X (X: GPU, OpenMP) using Kokkos parallel performant threading model.
- Starting from proven PERSEUS XMHD code to support crucial target physics.
- Added (static) mesh refinement and working towards full (dynamic) AMR to support:
  - Meshing to boundary features
  - Resolve evolving physics features
- Adding and refining multi-material treatment to properly model material contacts (e.g. beryllium and deuterium).

Holdback Slides

Code Validation with Lincoln Beryllium Liner Experiments

Z Liner Radiography (Shot 2060)

Sandia National Laboratories

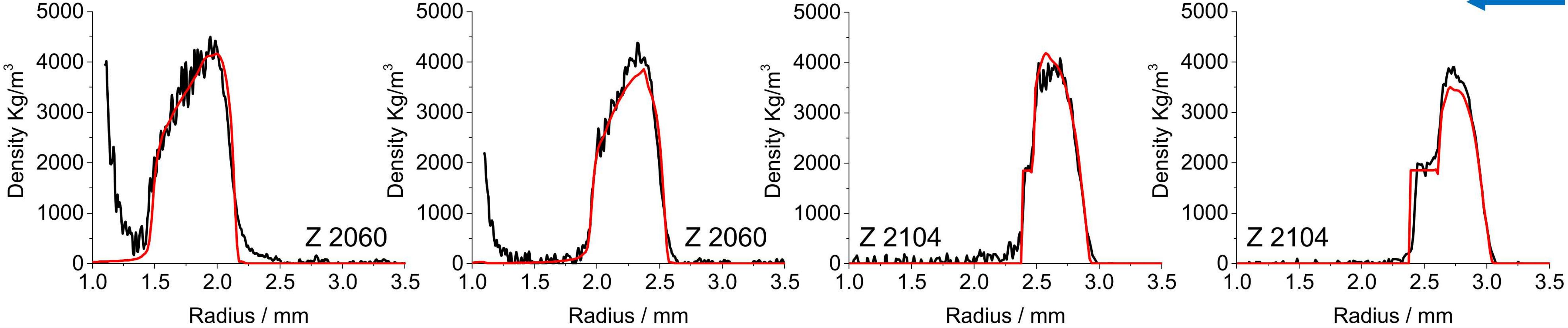


Citation: Physics of Plasmas 18, 056301 (2011); doi: 10.1063/1.3560911

29202 (LMD Be Conductivities)
LEOS40 (Be EOS)
Interfaced with 2D r-z version of Flexo/Perseus
~20 micron resolution
Preliminary results agree within uncertainties of experiment

Comparison of Abel inverted Z radiography data with simulated density (FLEXO/PERSEUS)

time



MM Hydro / Mag coupling:

- Multiple energy equations raises question of partitioning magnetic energy between components
- Internal energy equations (one per material):
  - Magnetic pressure added to single momentum equation.
  - Material internal energy equation update
  - Total energy (material internal plus kinetic) is not conserved.
  - Joule heating is partitioned.
  - ALEGRA approach
- Single total energy equation:
  - Multiple densities
  - EOS per material
  - Single (total) material energy
  - GORGON approach.

Numerous approaches to multi-material:

- Sharp Interface Methods (SIM) / interface tracking:
  - Lagrangian: not practical for large (fluid like) vorticities.
  - Eulerian, Level Set Methods: conservation is a research topic. Can't generate new interfaces
  - Eulerian, VOF reconstruction: can be problematic for unstable phenomena (K-H, R-T and R-M instabilities).
  - Not pursued here.
- Diffuse Interface Methods (DIM) / interface capturing:
  - Same algorithm in mixture and pure regions. Hyperbolic system in all regions of flow. Mixture model closure for multiphase regions.
  - "Interfaces" are created dynamically as needed.
  - Can handle interfaces between pure fluids and fluid mixtures.
  - Can be made to be conservative.
  - We will follow this general approach.

Terminology

- Multi-material flow: track/capture multiple distinct materials (air, steel, etc.).
- Multi-phase flow: track/capture multiple phases of a single material (gas, solid, liquid, plasma).

- Of course both can be present, e.g. Multi-material, multi-phase flow. Indeed we will be in this space (see later).

Our space:

- Multi-material:
  - More than two (algorithms designed for only two won't work here).
  - Materials may include Beryllium, etc…
- Multi-phase:
  - All phases present from solid to liquid to gas to plasma.
  - Target starts as a solid geometry but melts, vaporizes and finally becomes a plasma.
- Challenging because:
  - Significant demands on conservation equations (which set, DIM vs SIM, etc.).
  - Significant demands on EOS (huge phase space).
  - Significant demands on mixture models (e.g. solids have definitive boundaries with other phases, plasmas may be expected to mix).

