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Flexo: Development Activities for Z-Next Simulation

PRESENTED BY

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Motivations

- Develop a NGP performant eXtendend MagnetoHydroDynamic (XMHD) tool to support Z-Next design activities.
  - Starting from proven DG XMHD physics code (Perseus3D; Seyler and Martin, 2011).
  - Adding radiation transport to capture requisite target physics.
  - Incorporating AMR to maintain solution accuracy while remaining computationally feasible over wide range of length scales.
  - One of a suite of codes supporting different problem regimes.
- Designed from birth to support Next Generation Platforms using Kokkos:
  - Portably performant: runs efficiently on most modern hardware, especially NVIDIA GPUs.
  - Incorporates MPI to manage memory demands of large problems.
- And that is capable of impacting multiple Z-Next target needs:
  - NGS mesh generation
  - Extended Ohm's law magnetohydrodynamics (XMHD)
- The current path:
  - Extend an existing unstructured simplex adapt code to include cell-based AMR
  - Write a new XMHD application on top of the new AMR data structures
  - Add multi-material capability.
  - Add requisite radiation transport features.
  - Demo, profile, verify and deploy the resulting AMR XMHD code to impact Z-Next design.

Acknowledgements

Team:

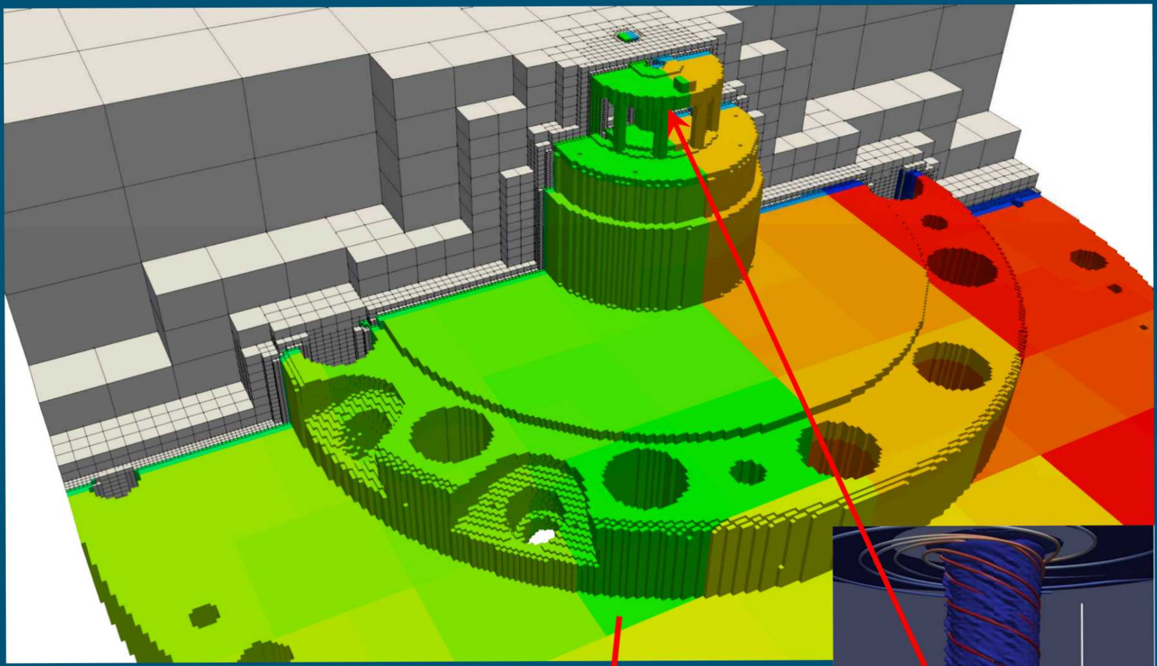
- Kris Beckwith
- Stephan Bond
- Brian Granzow
- Nat Hamlin
- Chris Jenning
- Matt Martin
- Andy Porwitzk
- Alan Stagg

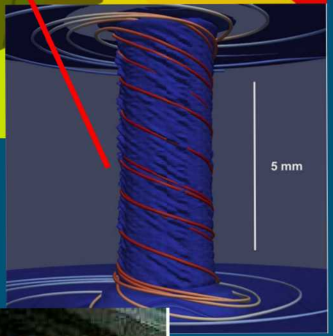
Original Perseus Fortran90:

