AsterX: a new open-source GPU-accelerated GRMHD code for dynamical spacetimes

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in collaboration with
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R. Haas, L. Ji, L.T. Sanches, E. Schnetter, J. Tsao, Y. Zlochower

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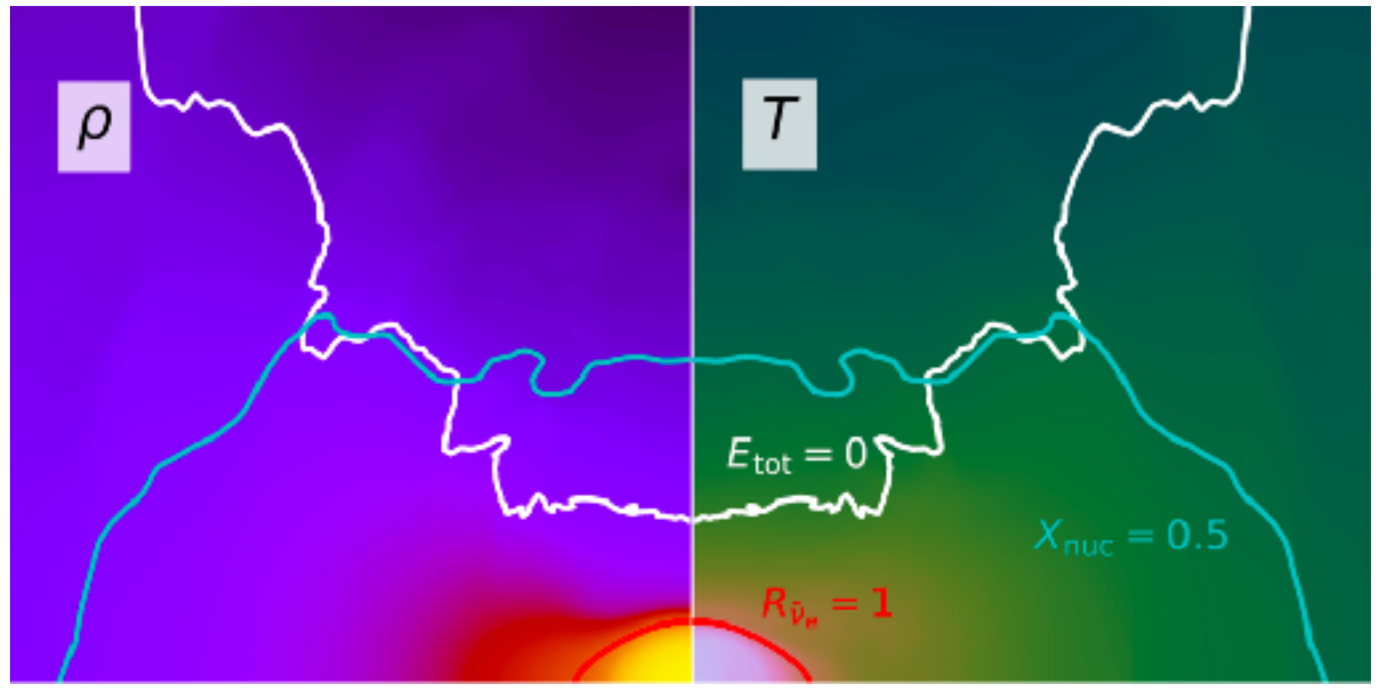
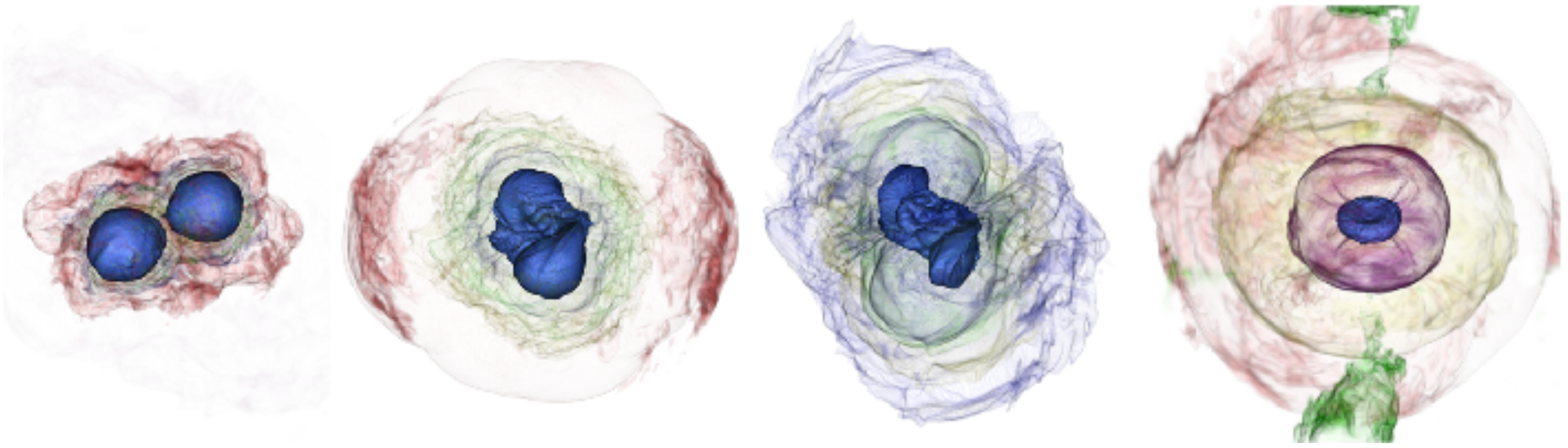
Overview

- Numerical background
- Code workflow
- AsterX code
- Test results
- Performance benchmarks
- Hands-on tutorial

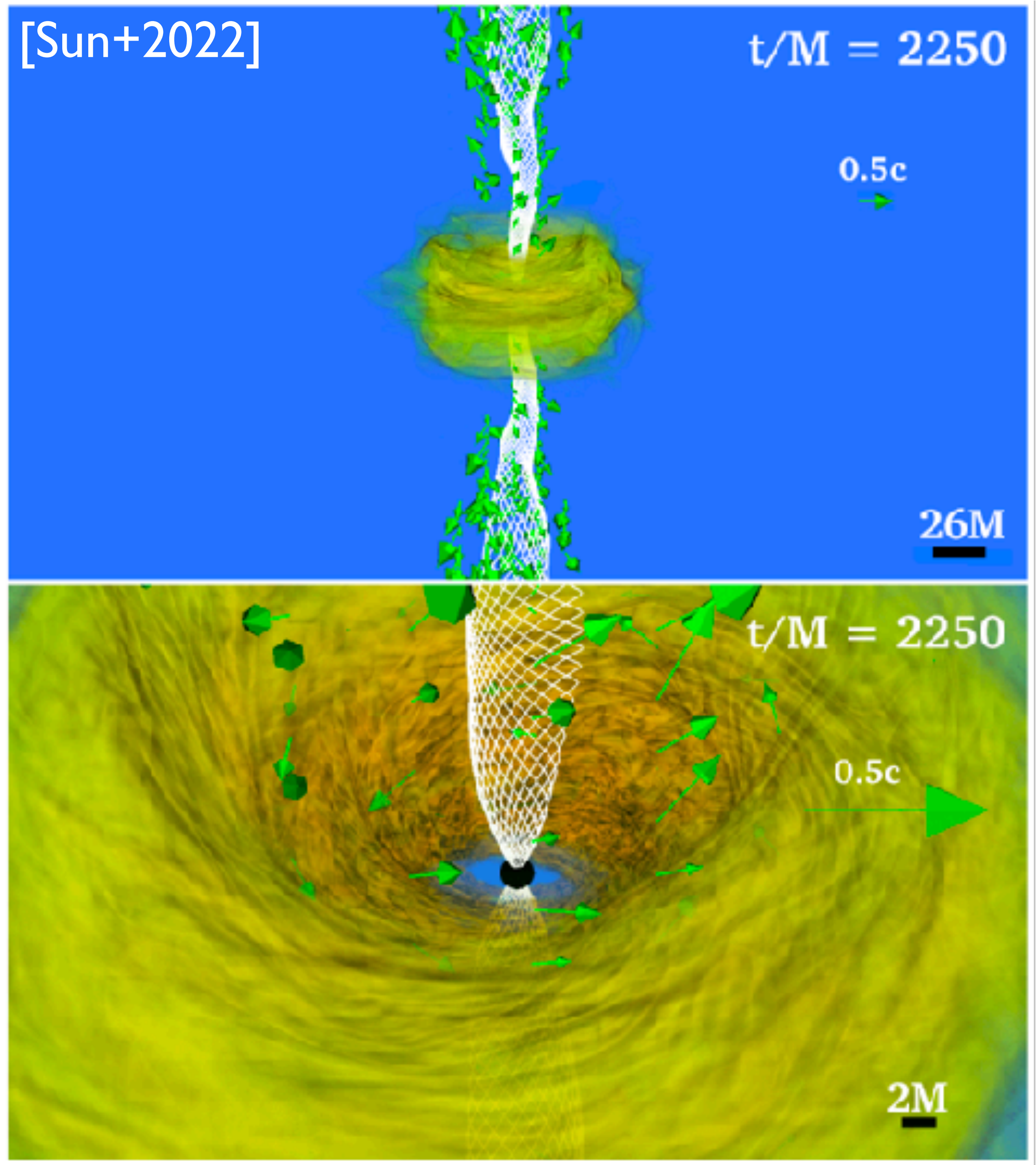
Need for GRMHD simulations

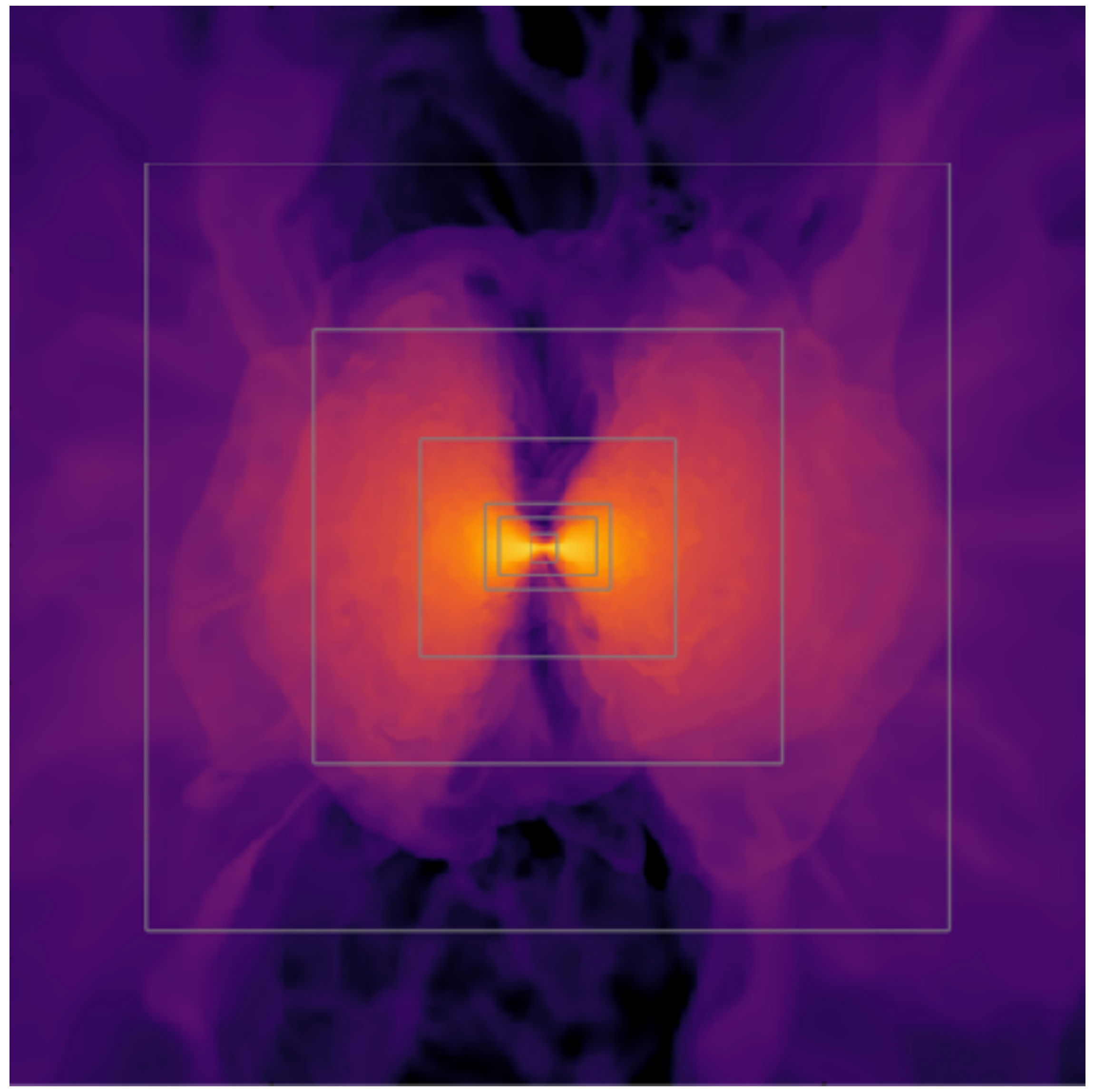


[Desai+2022]

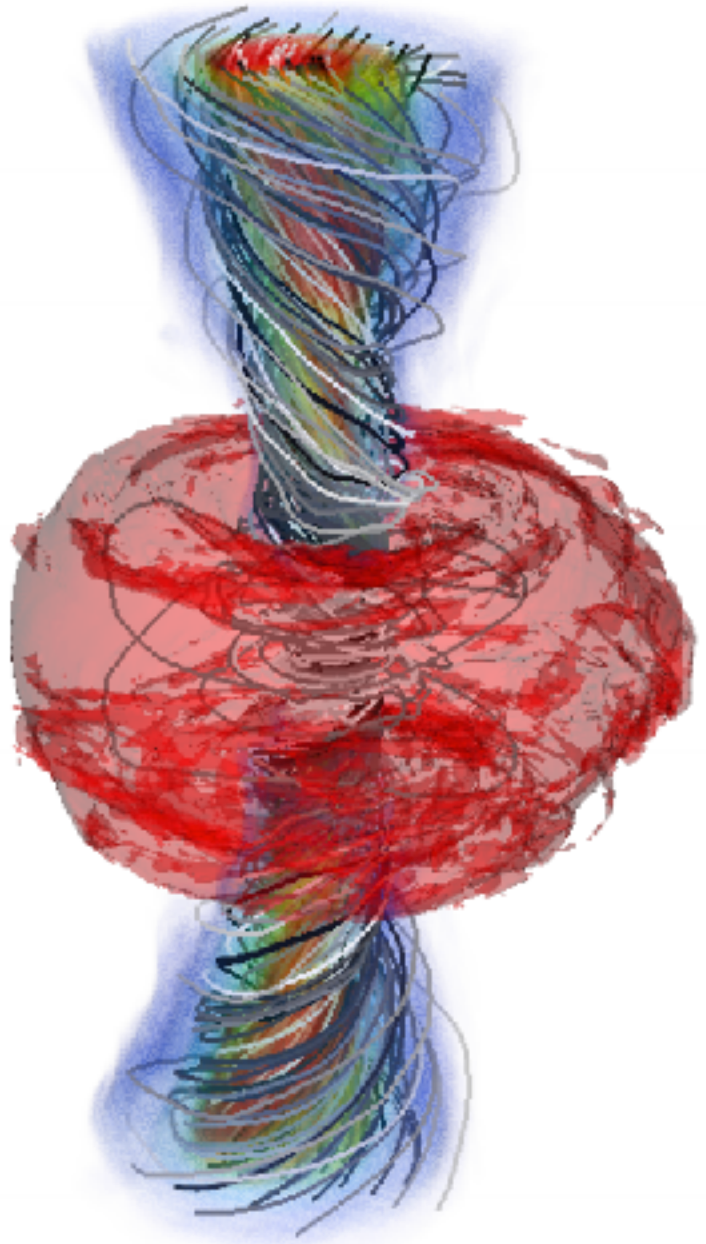


[Combi+2022]