Modeling complexities

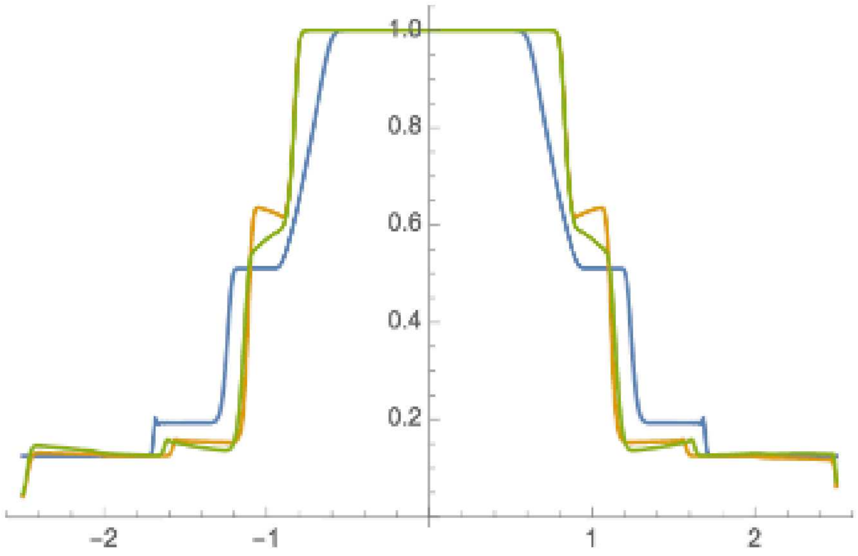
- Generally from Baer and Nunziato (1986)
- ... with restriction to single velocity (for XMHD)
- Many possibilities:
  - Miller and Puckett (1996)
  - Abgral and Saurel (1999)
  - … and others.
- Limiting at contact needed for high-order DG*

$$
\begin{aligned}
\gamma_g &= \gamma_l = 1.25 \\
x_1 = -1.0\ \text{mm}, \quad x_2 &= 1.0\ \text{mm} \\
x_1 \le x \le x_2 : \quad \rho(x) &= 1 \\
x < x_1,\ x > x_2 : \quad \rho(x) &= 0.125 \\
x_1 \le x \le x_2 : \quad P(x) &= 0.2 \\
x < x_1,\ x > x_2 : \quad P(x) &= 0.05 \\
\alpha_g(x) = 0.7, \quad \alpha_l(x) &= 0.3 \quad \text{everywhere}
\end{aligned}
$$

$$\frac{\partial \rho_m f_\alpha}{\partial t} + \nabla \cdot (f_\alpha \rho_m \mathbf{v}_m) = \rho_m \mu (P_\alpha - P_m)$$

$$\frac{\partial f_\alpha}{\partial t} + \mathbf{v}_m \cdot \nabla \cdot f_\alpha = \mu (P_\alpha - P_m)$$

Out[933]=



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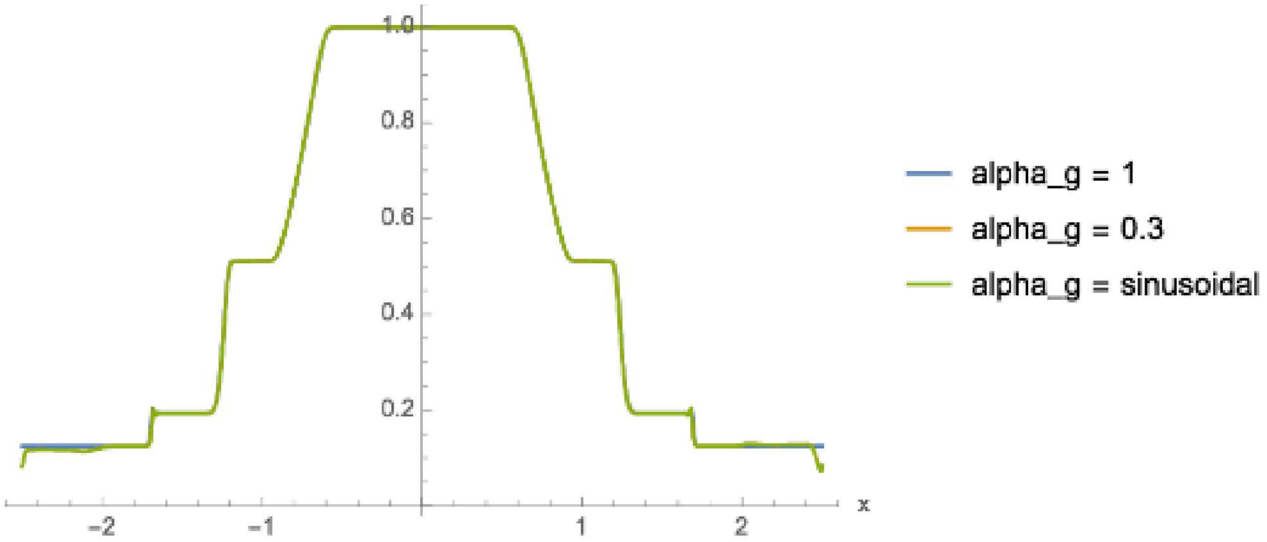

* Qiu and Shu, 2003, Zhu et al., 2008, Dumbster and Loubere, 2016