- Matt Martin
- Charles Seyler
- Yang Yang
- Xuan Zhao

Challenges

- Low density electrode plasmas
- Must include Hall term
- Multiple materials / EOS
- Complex geometries
- Wide range of spatial and temporal scales
- Incorporate radiation physics
- Advanced computational architectures





PERSEUS GOL equations

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0$$ Density

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u} + \mathbf{I}P) = \mathbf{J} \times \mathbf{B}$$ Momentum

$$\partial_t \mathcal{E}_n + \nabla \cdot (\mathbf{u}(\mathcal{E}_n + P)) = \mathbf{u} \cdot (\mathbf{J} \times \mathbf{B}) + \eta \|\mathbf{J}\|^2$$ Total Energy

$$\partial_t \mathbf{B} + \nabla \times \mathbf{E} = 0$$ Magnetic Field

$$\partial_t \mathbf{E} - c^2 \nabla \times \mathbf{B} = -\frac{1}{\varepsilon_0} \mathbf{J}$$ Electric Field

$$\partial_t \mathbf{J} + \nabla \cdot \left(\mathbf{u}\mathbf{J} + \mathbf{J}\mathbf{u} - \frac{1}{n_e e}\mathbf{J}\mathbf{J} - \frac{e}{m_e}\mathbf{I}P_e\right) = \frac{n_e e^2}{m_e}\left(\mathbf{E} + \mathbf{u} \times \mathbf{B} - \eta \mathbf{J} - \frac{1}{n_e e}\mathbf{J} \times \mathbf{B}\right)$$ Current Density

$$\partial_t S_e + \nabla \cdot (\mathbf{u}_e S_e) = (\gamma - 1) n_e^{1-\gamma} \eta \|\mathbf{J}\|^2$$ Electron Entropy