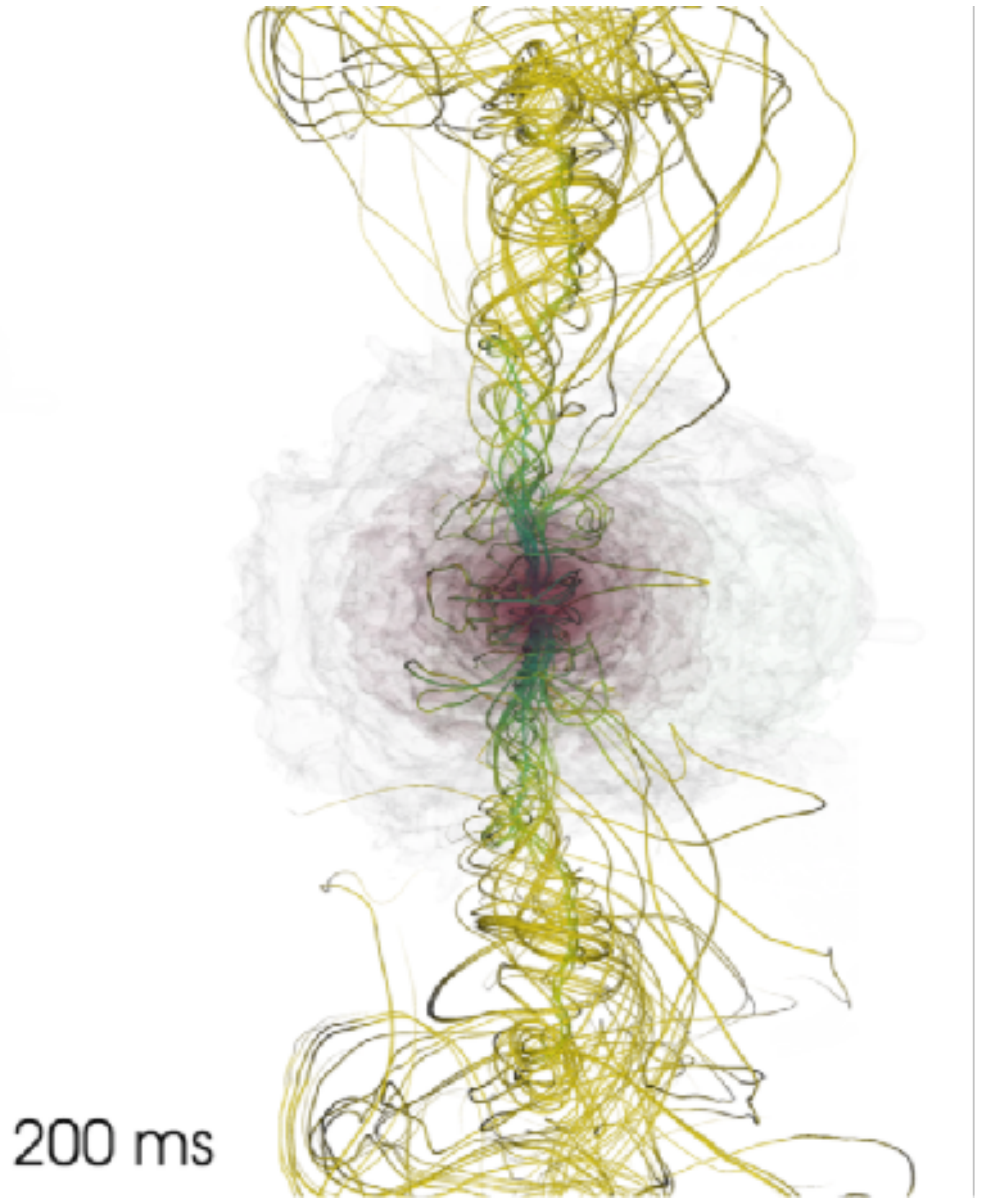




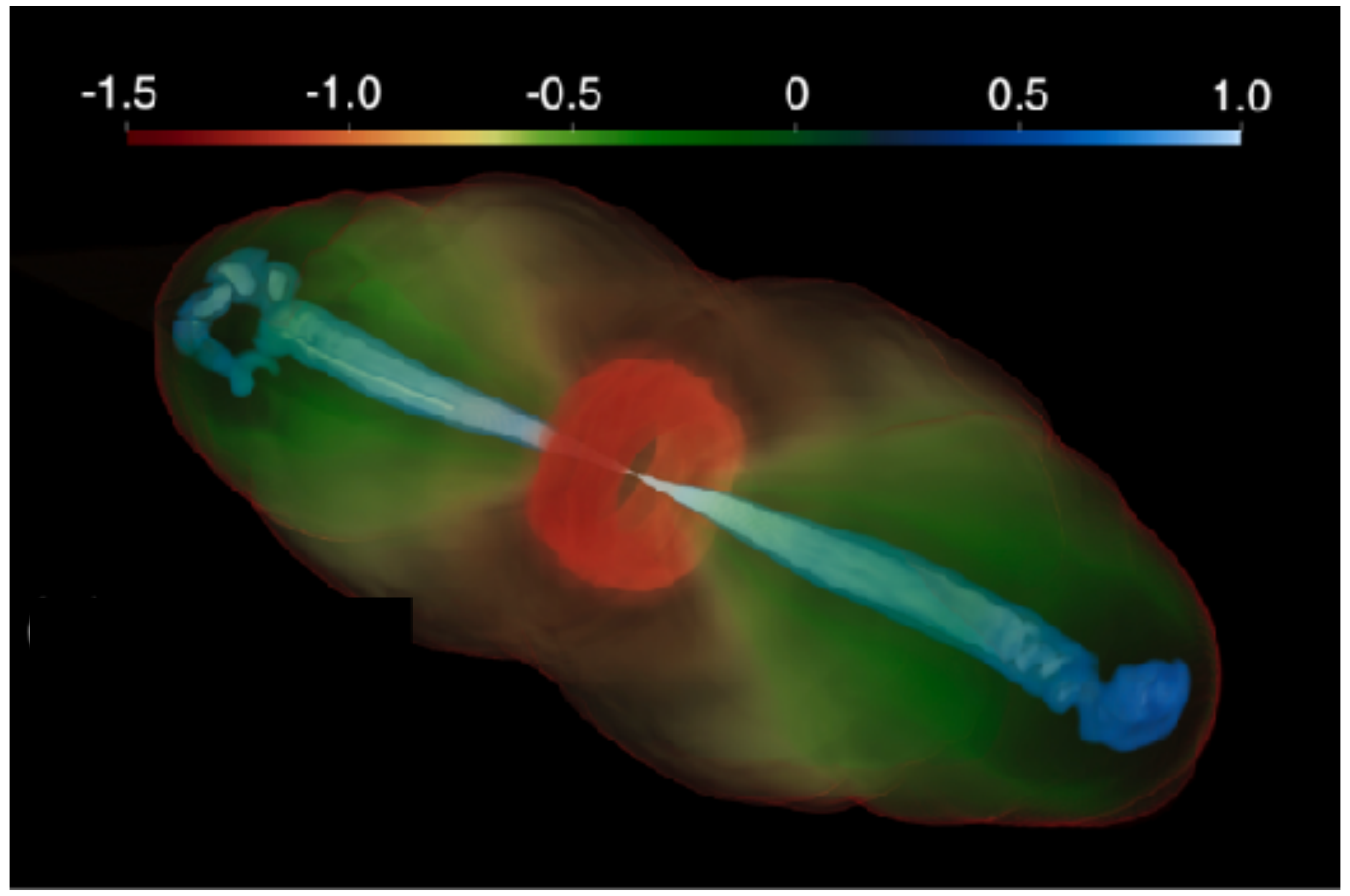
[Lopez-Armengol+2021]



[Moesta+2020]



[Ciolfi 2020]



Numerical Background

Einstein field equations: $G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = 8\pi T_{\mu\nu}$

Maxwell equations: $\nabla^*_\nu F^{\mu\nu} = 0; \quad \nabla_\nu F^{\mu\nu} = 4\pi \mathcal{J}^\mu$

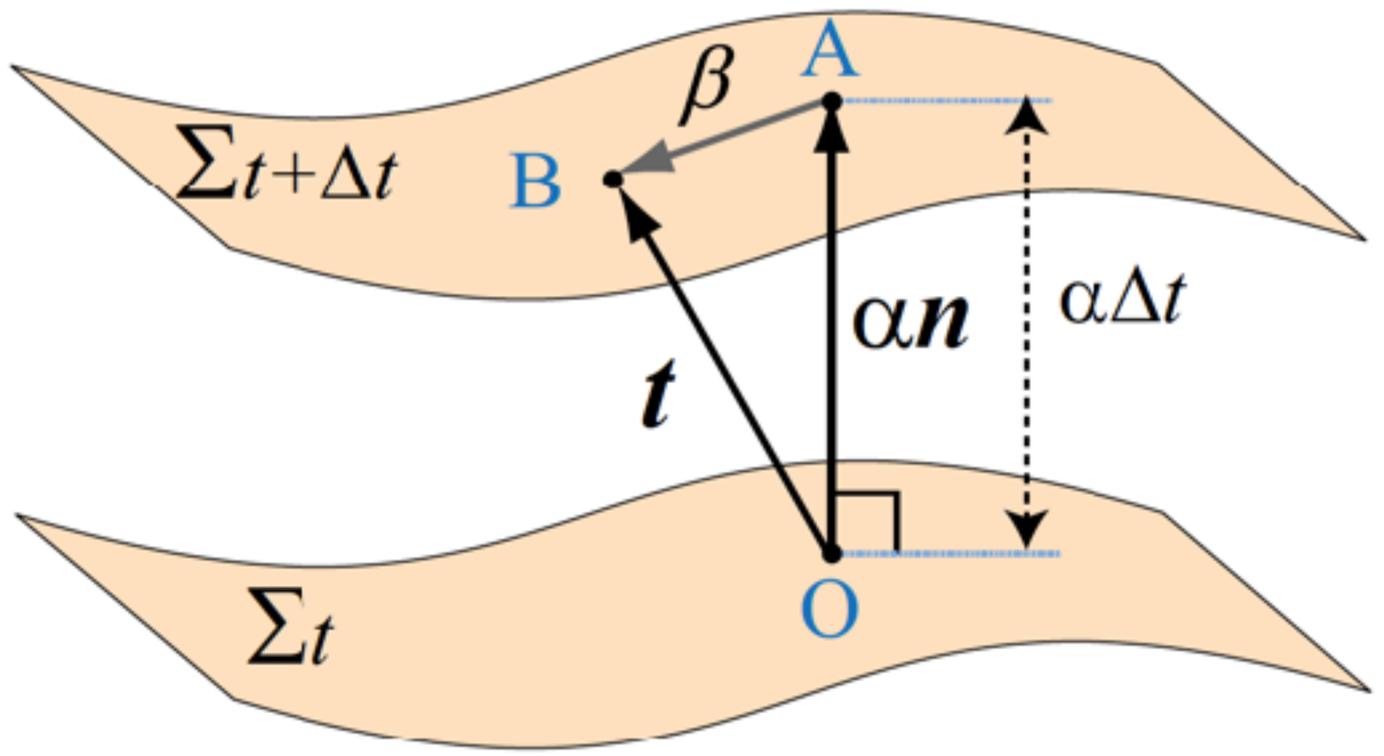
4-current density: $\mathcal{J}^\mu = q u^\mu + \sigma F^{\mu\nu} u_\nu$

Energy conservation: $\nabla_\mu T^{\mu\nu} = 0$

Mass conservation: $\nabla_\mu (\rho u^\mu) = 0$

Equation of state: $P = P(\rho, \epsilon)$

- Numerical Relativity: solve non-linear Einstein equations coupled with MHD equations in GR
- 3+1 foliation: treating the system as *initial value problem* - solution in future based on initial data



[Shibata 2015]

Line element: $ds^2 = g_{\mu\nu} dx^\mu dx^\nu = -\left(\alpha^2 - \beta^i \beta_i\right) dt^2 + 2\beta_i dx^i dt + \gamma_{ij} dx^i dx^j$

Time-like unit normal: $n^\mu = \frac{1}{\alpha}\left(1, -\beta^i\right); \quad n_\mu = (-\alpha, 0, 0, 0)$

Eulerian 3-velocity: $v^i = \frac{1}{\alpha}\left(\frac{u^i}{u^0} + \beta^i\right)$

Numerical Background

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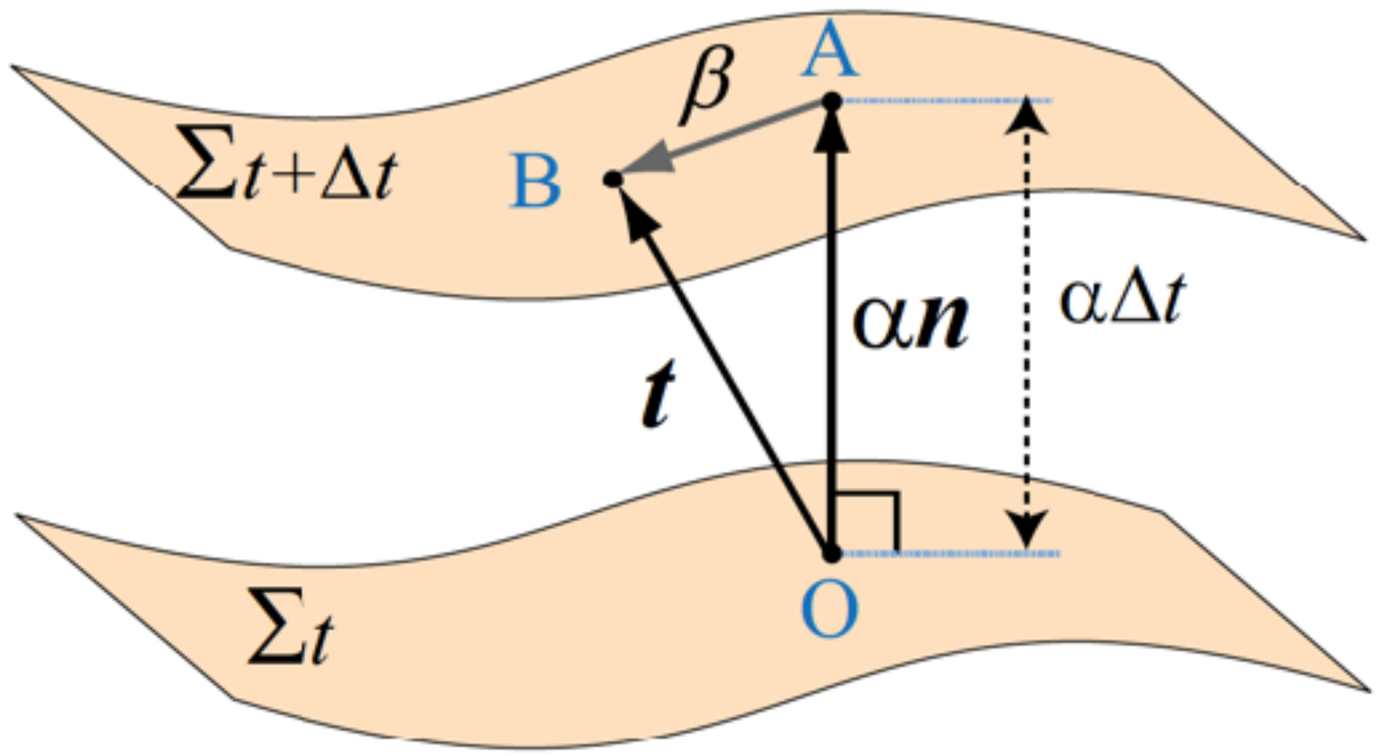


[Shibata 2015]

- Spacetime evolution: based on BSSN/Z4c formulation (via McLachlan, Baikal, Z4c)
- GRMHD evolution: based on Valencia formulation (via WhiskyMHD, IllinoisGRMHD, GRHydro, Spritz, GRHayl)

Sam Cupp's talk on Tuesday!

GRMHD Equations

First order flux-conservative hyperbolic Valencia formalism

$$\frac{1}{\alpha\sqrt{\gamma}}\left[\partial_t\left(\sqrt{\gamma}\mathbf{U}\right)+\partial_i\left(\sqrt{\gamma}\mathbf{F}^{\mathbf{i}}\right)\right]=\mathbf{S}$$

State vector

$$\mathbf{U}\equiv\begin{pmatrix} D \\ S_j \\ \tau \\ B^k \\ DY_e \end{pmatrix}$$

Fluxes

$$\mathbf{F}\equiv\begin{pmatrix} D\tilde{v}^i \\ S_j\tilde{v}^i+\alpha\left(P+P_{\text{mag}}\right)\delta^i_j-\alpha b_j B^i/W \\ \tau\tilde{v}^i+\alpha\left(P+P_{\text{mag}}\right)v^i-\alpha^2 b^0 B^i/W \\ B^k\tilde{v}^i-B^i\tilde{v}^k \\ DY_e\tilde{v}^i \end{pmatrix}$$

Source terms

$$\mathbf{S}\equiv\begin{pmatrix} 0 \\ T^{\mu\nu}\left(\partial_\mu g_{\nu j}-\Gamma^\delta_{\nu\mu}g_{\delta j}\right) \\ \alpha\left(T^{\mu 0}\partial_\mu \ln\alpha-T^{\mu\nu}\Gamma^0_{\nu\mu}\right) \\ 0 \\ 0 \end{pmatrix}$$

$$T^{\mu\nu}=\left(\rho h+b^2\right)u^\mu u^\nu+\left(p_{\text{gas}}+p_{\text{mag}}\right)g^{\mu\nu}-b^\mu b^\nu$$

fluid can interchange energy and momentum with the spacetime

Prim2Con

primitives

ρ	rest-mass density
v^i	fluid 3-velocity
ϵ	specific internal energy
Y_e	electron fraction

P	gas pressure
$P_{\mathrm{mag}} \equiv b^2/2$	magnetic pressure
$W = 1/\sqrt{1-v^2}$	Lorentz factor
$h = 1 + \epsilon + P/\rho$	specific enthalpy
$\vec{A}$	vector potential

conservatives

conserved density	$D \equiv \rho W$
conserved momentum	$S_j \equiv \left(\rho h + b^2\right) W^2 v_j - \alpha b^0 b_j$
conserved internal energy	$\tau \equiv \left(\rho h + b^2\right) W^2 - \left(P + P_{\mathrm{mag}}\right) - \alpha^2 \left(b^0\right)^2 - D$
conserved magnetic field	$\vec{B} \equiv \vec{\nabla} \times \vec{A}$
conserved electron fraction	DY_e

Evolution Equations for B

Ideal MHD

$$\sigma \to \infty; \quad F^{\mu\nu} u_\nu \to 0$$

co-moving observer measures no electric field

Maxwell equations

$$\nabla^*_\nu F^{\mu\nu} = \frac{1}{\sqrt{-g}} \partial_\nu \left(\sqrt{-g} \left(b^\mu u^\nu - b^\nu u^\mu \right) \right) = 0$$

written solely in terms of b

Divergence-free condition: $\partial_i \tilde{B}^i = 0$

Induction equations: $\partial_t \tilde{B}^i = \partial_j \left(\tilde{v}^i \tilde{B}^j - \tilde{v}^j \tilde{B}^i \right)$

where $\tilde{B}^i \equiv \sqrt{\gamma} B^i; \quad \tilde{v}^i \equiv \alpha v^i - \beta^i$

Co-moving magnetic field components

$$b^0 = \frac{W B^i v_i}{\alpha}, \qquad b^i = \frac{B^i + \alpha b^0 u^i}{W}, \qquad b^2 \equiv b^\mu b_\mu = \frac{B^2 + \alpha^2 \left(b^0\right)^2}{W^2}$$