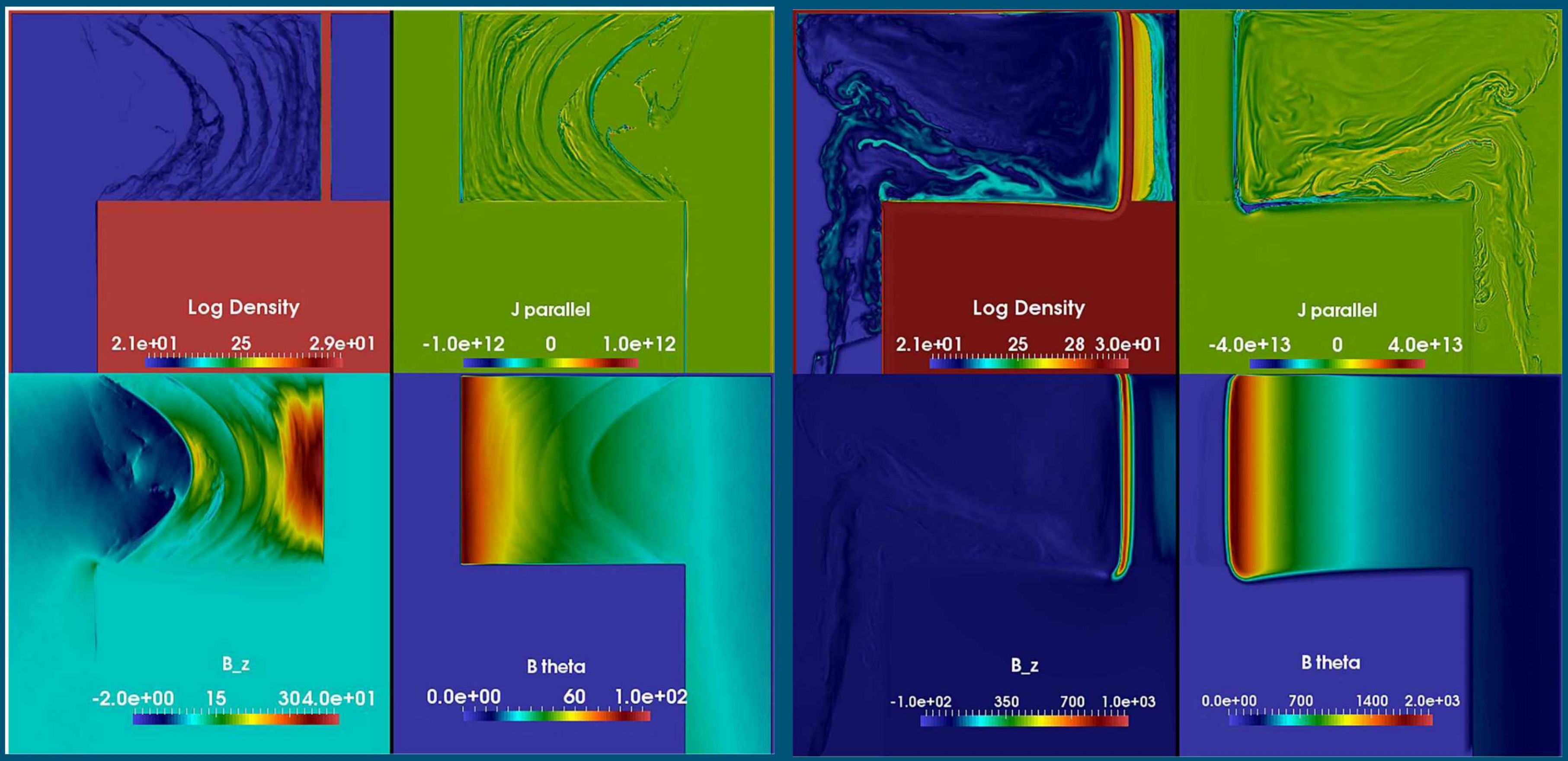
Code History

- Finite Volume Fortran90 code: M. Martin and C. Seyler 2011
  - **P**lasma as an **E**xtended-MHD **R**elaxation **S**ystem using and **E**fficient **U**pwind **S**cheme
  - Generalized Ohm's Law 2-Fluid model (14 moment)
  - Relaxation system of equations
  - Finite Volume / Uniform Grid
  - Implicit-Explicit Monotone Upwind Scheme for Conservation Laws
  - Modified Local Lax-Friedrichs
  - Locally linearly implicit (local 3 x 3 linear solves)
  - Able to recover resistive-MHD limit

- DG Perseus Fortran90 code: X. Zhao, Y. Yang and C. Seyler 2014
  - Generalized Ohm's Law 2-Fluid model (15 moment)
  - Discontinuous Galerkin extension of FV Perseus
  - Modified HLLC flux
  - Locally linearly implicit (local 3 x 3 solves)
  - Positivity preserving