Evolution Equations for A

4-vector potential: $\mathscr{A}_\nu = n_\nu \Phi + A_\nu$

Induction equations: $\partial_t A_i = -E_i - \partial_i \left(\alpha\Phi - \beta^j A_j \right)$

Computing B: $B^i = \epsilon^{ijk} \partial_j A_k$

Algebraic gauge: $\Phi = \frac{1}{\alpha} \left(\beta^j A_j \right) = -n^j A_j$

$$\partial_t A_i = \epsilon_{ijk} v^j B^k$$

Generalised Lorenz gauge: $\nabla_\nu \mathscr{A}^\nu = \xi n_\nu \mathscr{A}^\nu$

$$\partial_t \left(\sqrt{\gamma}\Phi \right) + \partial_i \left(\alpha\sqrt{\gamma}A^i - \sqrt{\gamma}\beta^i\Phi \right) = -\xi\alpha\sqrt{\gamma}\Phi$$

Equation of State

- Analytical

  - ideal gas $P(\rho, \epsilon) = (\Gamma - 1)\rho\epsilon; \;\; \epsilon_{\text{min}} = 0$

  - polytrope $P(\rho) = k\rho^{\Gamma}; \quad \Gamma = 1 + 1/n$

- Tabulated

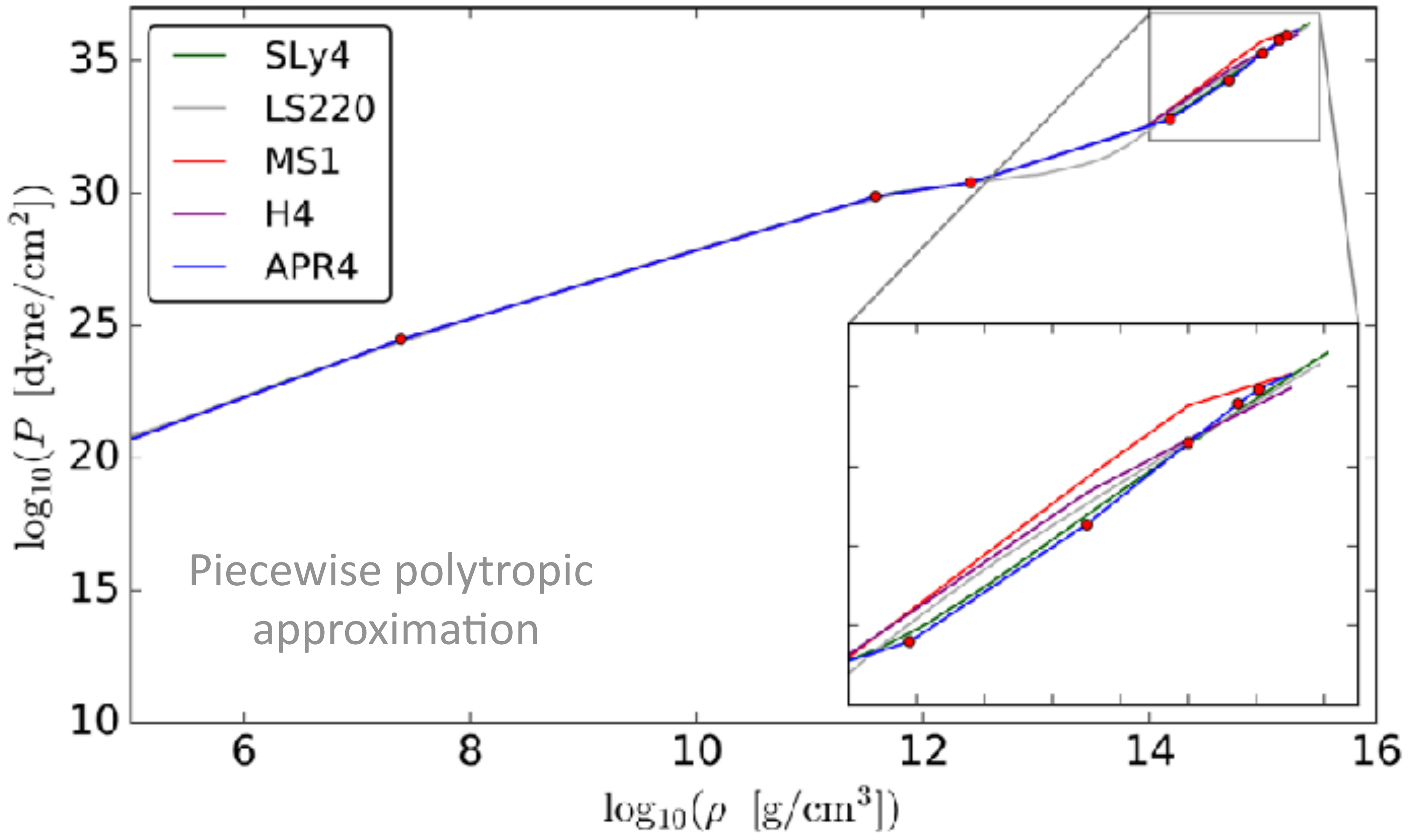
  - 1 parameter $P = P(\rho)$

  - 3 parameter $P = P(\rho, T, Y_e)$

- Hybrid

$$P(\rho, \epsilon) = P_{\text{cold}}(\rho) + (\Gamma_{\text{th}} - 1)\rho \left(\epsilon - \epsilon_{\text{cold}}(\rho)\right)$$

$$\epsilon_{\text{min}}(\rho) = \epsilon_{\text{cold}}(\rho)$$

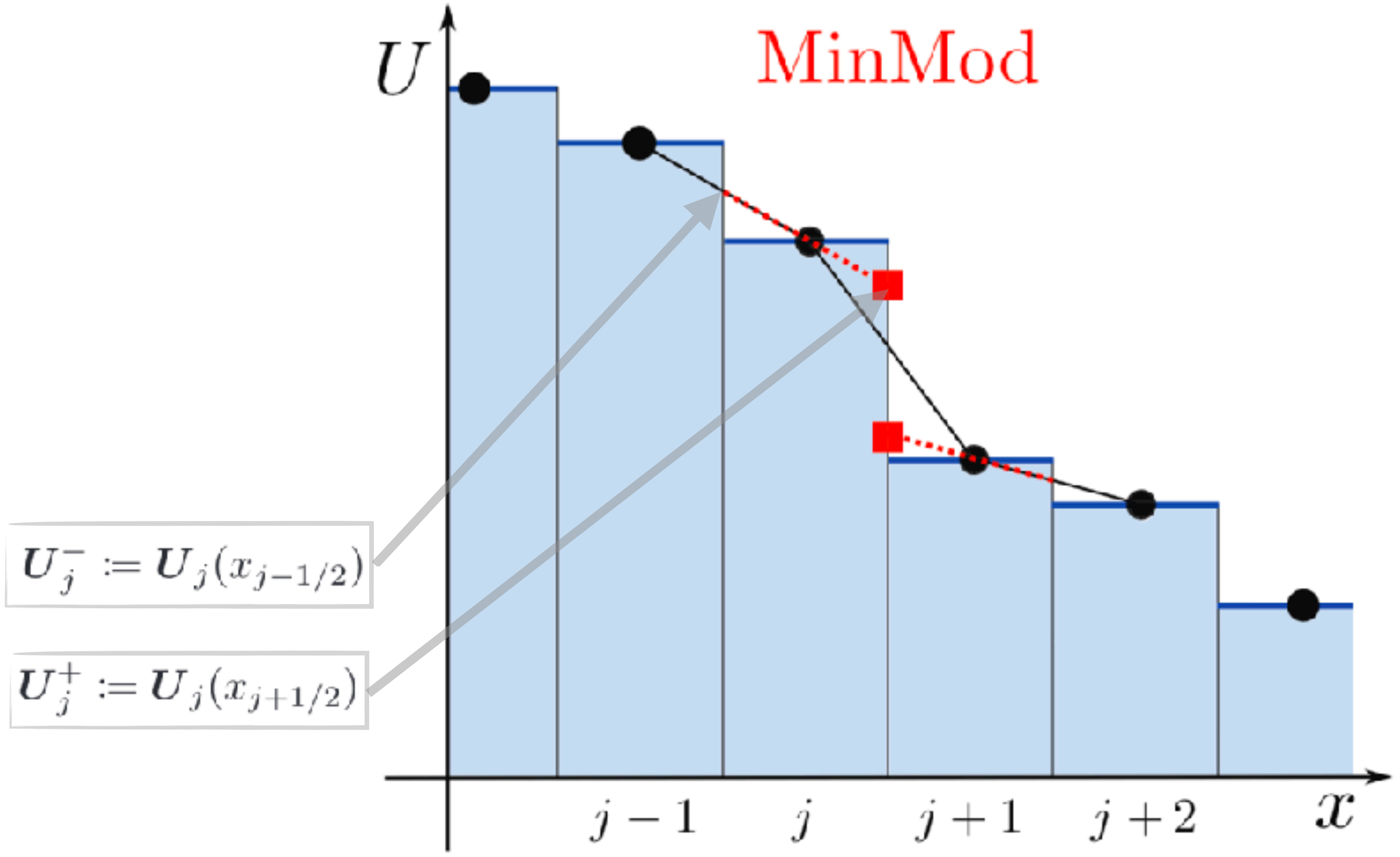


[Endrizzi et al 2016]

HRSC Methods

- **Reconstruction methods:**
  reconstruct the variables to the left and right of the grid-interfaces
  ➡ Minmod
  ➡ Piecewise parabolic method (PPM)

- **Approximate Riemann solvers:**
  compute the fluxes at cell-interfaces
  ➡ Lax-Friedrichs
  ➡ HLLE solver



[Rezzolla+2013]

Con2Prim

- Recover primitive variables from evolved conservative ones: C2P
  - no analytical solution in GRMHD
  - needs numerical approach: root finding algorithms
- Currently known C2P schemes (e.g., Noble+2006, Duran+2008, Neilsen+2014, Newman+2014, **Siegel+2018**) could all fail in certain regimes, e.g. for high magnetizations and Lorentz factors

Types of methods:

- Newton-Raphson schemes
  - unbounded; usually need initial guess; depend on EOS derivatives
- Root-bracketing schemes
  - bounded; might not depend on initial guess and on EOS derivatives

Code Workflow

$$\frac{1}{\alpha\sqrt{\gamma}}\left[\partial_t\left(\sqrt{\gamma}\mathbf{U}\right)+\partial_i\left(\sqrt{\gamma}\mathbf{F^i}\right)\right]=\mathbf{S}$$

Initialisation: primitive variables defined at each grid point

Prim2Con: conserved variables computed from primitives

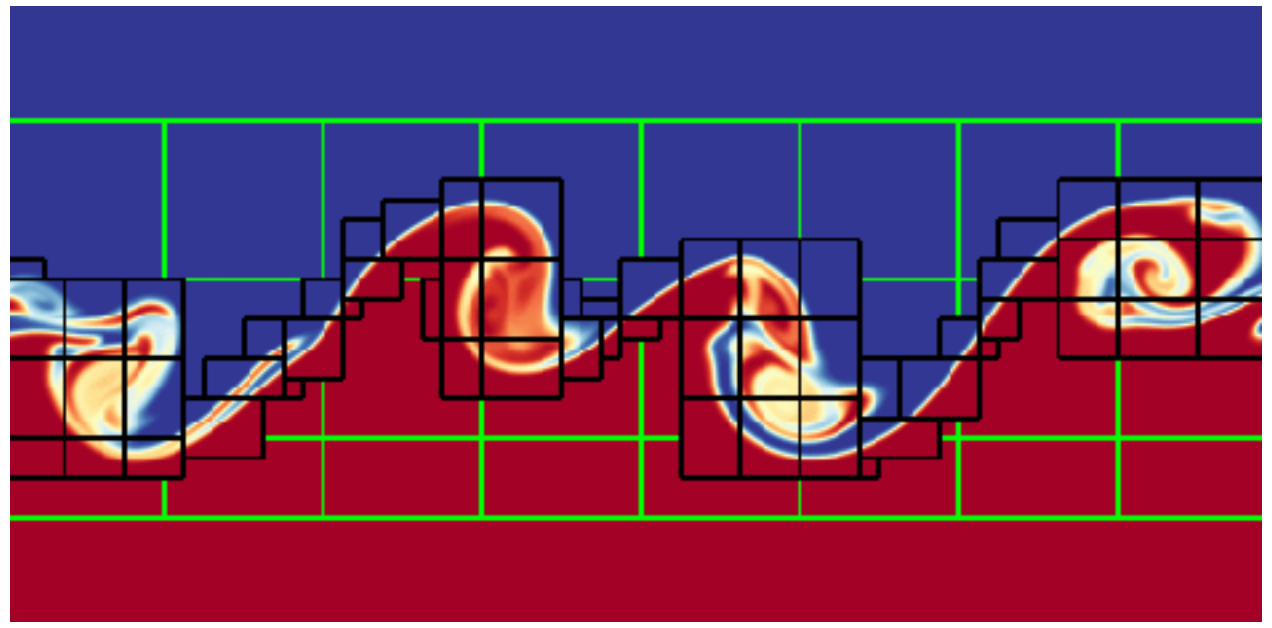
Source terms: evaluated using FD schemes

Flux terms: computed using HRSC methods (reconstruction + approx Riemann solvers)

Time update: ODEs for conserved variables solved using time integrator (such as RK4)

Con2Prim: computes primitives from evaluated conserved variables for next time step

AMReX

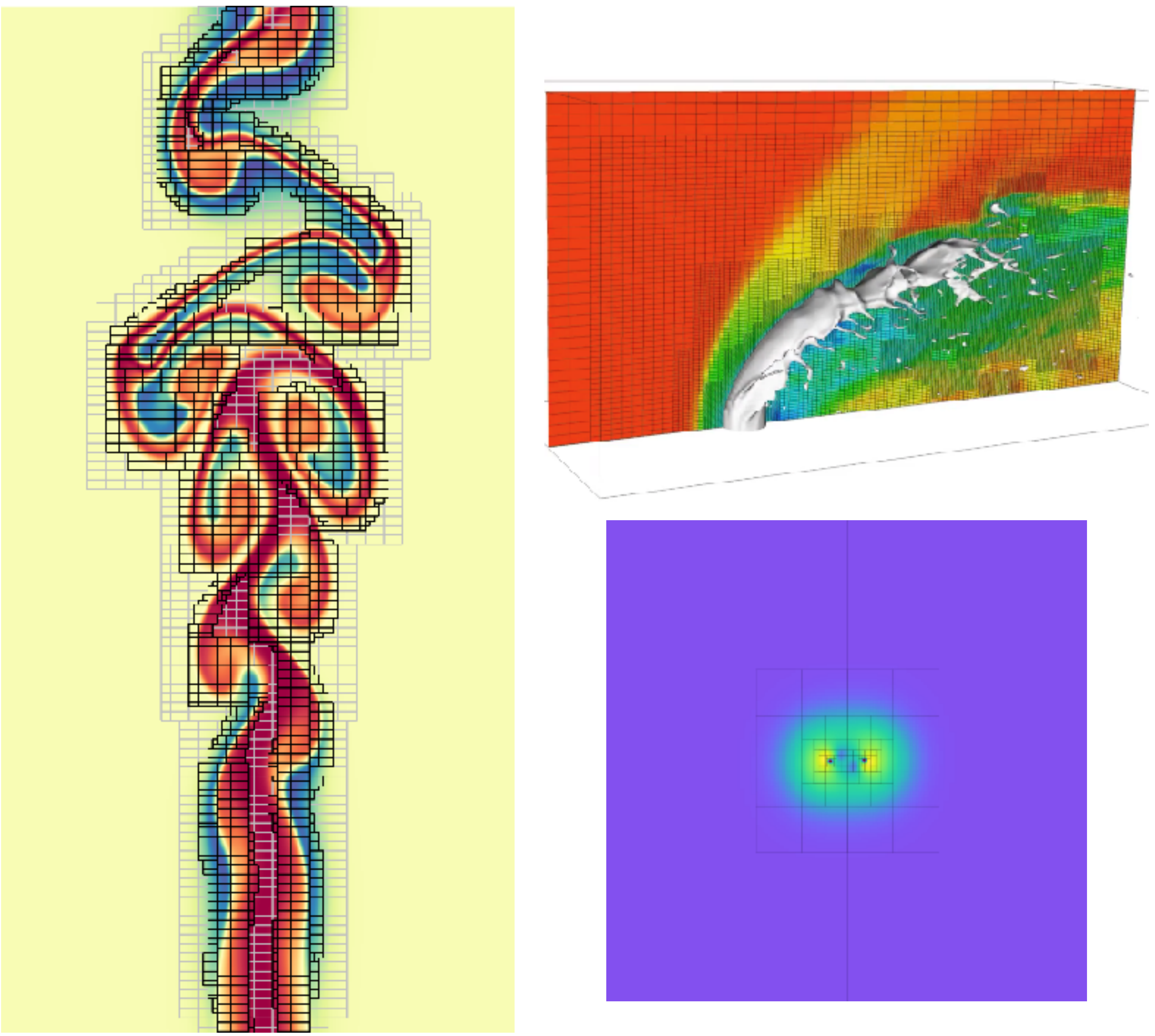


AMReX

- Software framework for massively parallel, block-structured adaptive mesh refinement (AMR) applications

- Developed at **LBNL**, **NREL** and **ANL** as a part of DOE's Exascale Computing Project

- **Key features:**
    - C++ and Fortran interfaces
    - 1-, 2- and 3-D support
    - Support for cell-, face-, vertex-, edge-centered data
    - Support for hyperbolic, parabolic, and elliptic solvers
    - Optional subcycling in time for time-dependent PDEs
    - Support for particles
    - **Performance portability**: parallelization via flat MPI, OpenMP, hybrid MPI/OpenMP, hybrid MPI/(**CUDA** or **HIP** or DPC++)
    - Parallel I/O