PERSEUS Results

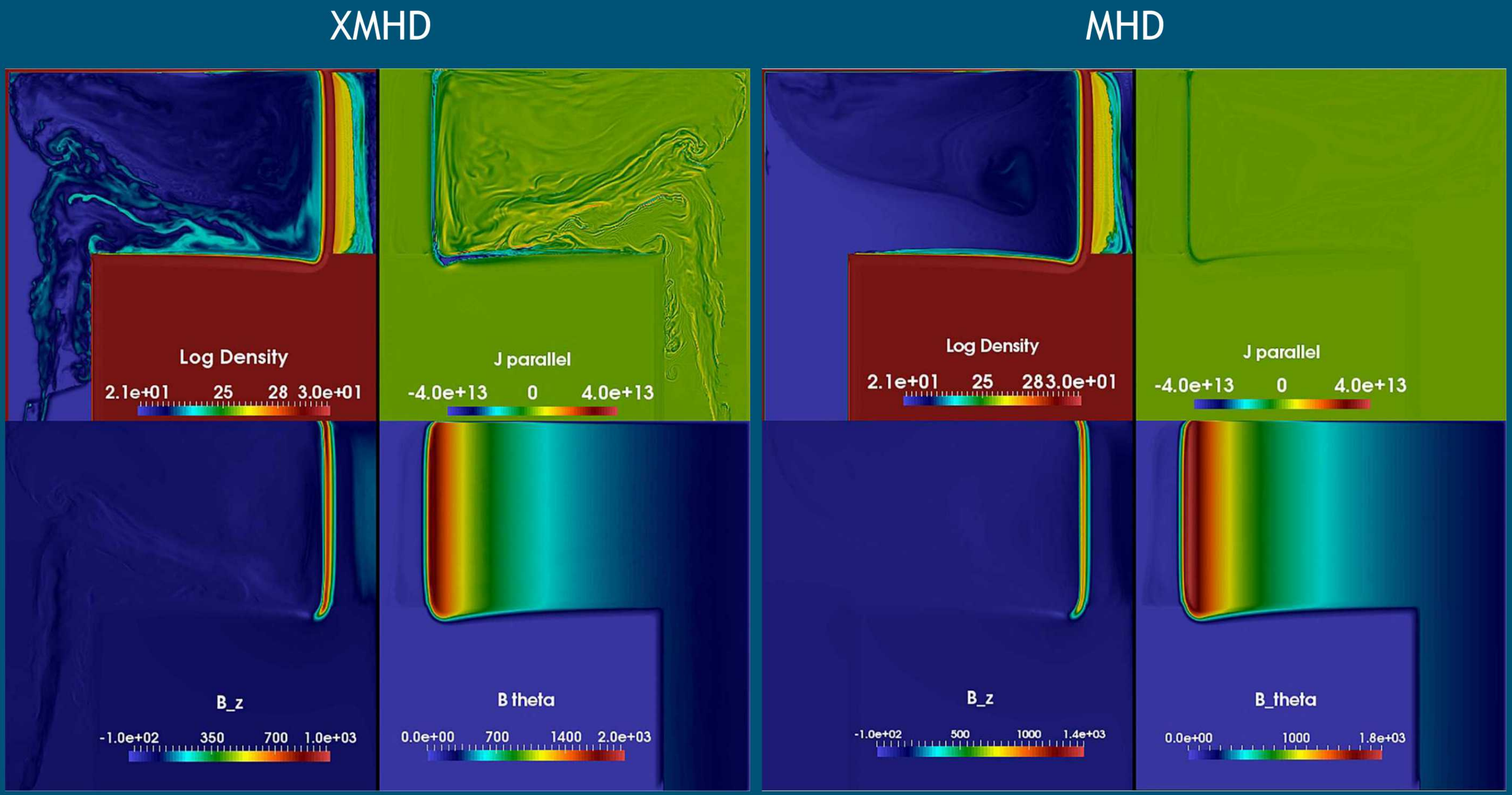
t = 20ns   t = 90ns



XMHD: No plasma layer initialized on feed walls

* C.E. Seyler, M.R. Martin, N.D. Hamlin, Phys. Plasmas, 25 (2018)