Taken from https://amrex-codes.github.io/amrex/

AMReX

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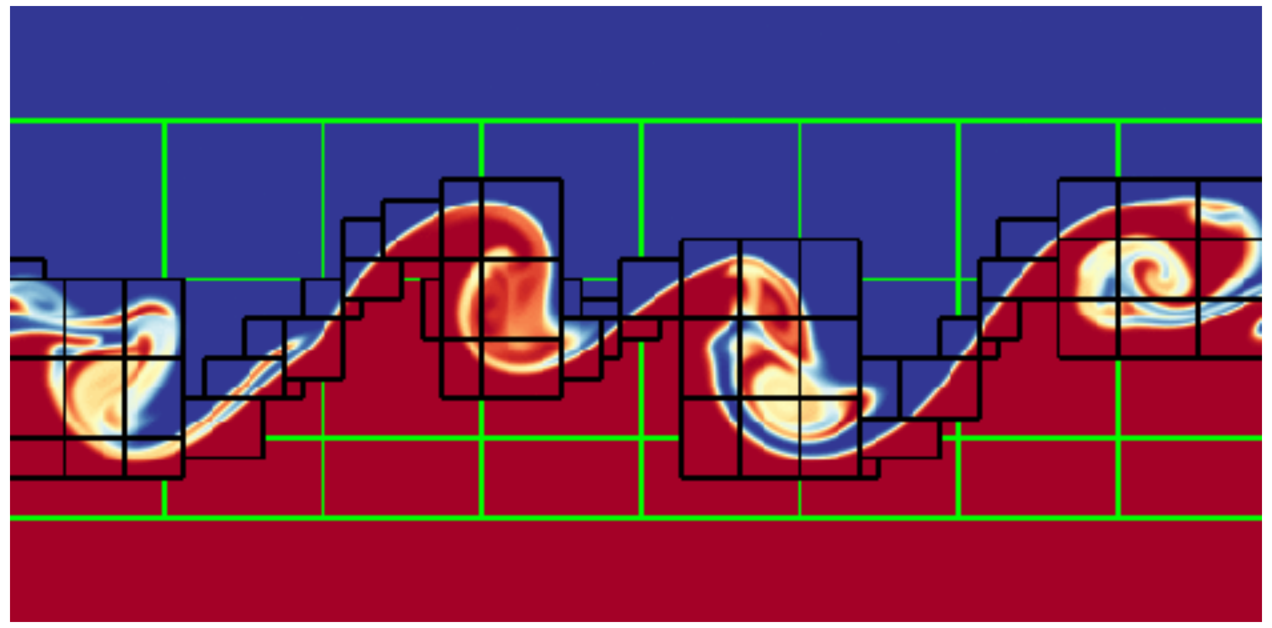
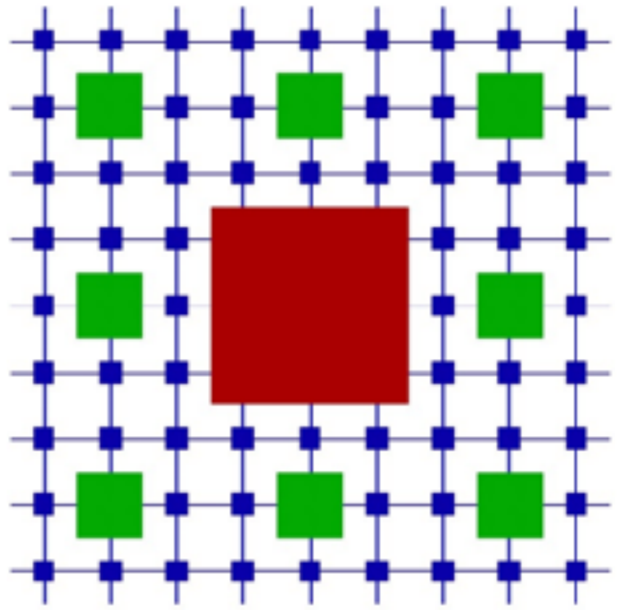
CarpetX

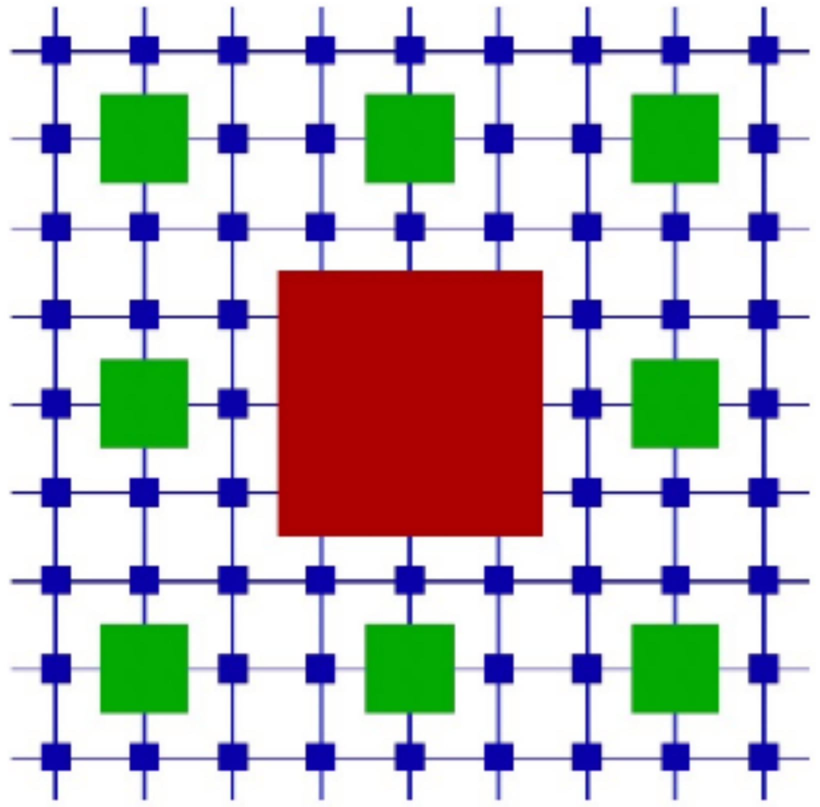


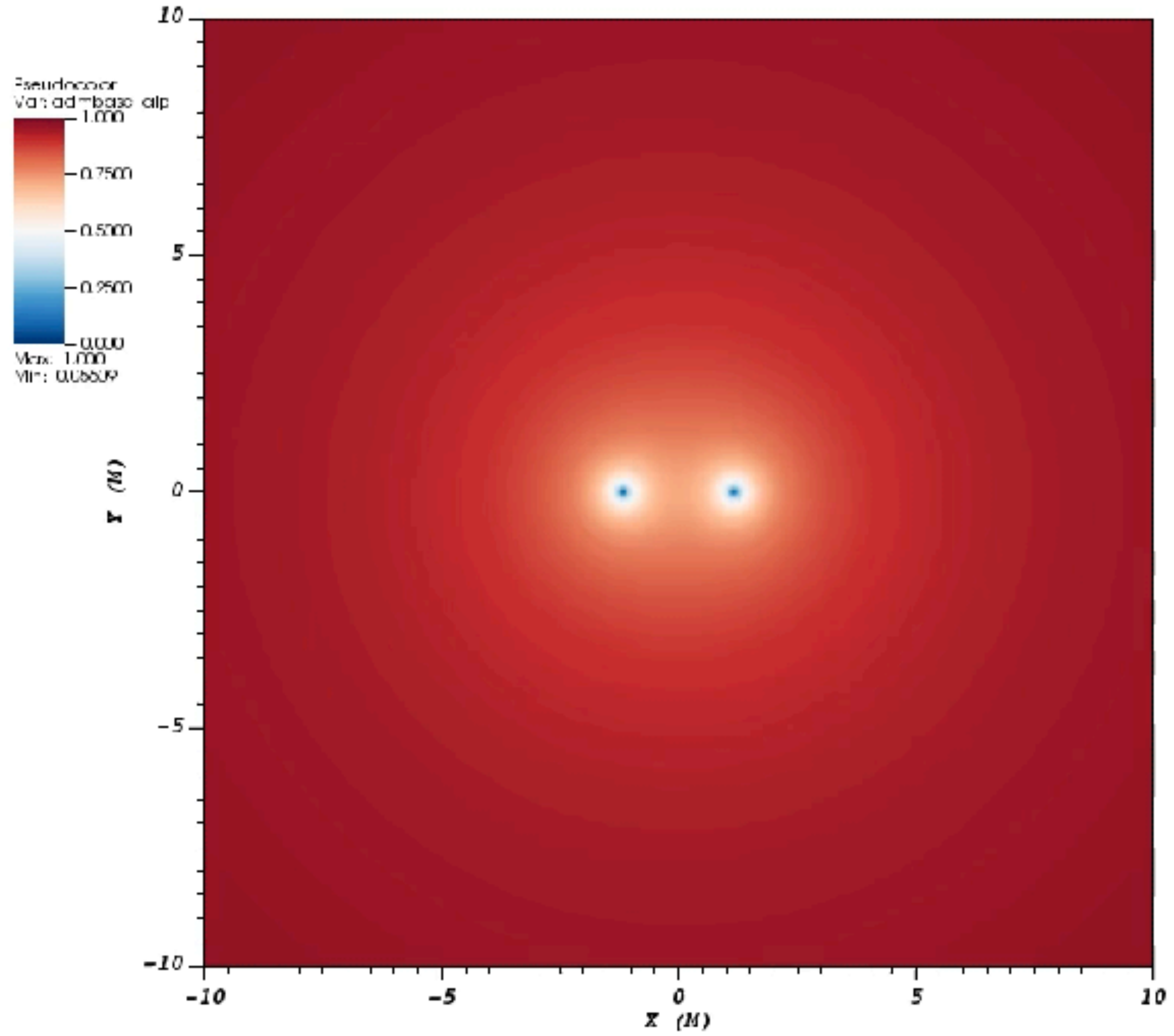


Erik Schnetter’s talk on Tuesday!

CarpetX: a new driver for the Einstein Toolkit

- **Support for accelerators (e.g. GPUs)**
- AMR based on local criteria
- Scalable → Exascale
- Hydro refluxing
- Elliptic solvers
- I/O in HDF5 (Silo, openPMD) or ASCII
- GitHub: https://github.com/EinsteinToolkit/CarpetX
- Applications:
  - **WaveToyX:** solves a scalar wave equation
  - **Z4c:** Einstein field equations in vacuum
  - **GRaM-X:** a new GRMHD code [Shankar et al. 2022]





BBH merger simulations by
Allen Wen (RIT)

AMReX

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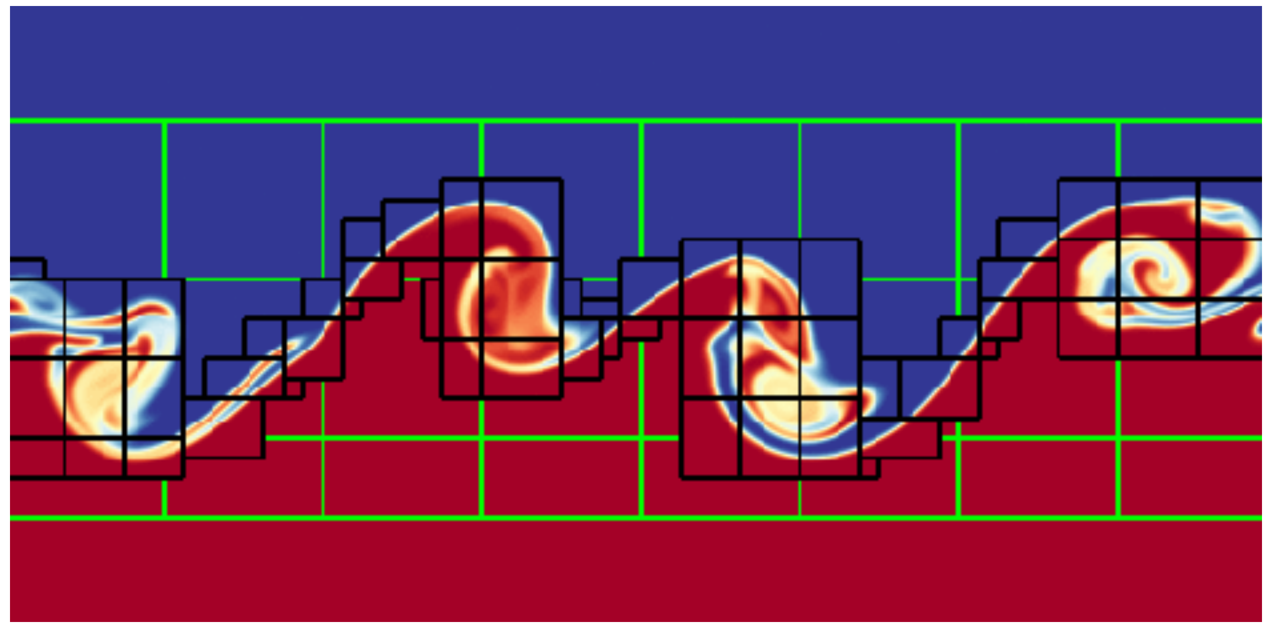
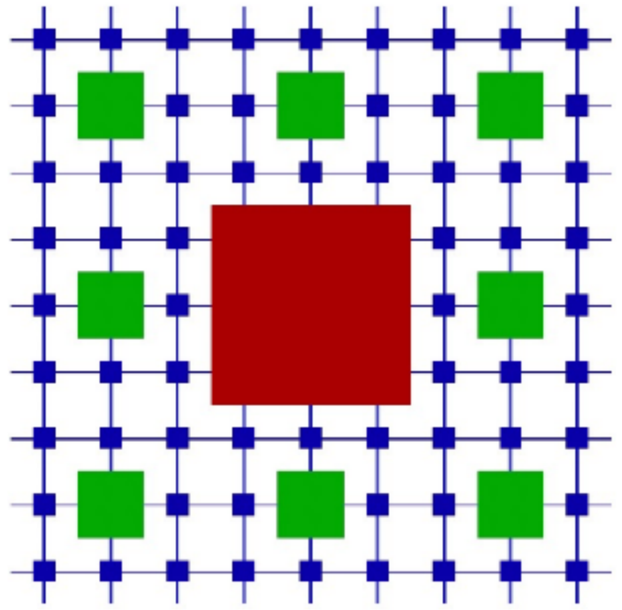
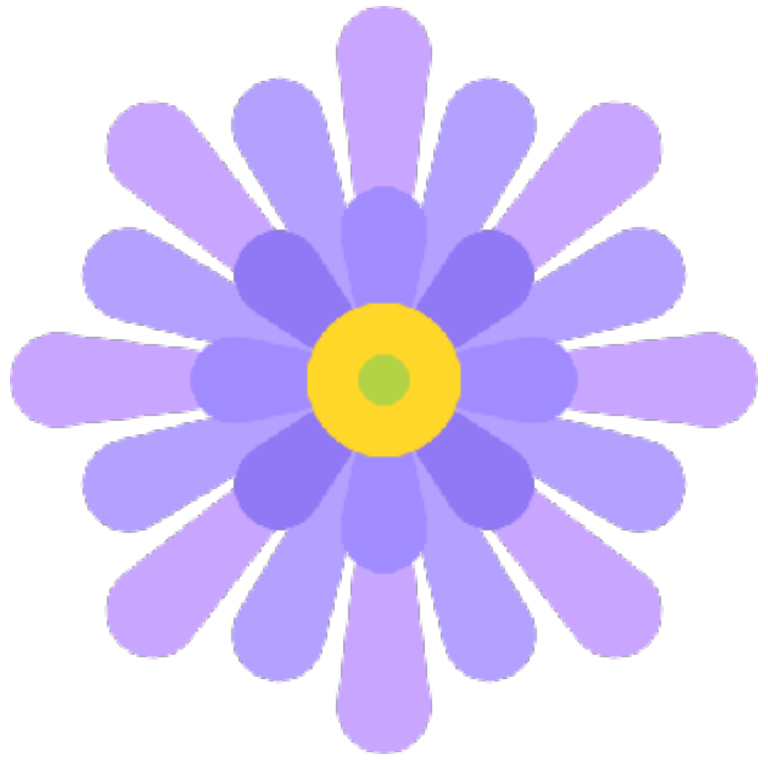
CarpetX