PERSEUS Results

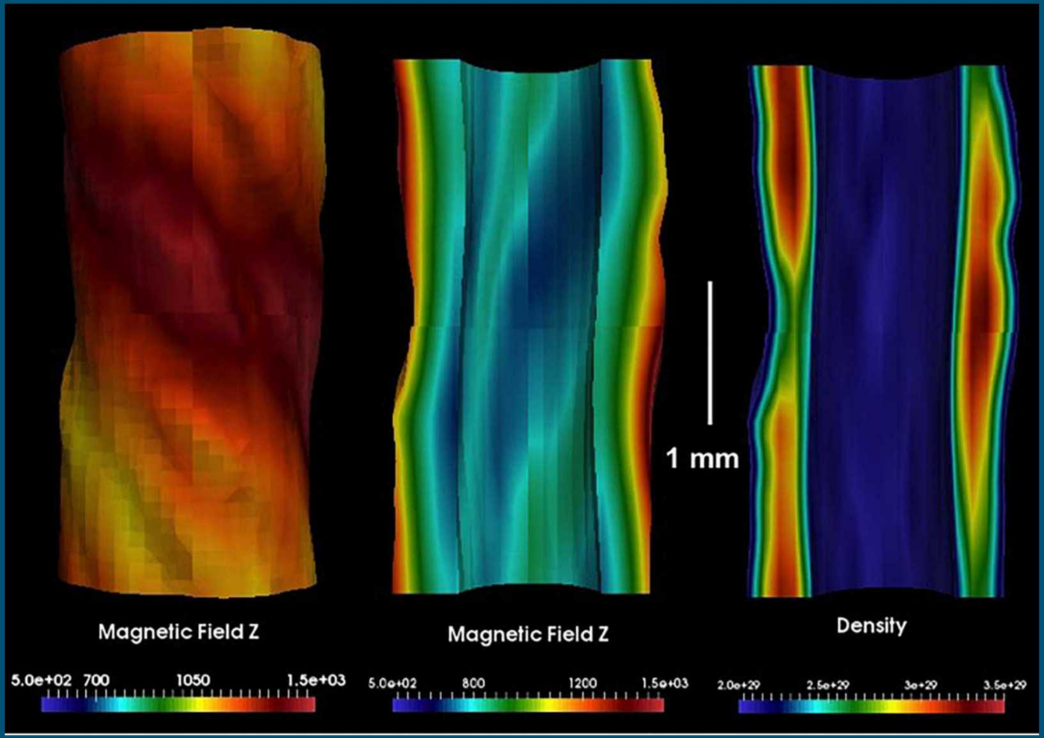


XMHD: No plasma layer initialized on feed walls, t = 90ns

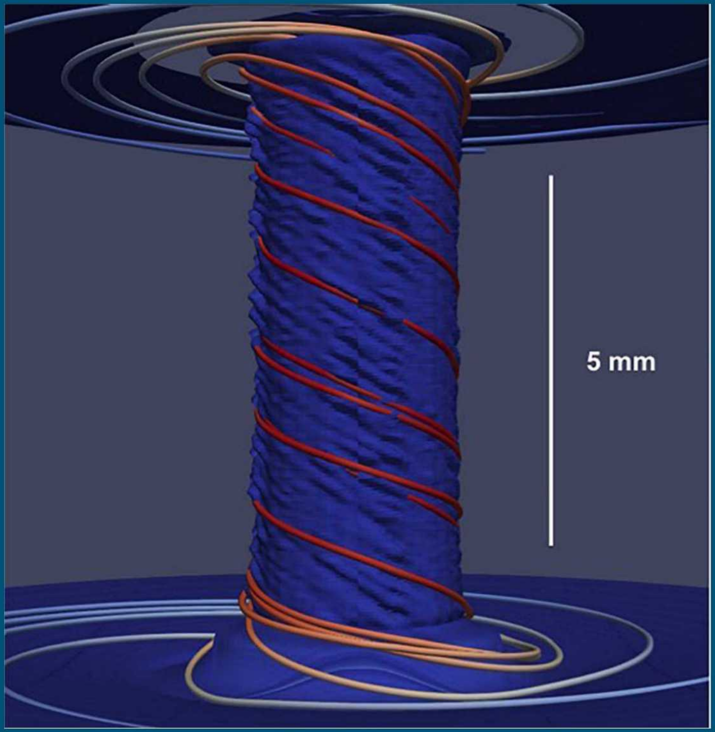
* C.E. Seyler, M.R. Martin, N.D. Hamlin, Phys. Plasmas, 25 (2018)