↓

AsterX



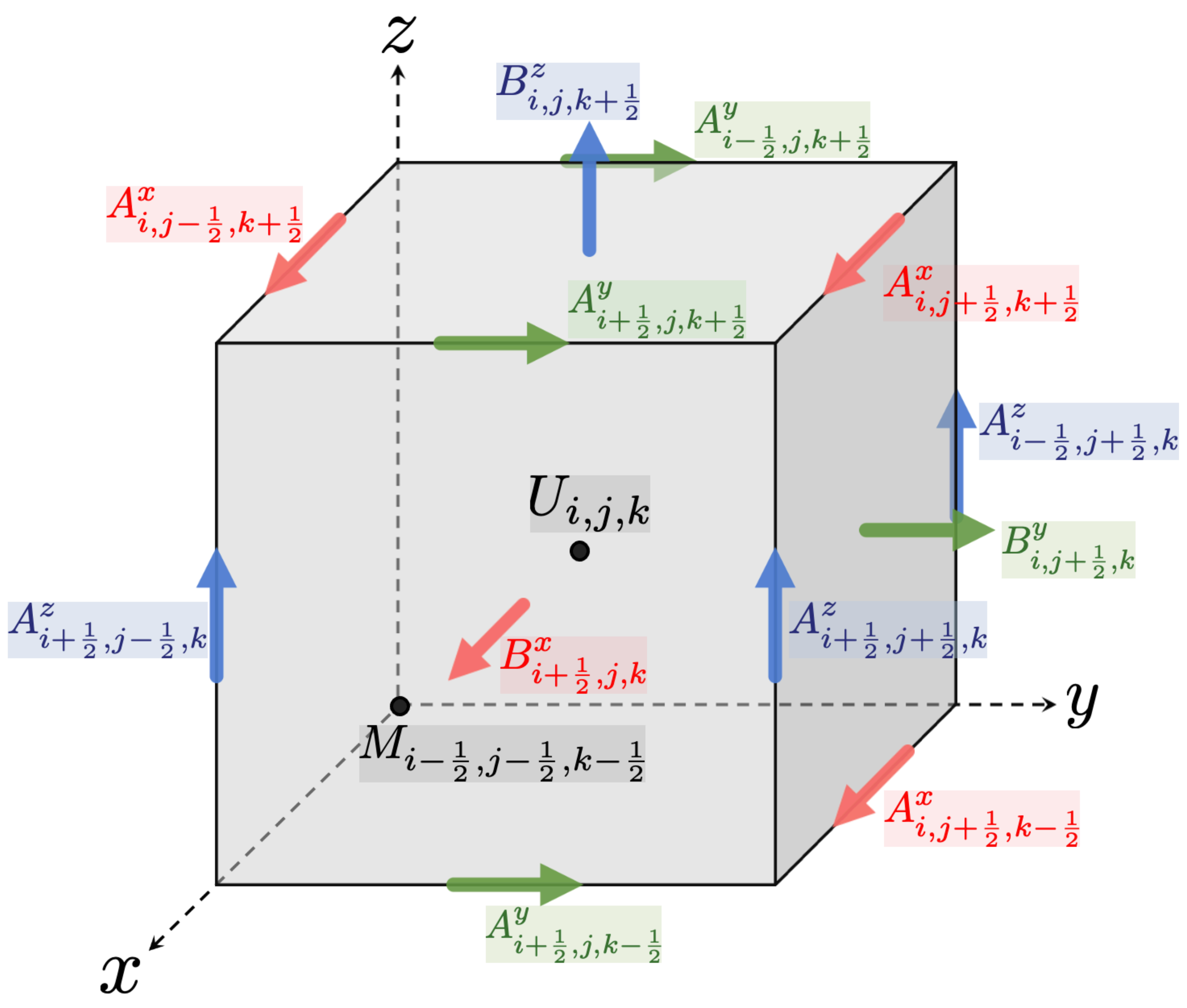




AsterX: General Relativistic MHD code

Heavily derived from the Spritz code

- ReconX:
  - MinMod (TVD)
  - Piecewise Parabolic Method (PPM)
  - WENO-Z (weighted essentially non-oscillatory)
  - MP5 (5th order monotonicity-preserving)
- Flux solvers:
  - Lax-Friedrichs
  - HLLE
- Con2PrimFactory:
  - 2D Noble et al.
  - 1D Palenzuela et al.
  - 1D RePrimAnd (only CPU-compatible)
  - 3D Anton et al.
  - 1D Newman & Hamlin



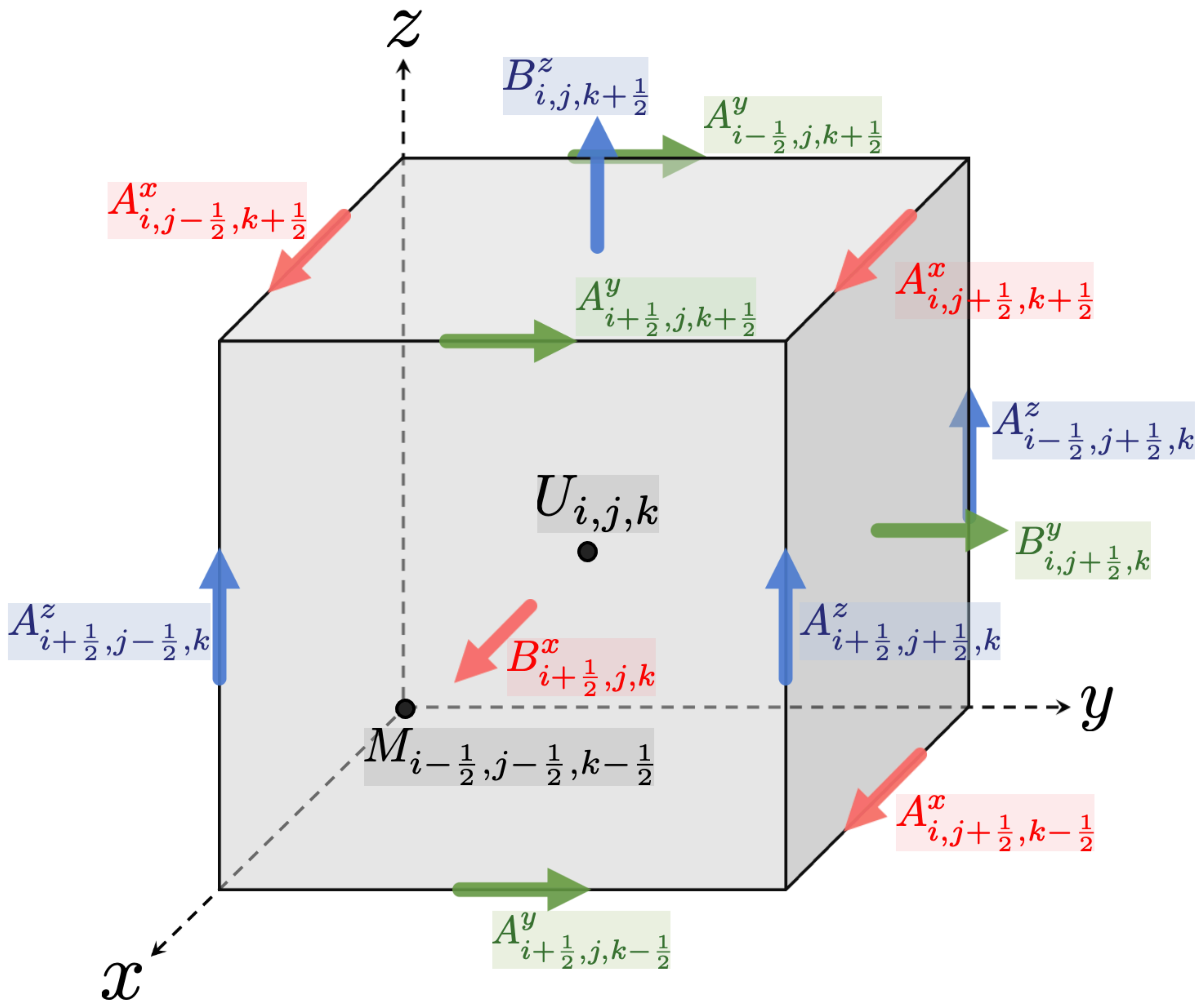
Locations of different grid-functions in a grid-cell

AsterX: General Relativistic MHD code

Heavily derived from the Spritz code

- EOSX:
  - Analytical: Ideal gas, Polytropic
  - Hybrid
  - Finite temperature tabulated
- Vector potential evolution:
  - Flux CT
  - Upwind CT (HLLE)
- GitHub:

https://github.com/jaykalinani/AsterX

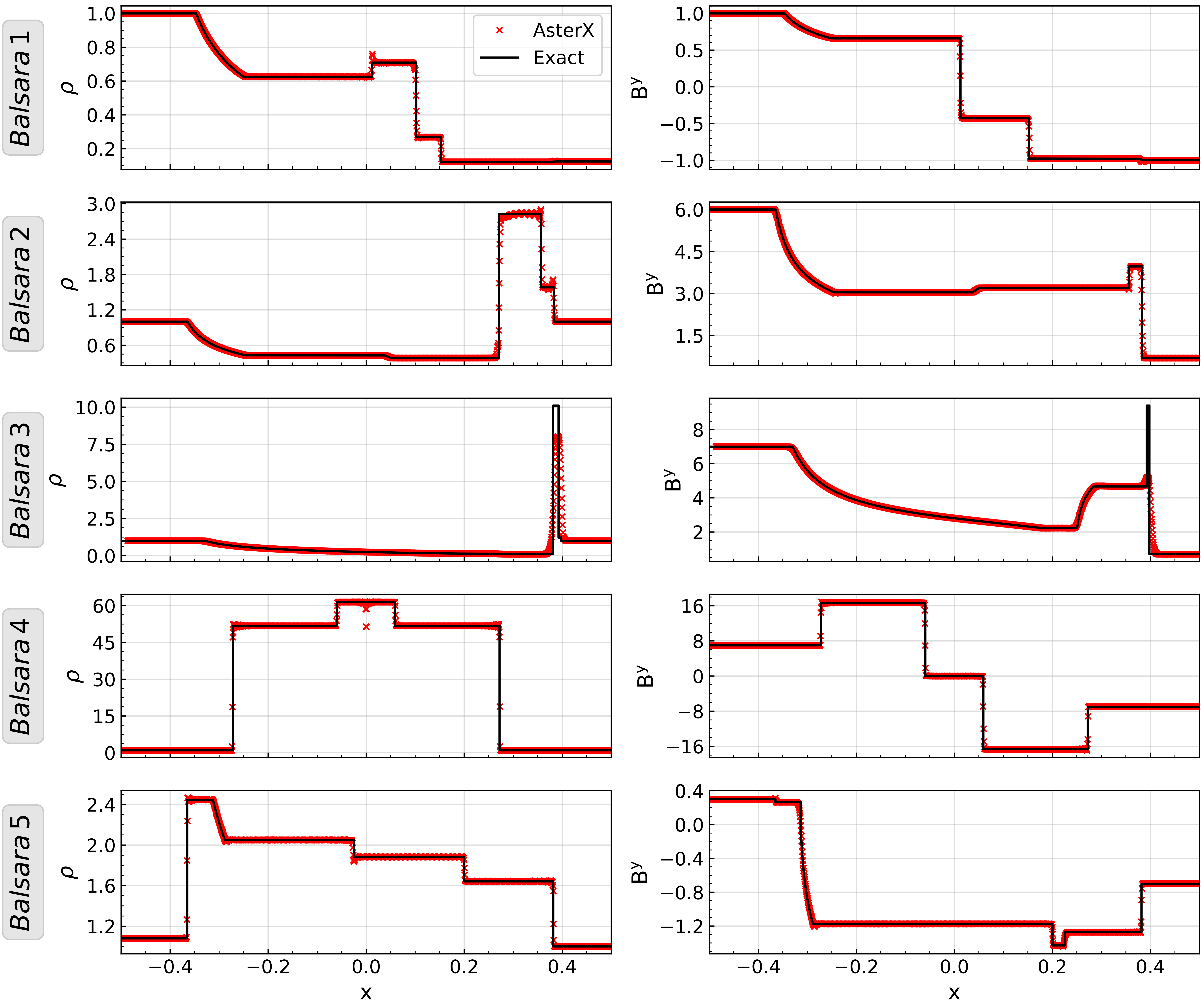


Locations of different grid-functions in a grid-cell

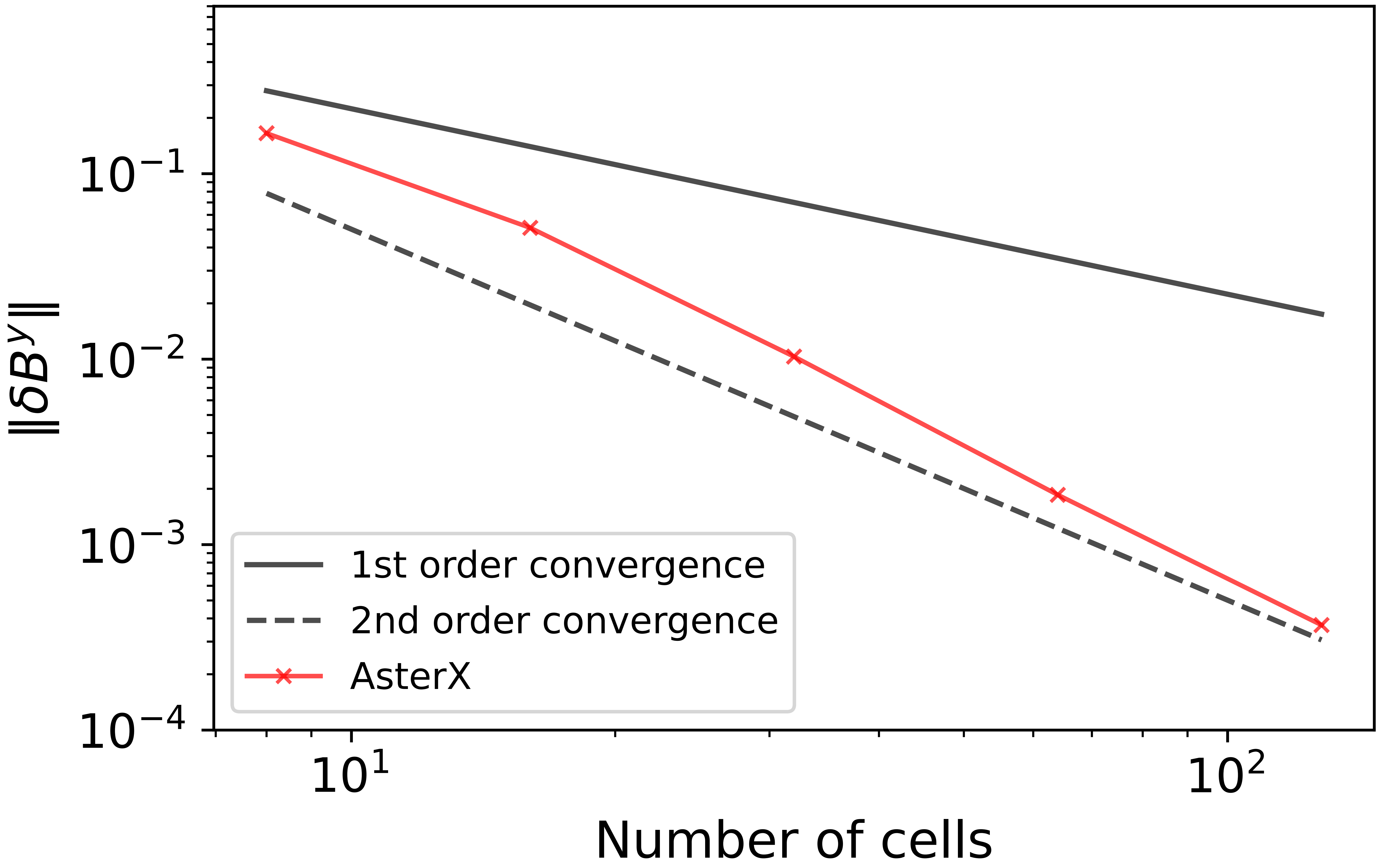
Balsara Shocktube

Rest-mass density

Magnetic field: By

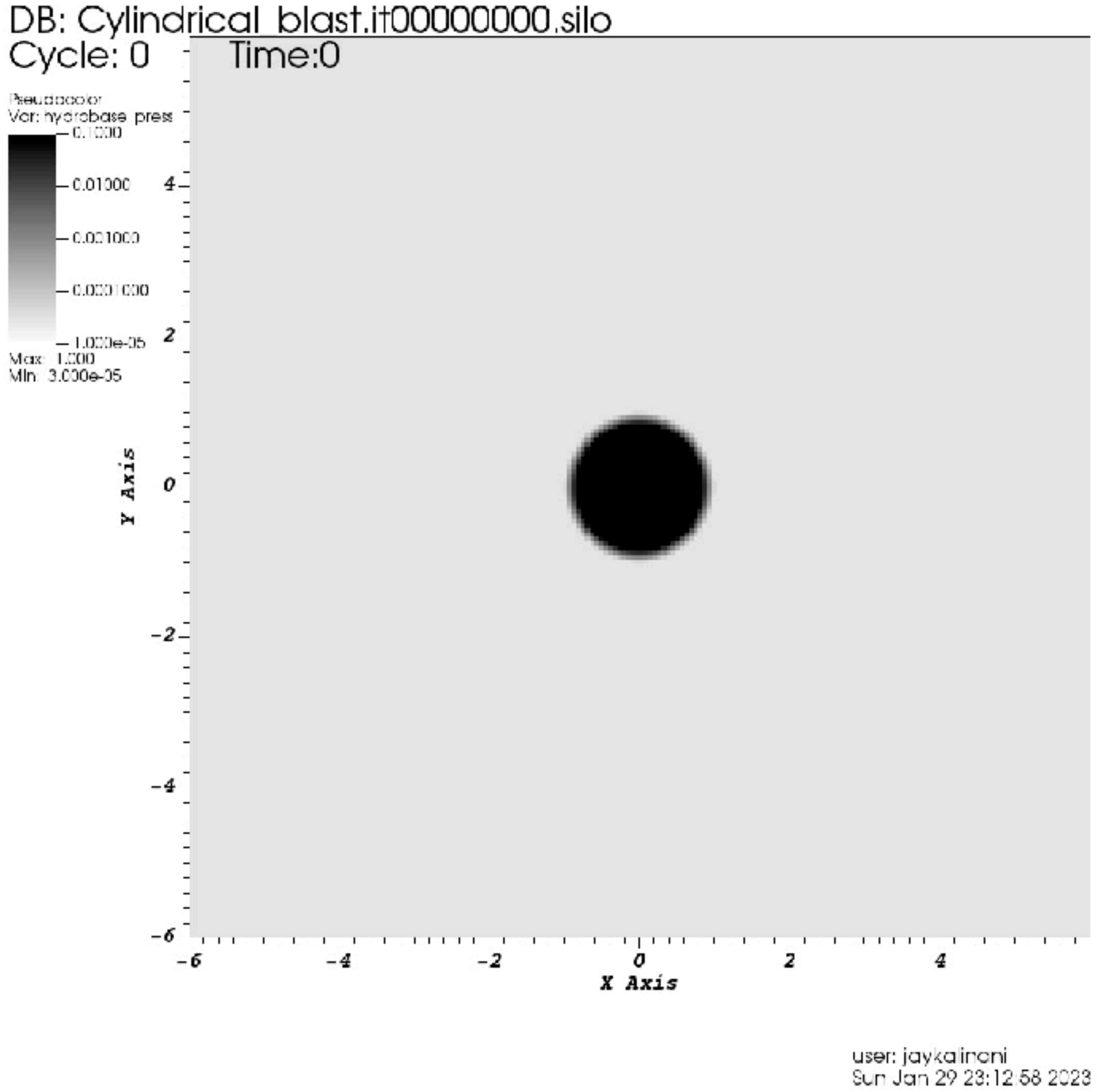


Convergence study: Alfvén wave

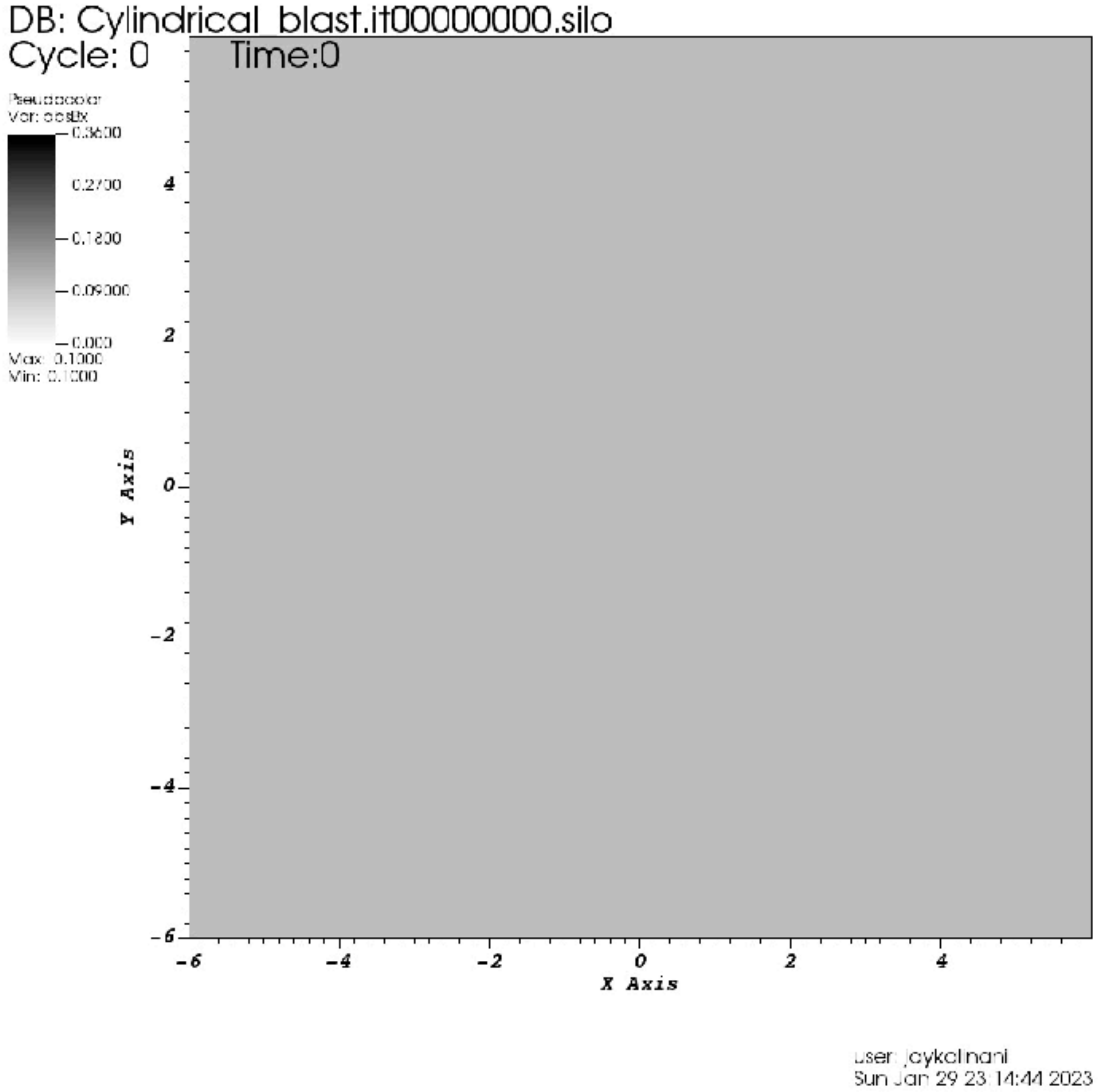


Cylindrical Explosion

Rest-mass density

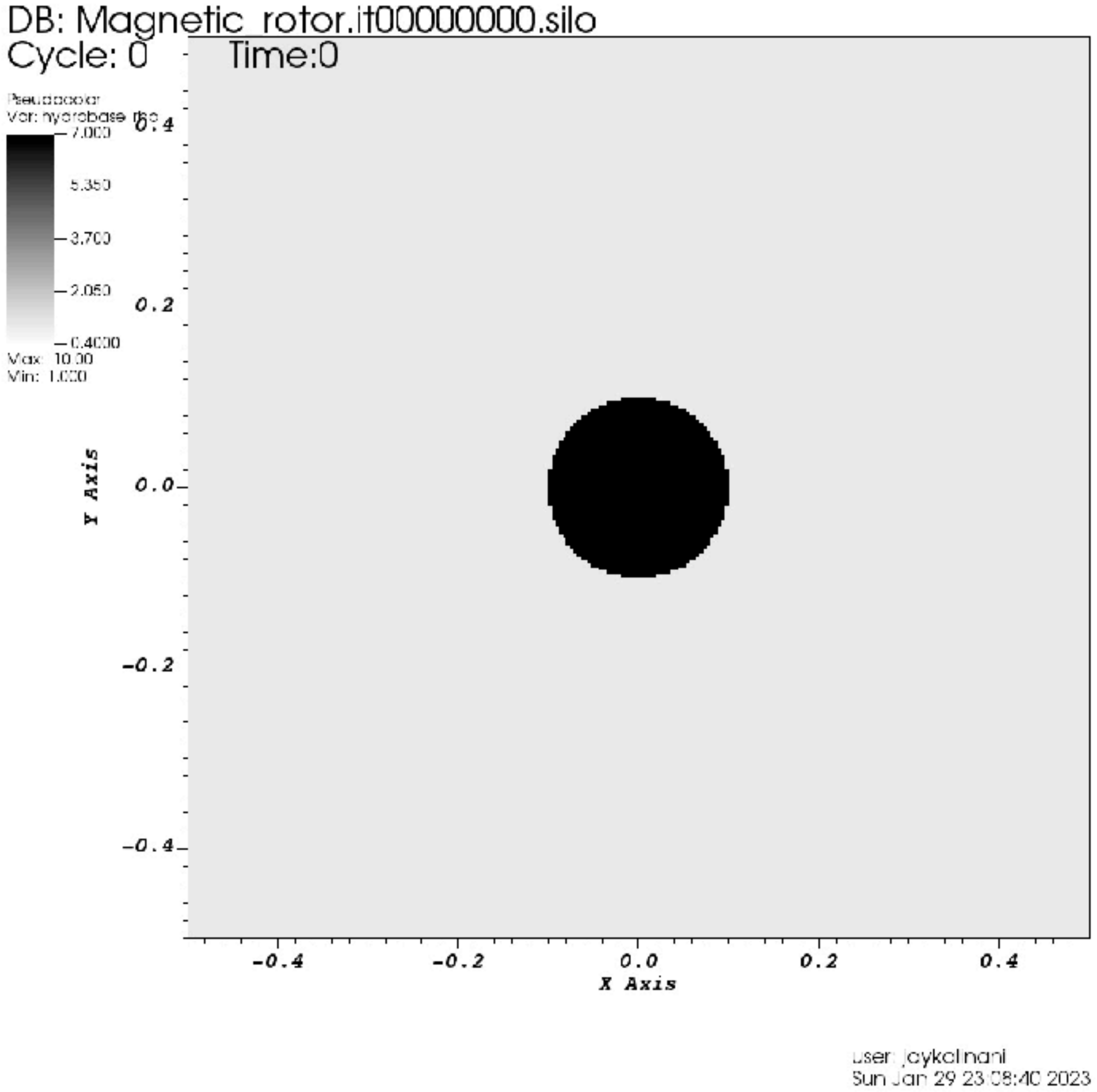


Magnetic field: abs(Bx)



Magnetic Rotor

Rest-mass density



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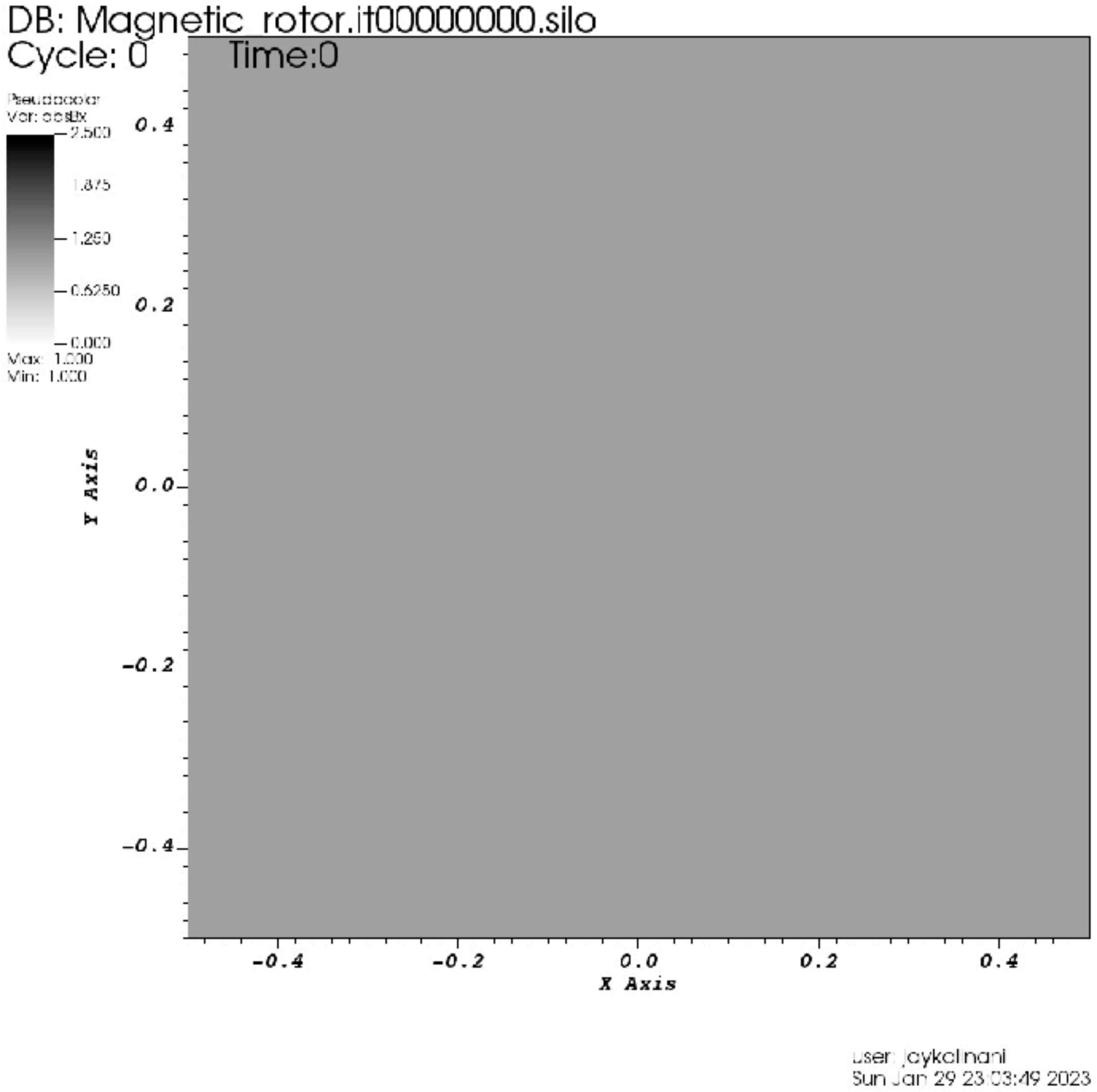
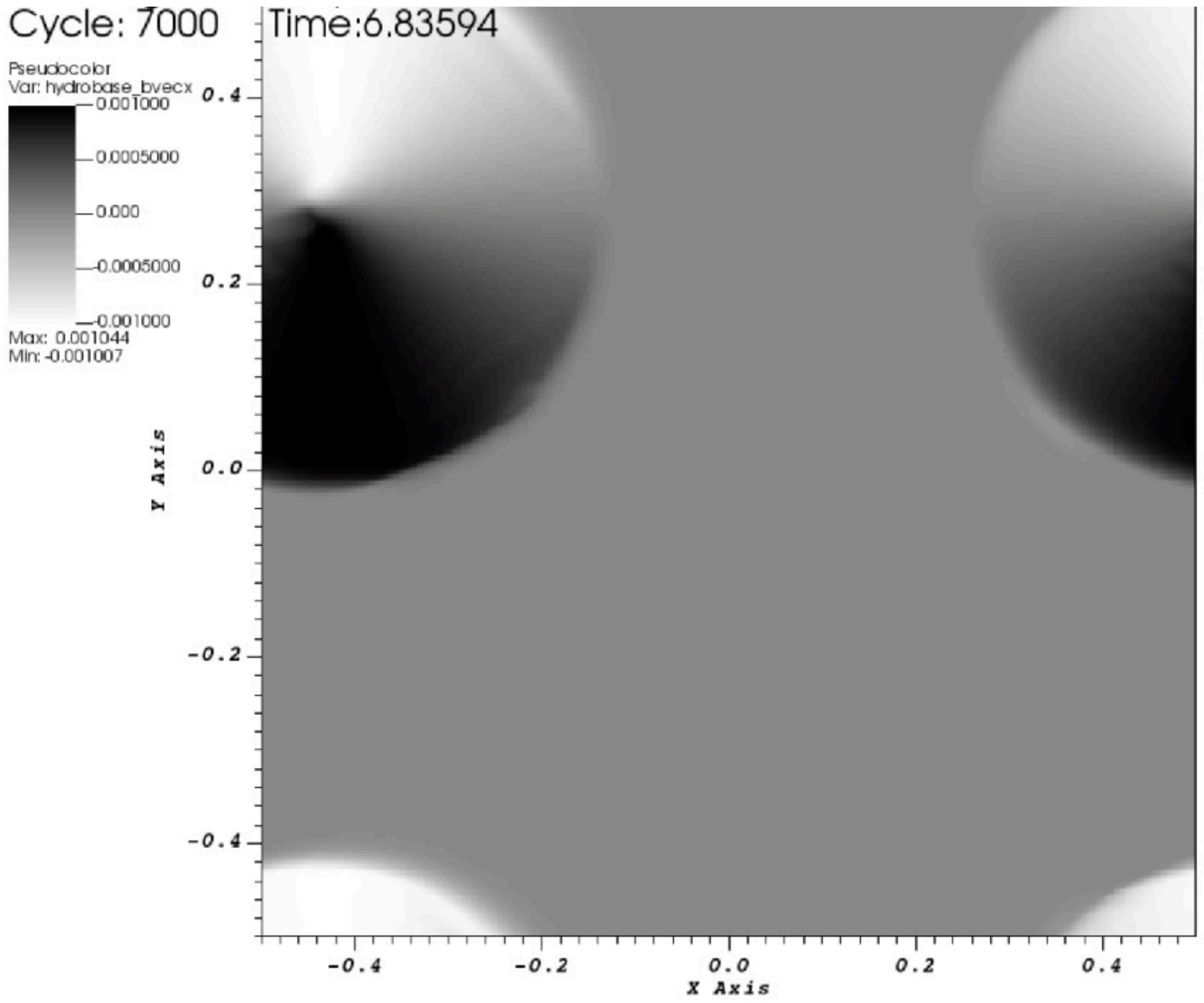