PERSEUS Results

iso contours



density

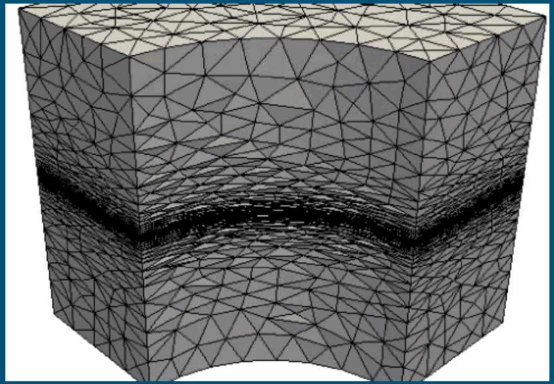


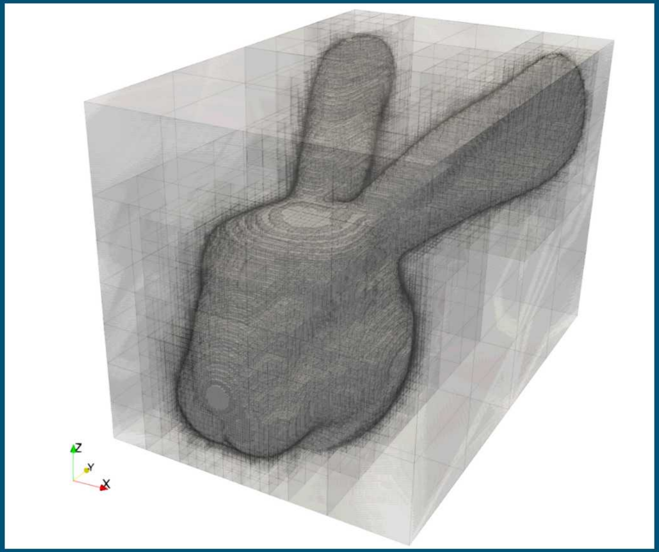
* C.E. Seyler, M.R. Martin, N.D. Hamlin, Phys. Plasmas, 25 (2018)

A Cell-Based AMR library for NGP

- Omega_h was:
  - Array-based C++ simplex adapt code
  - Conforming unstructured adaptation
    - Isotropic
    - Anisotropic
    - Local mesh modification on cavities
  - Built with MPI + X parallelism
    - CUDA
    - OpenMP
    - Enabled via Kokkos

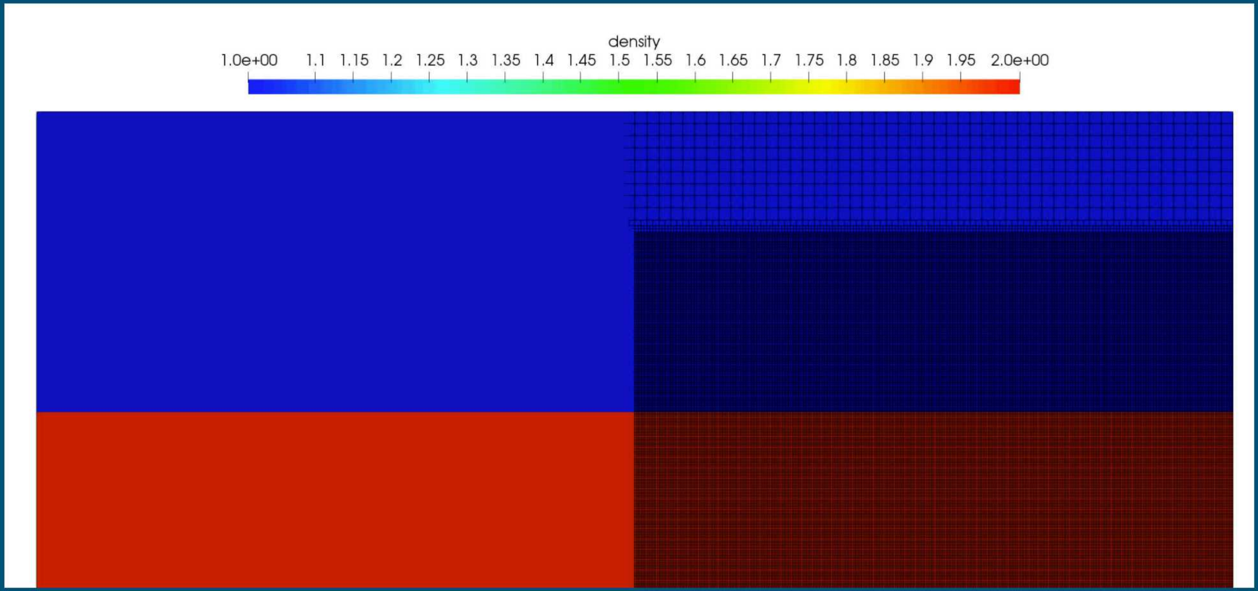
- Omega_h is now:
  - Everything it was before plus:
  - Unstructured cell-based AMR:
    - Hanging node refinement
    - Currently a single refinement template
    - Quads split into 4 quads
    - Hexes split into 8 hexes