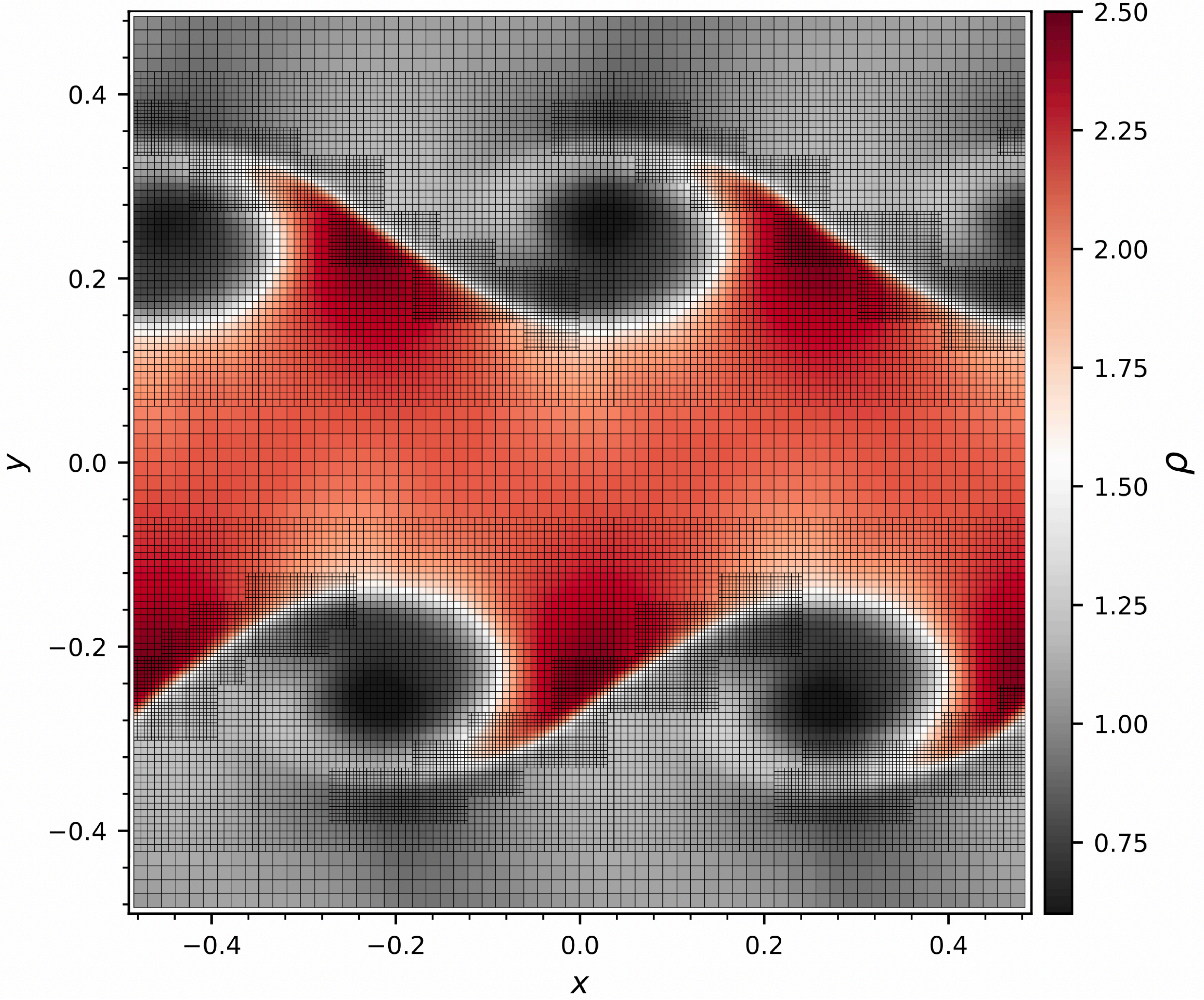
Magnetic Loop Advection

Magnetic field: Bx



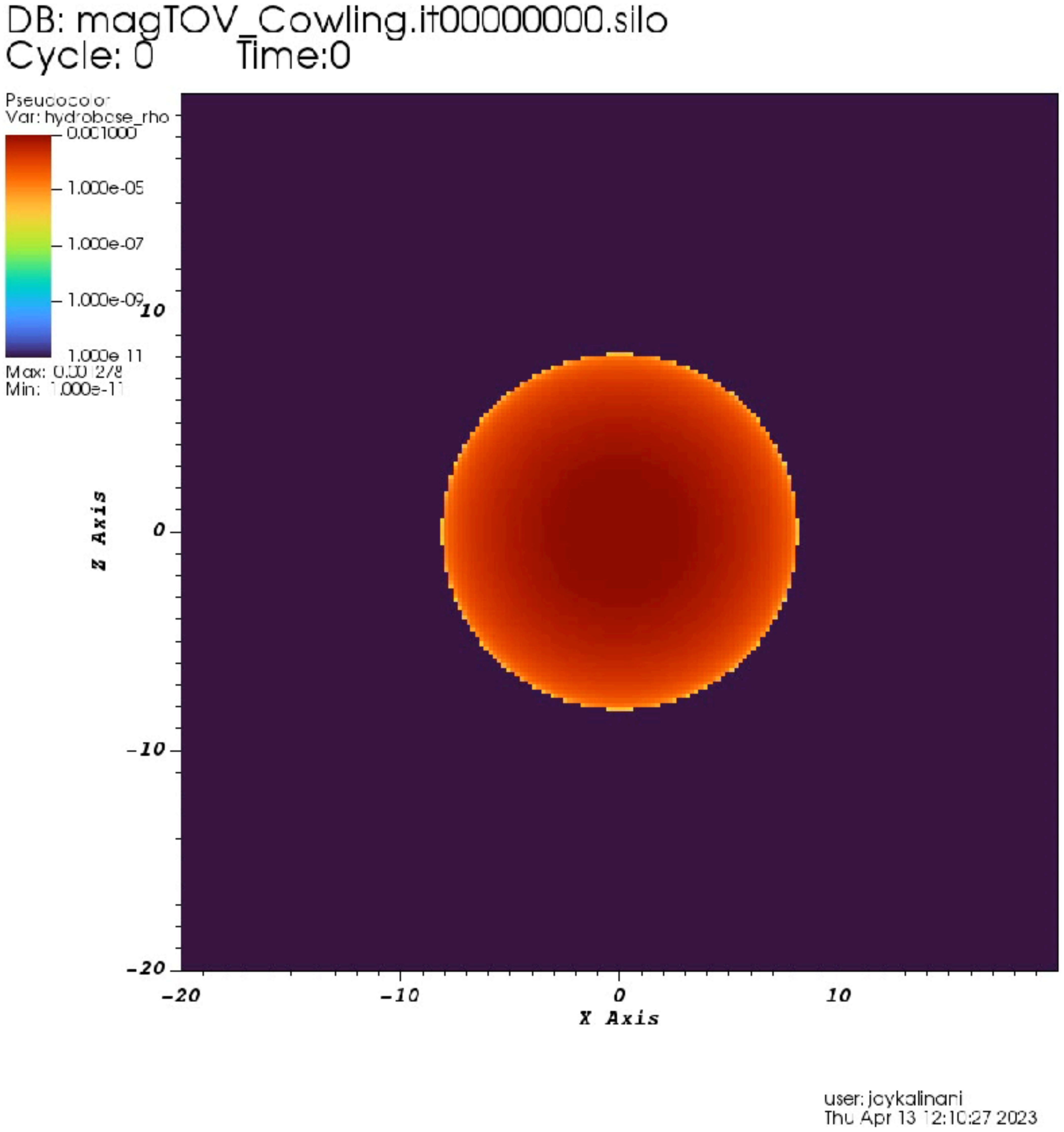
Kelvin Helmholtz Instability

Rest-mass density

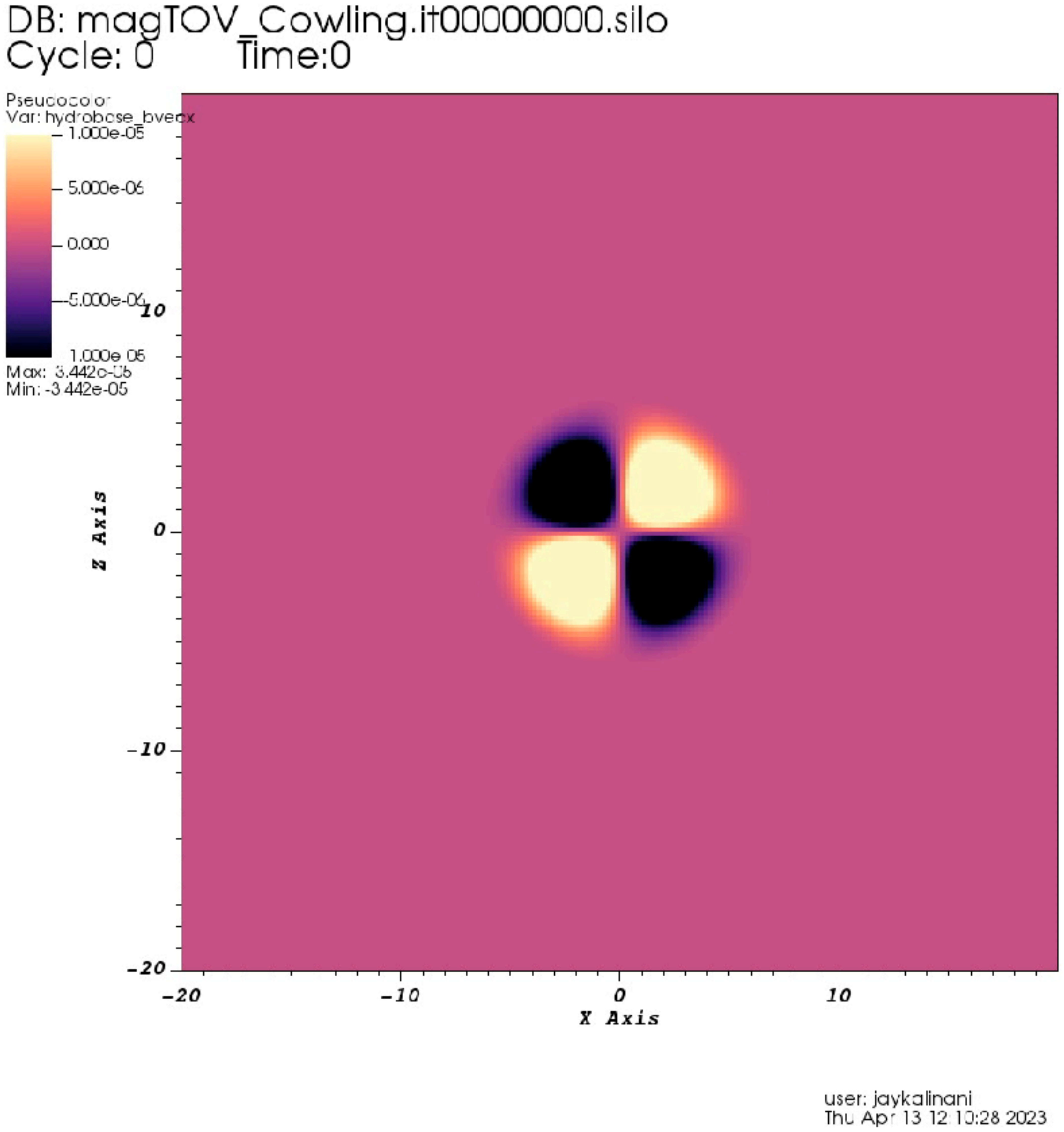


Magnetized TOV

Rest-mass density

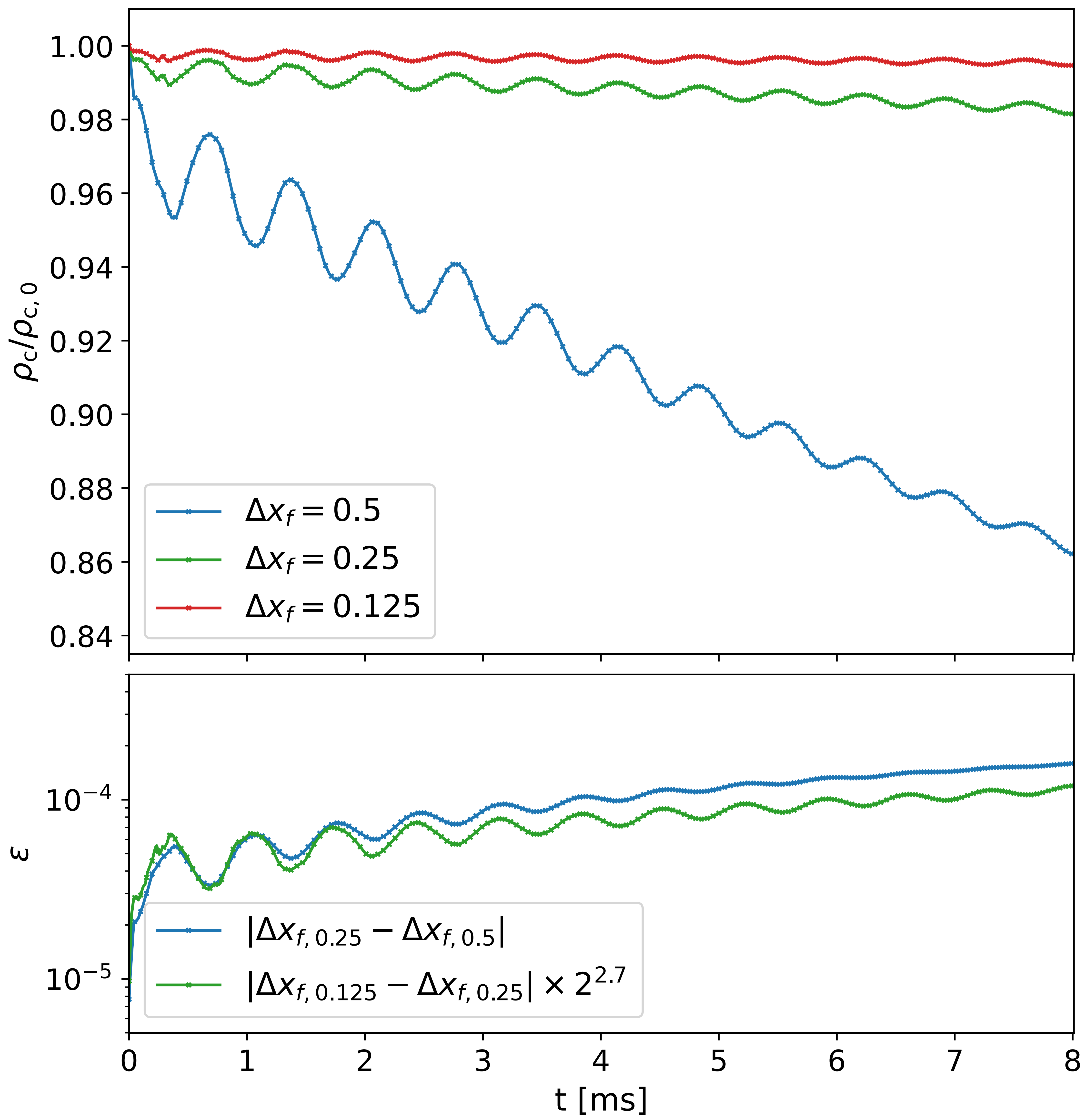


Magnetic field: Bx

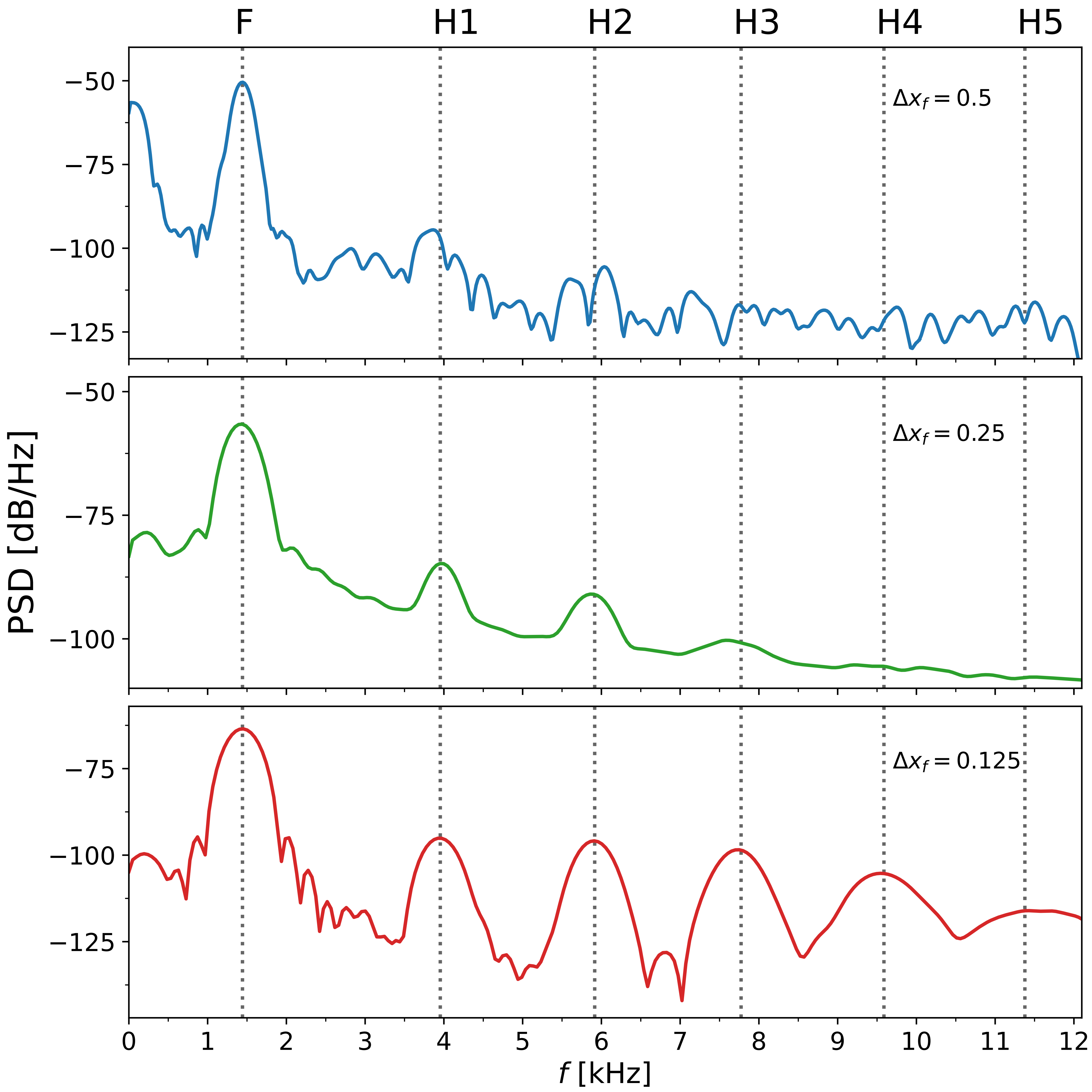


Magnetized TOV

Max. rest-mass density evolution

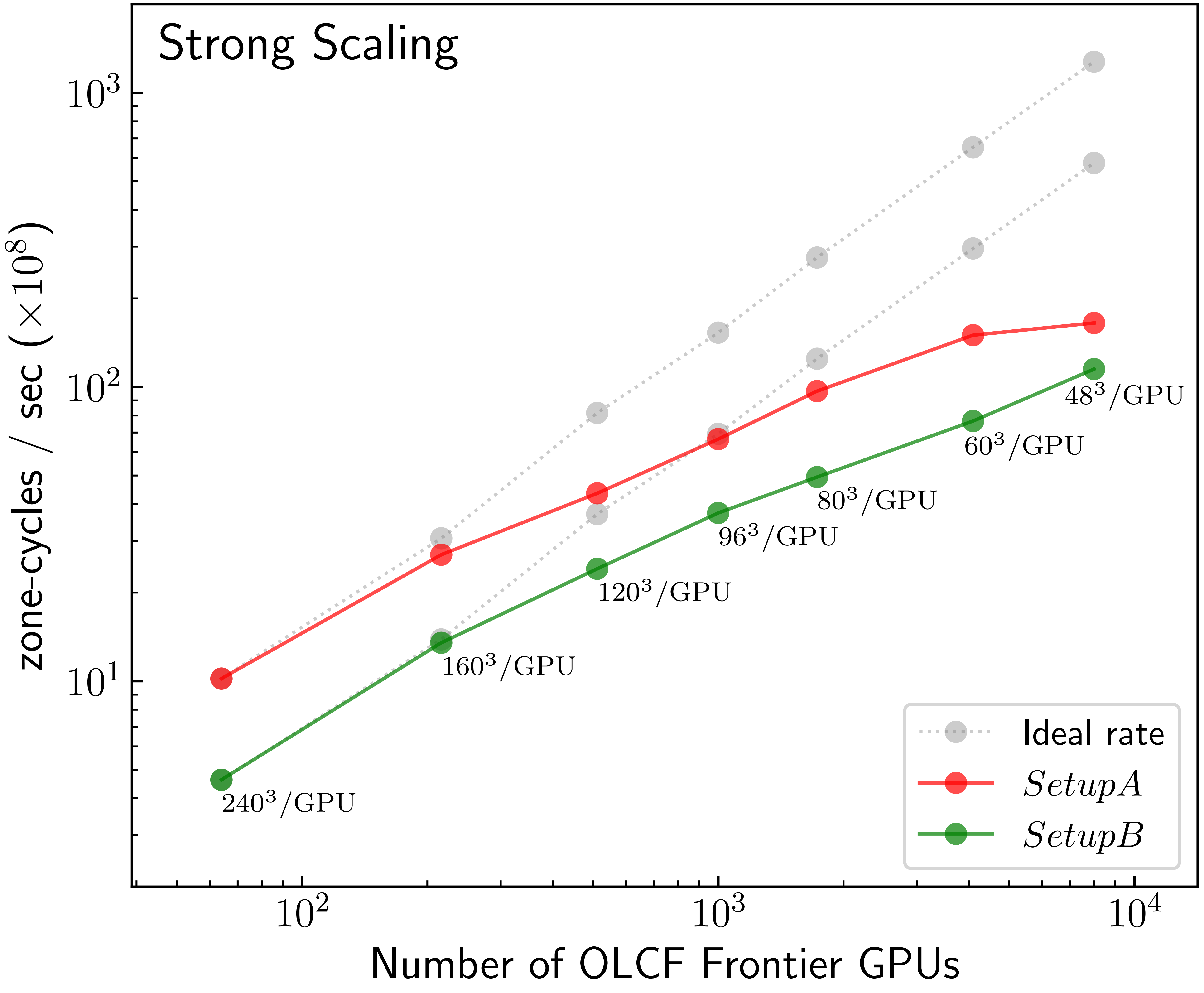


Power spectral density

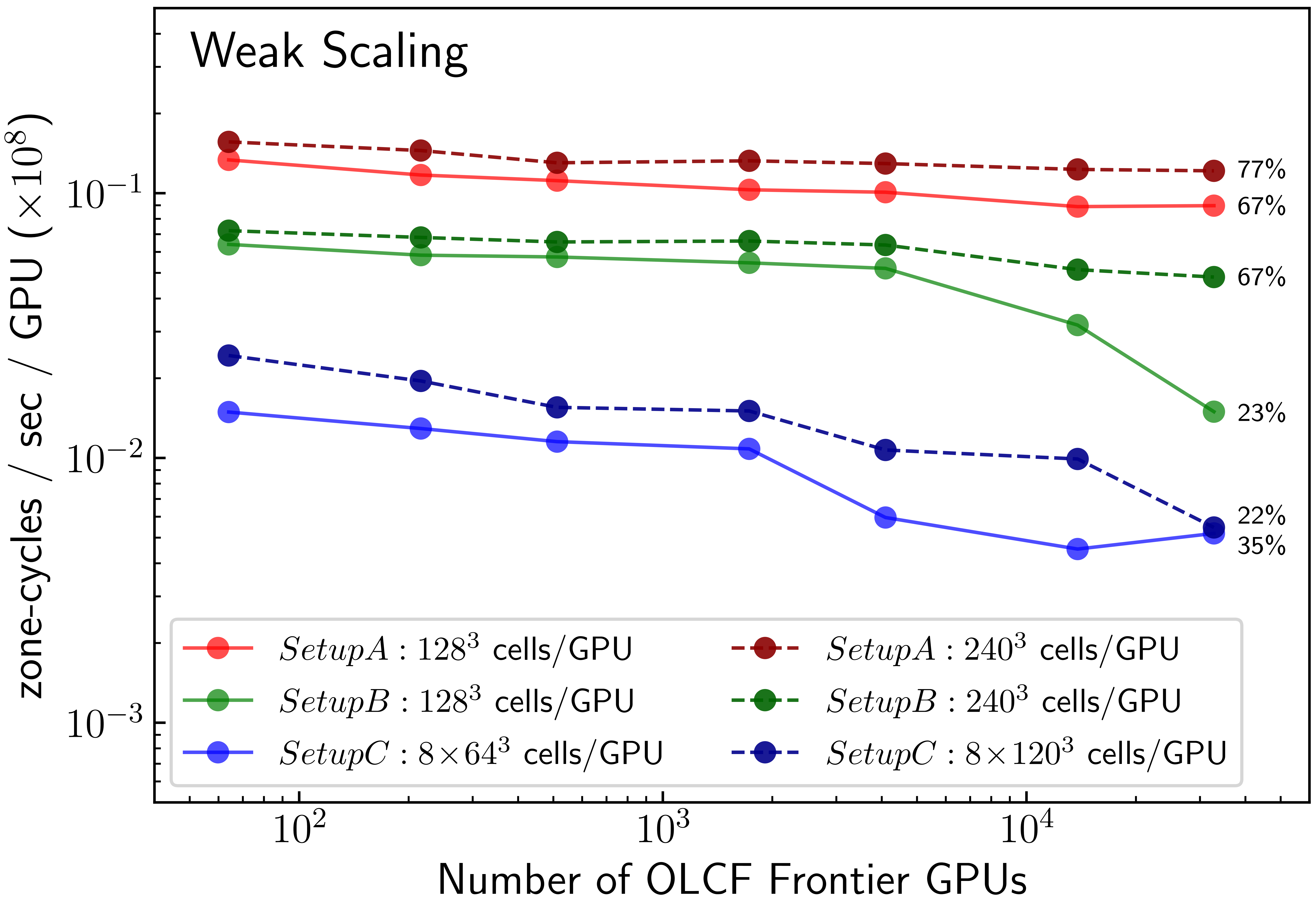