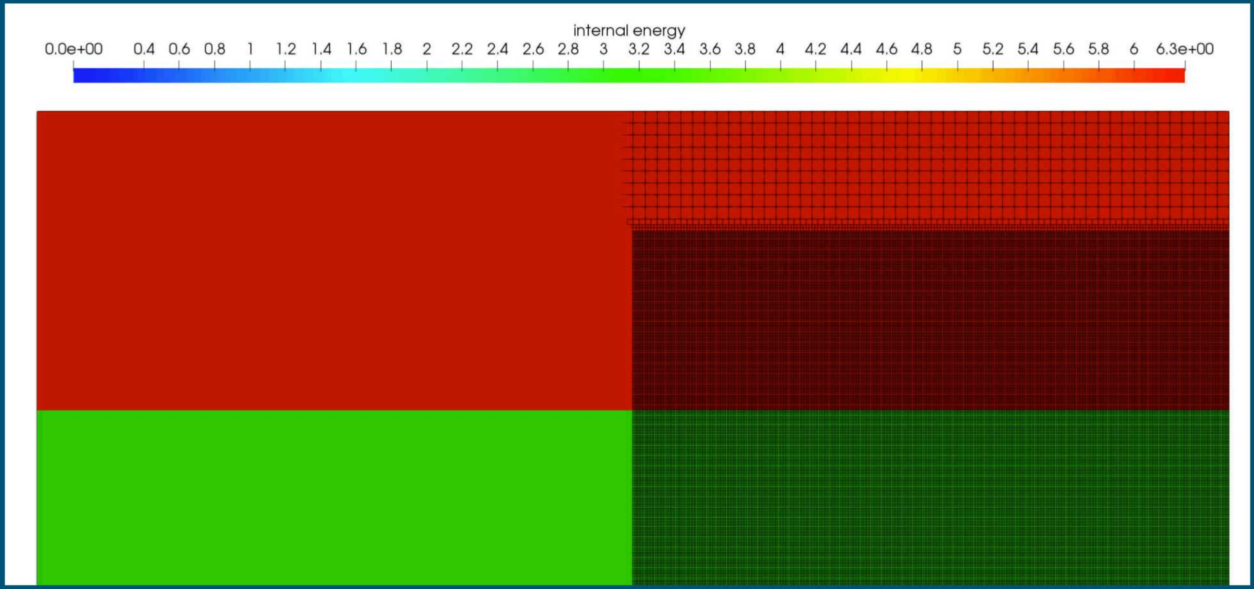




Ibanez, Daniel Alejandro. *Conformal Mesh Adaptation on Heterogeneous Supercomputers*. Diss. Ph. D. thesis, Rensselaer Polytechnic Institute, 2016.

FLEXO Time Static AMR Mesh Example: KH Instability





Radiation Transport

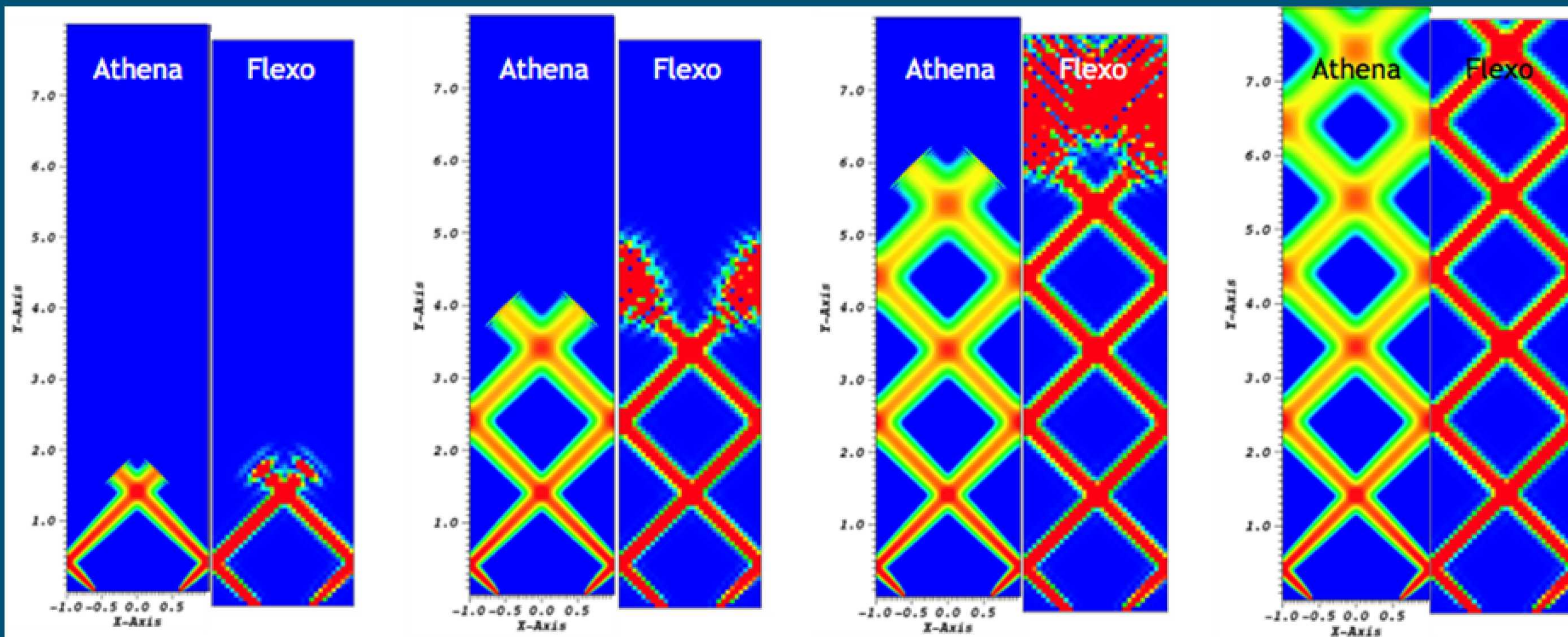
Imposes significant computational cost (performance and/or memory) attacked using moment formalisms:

- However requires closure relation
- Flux limited diffusion is robust and easy to implement but has deficiencies in optically thin regions
- M1 closure rectifies these defects but is unable to treat multiple radiation sources.
- VET (Variable Eddington Tensor) methods are not subject to these limitations but are based on the assumption that the time-scale for radiative transport is short compared to flow dynamical time-scales.

Must accurately couple the radiation field to the magneto-hydrodynamic equations:

- Follow approach of Sekora and Stone (2010) extended to multi-dimensions by Jiang et al. (2012) using the VET closure of Davis et al. (2012).
- Methods used here is described by Jiang et al. (2014) and are publically available as part of the Athena MHD code.
- Use extensive test suite of Jiang et al. (2014) to verify algorithms.

Radiation Transport: Crossing Beams Problem



- Athena resolutions: 512x1024 zones; Flexo resolution: 32x128 zones

Multi-Material Treatment

- Single temperature and velocity
- Multiple mass and internal energy densities
- Conservative form: Partial densities

$$\rho := \rho_1 + \rho_2 + \cdots \rho_n$$

$$\partial_t \rho_i + \nabla \cdot (\rho_i \mathbf{u}) = 0$$

- Non-conservative form: Density fractions

$$\rho_i = Y_i \rho, \qquad Y_1 + Y_2 + \cdots Y_n = 1$$

$$\partial_t Y_i + \mathbf{u} \cdot \nabla Y_i = 0$$

- Non-conservative form: Inverse density fractions

$$\rho_i = V_i^{-1} \rho, \qquad V_1^{-1} + V_2^{-1} + \cdots V_n^{-1} = 1$$

$$\partial_t V_i + \mathbf{u} \cdot \nabla V_i = 0$$

M.T.H. de Frahan, S. Varadan, E. Johnsen, J. Comput. Phys. 280 (2015) 489-509

Conclusions and Future Work

- Conclusions
  - Extended existing unstructured simplex adapt code to include cell-based AMR
  - AMR library written from the get-go with MPI + X parallelism in mind
  - Demonstrated AMR abilities in FLEXO prototype code.
- Future Work
  - Omega_h AMR
    - MPI implementation (already in progress)
    - Add different refinement templates (anisotropic AMR)?
    - Coarsening
  - FLEXO
    - Radiation transport (already in progress)
    - XMHD implementation (already in progress)
    - MPI implementation using Omega_h
    - Time-dynamic AMR meshes
    - Local solution transfer operators during AMR
- Questions?