GPU Scaling Tests: Frontier

- Setup A: static (Cowling) spacetime + uniform grid
- Setup B: dynamic (Z4c) spacetime + uniform grid
- Setup C: dynamic (Z4c) spacetime + 8-level AMR

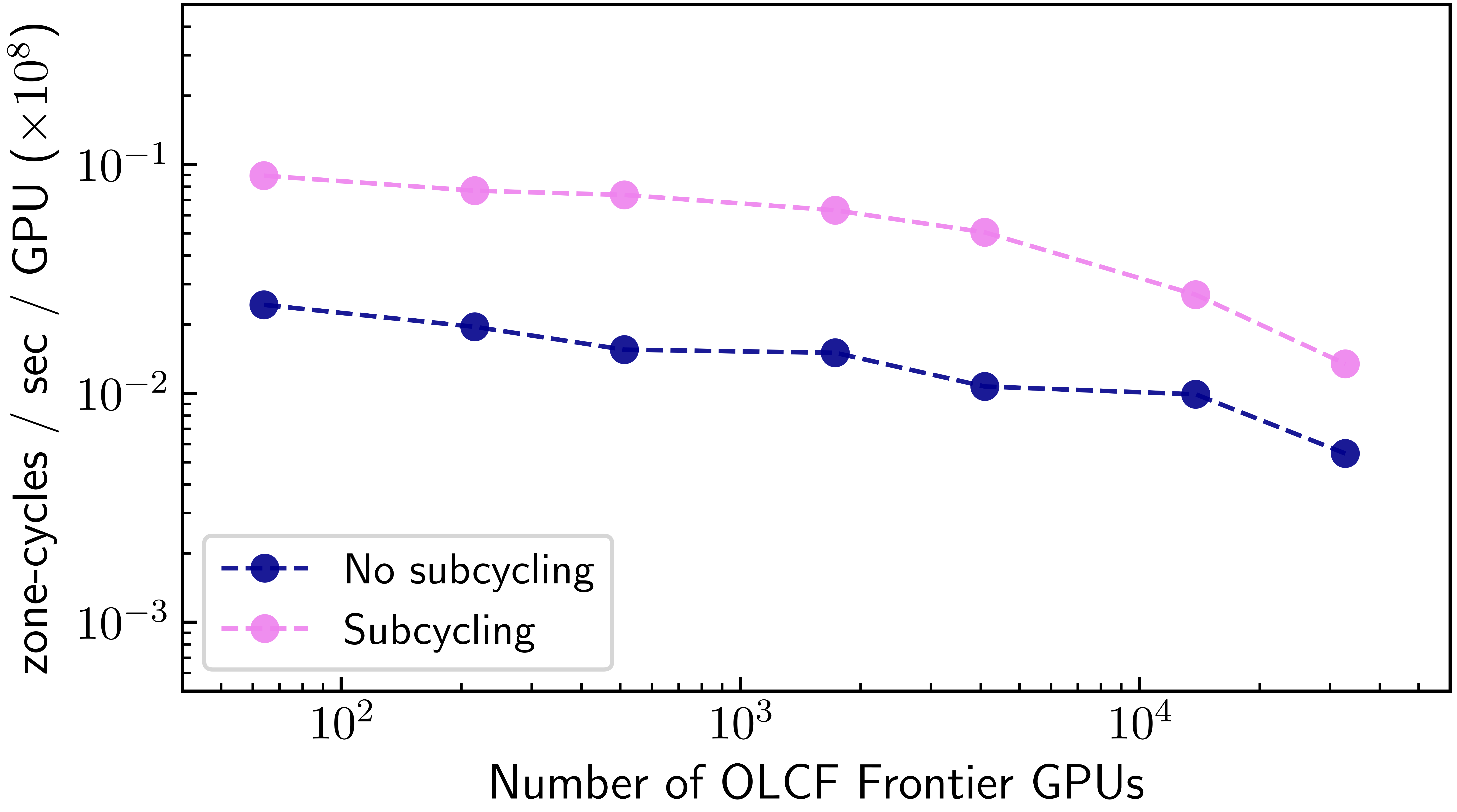


GPU Scaling Tests: Frontier



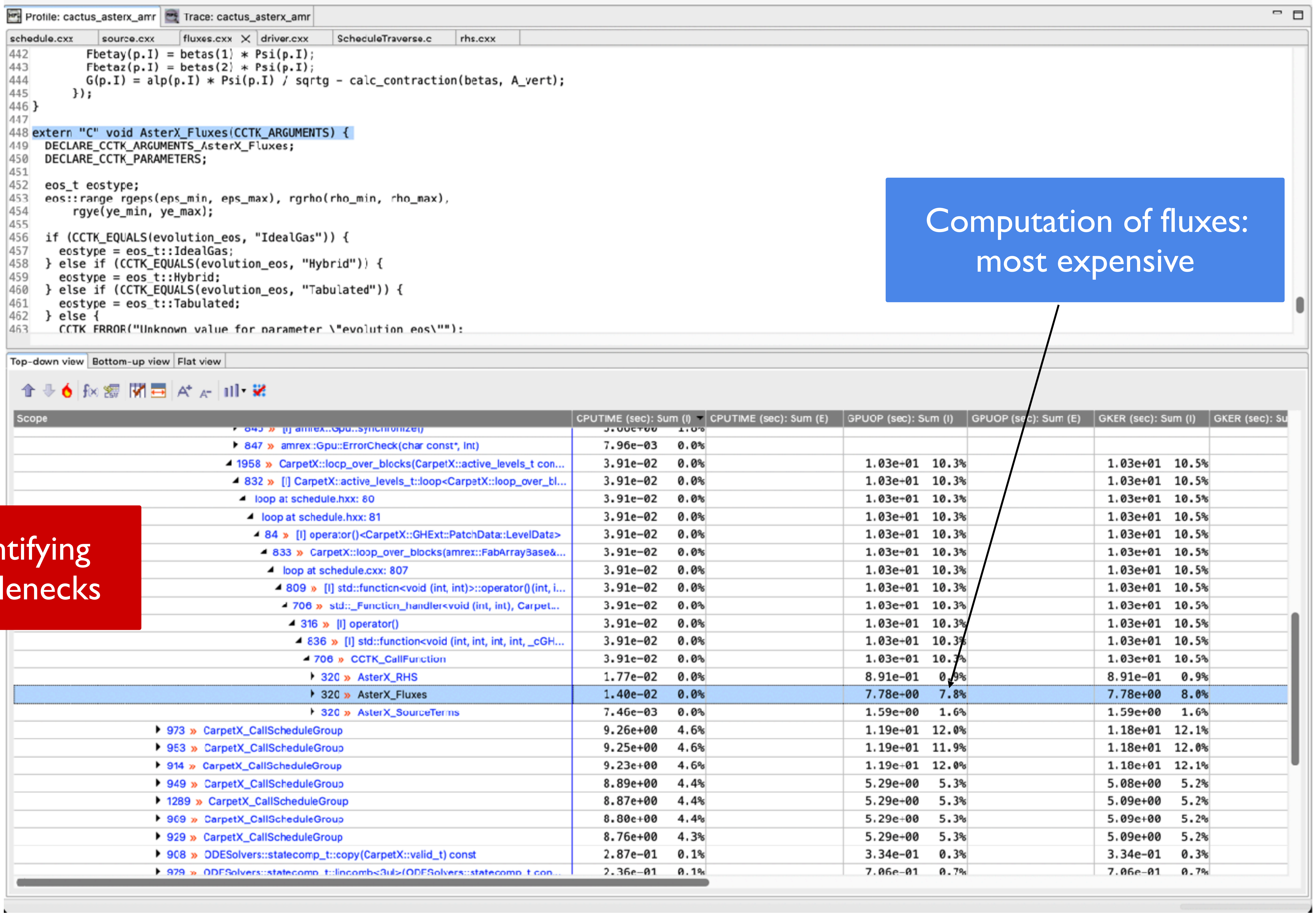
GPU Scaling Tests: Frontier

Subcycling in time: Liwei Ji's talk on Tuesday!



Profiling: Nvidia Nsight Systems

Profiling: HPCToolkit

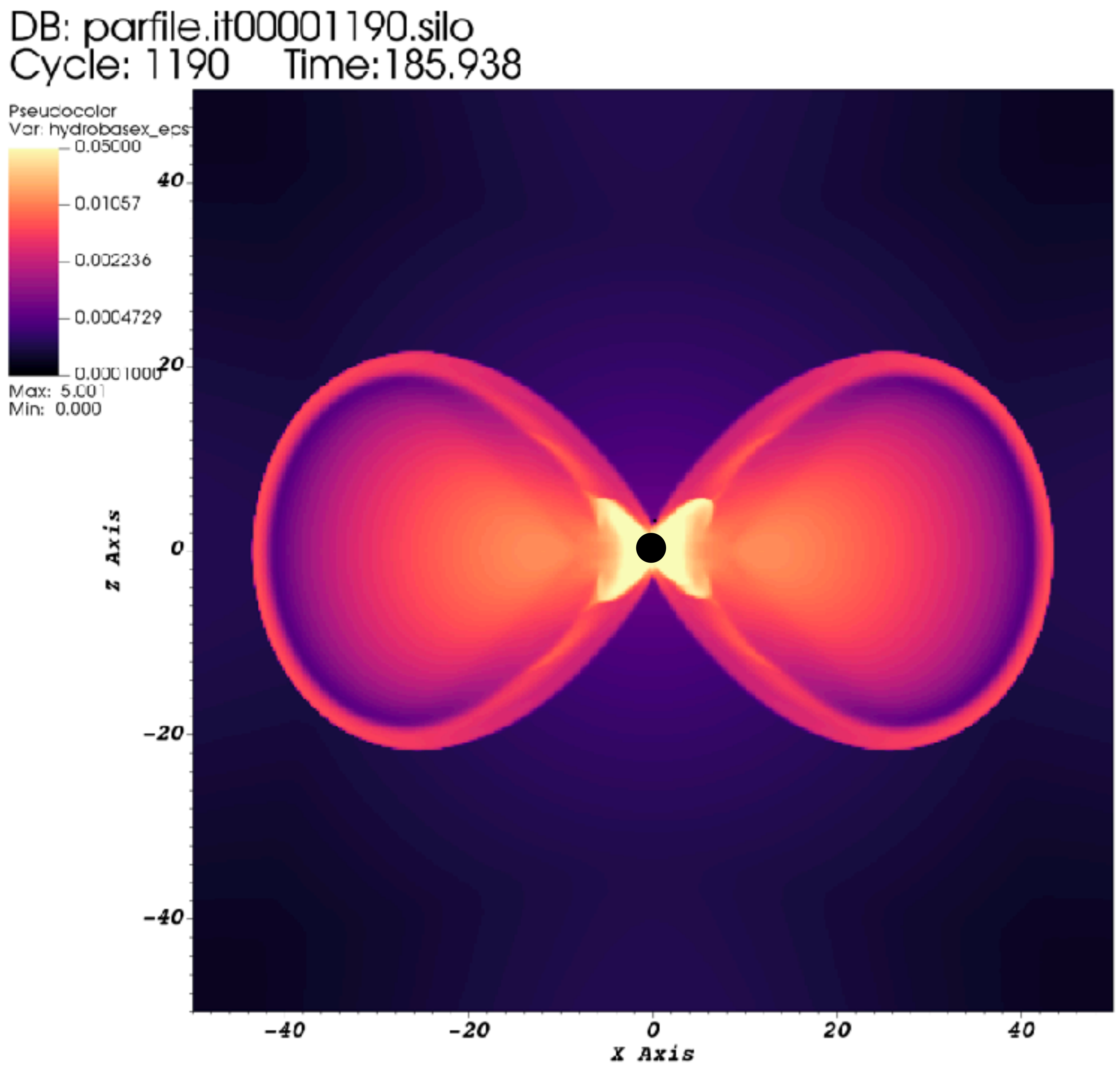


Identifying Bottlenecks

Ongoing developments

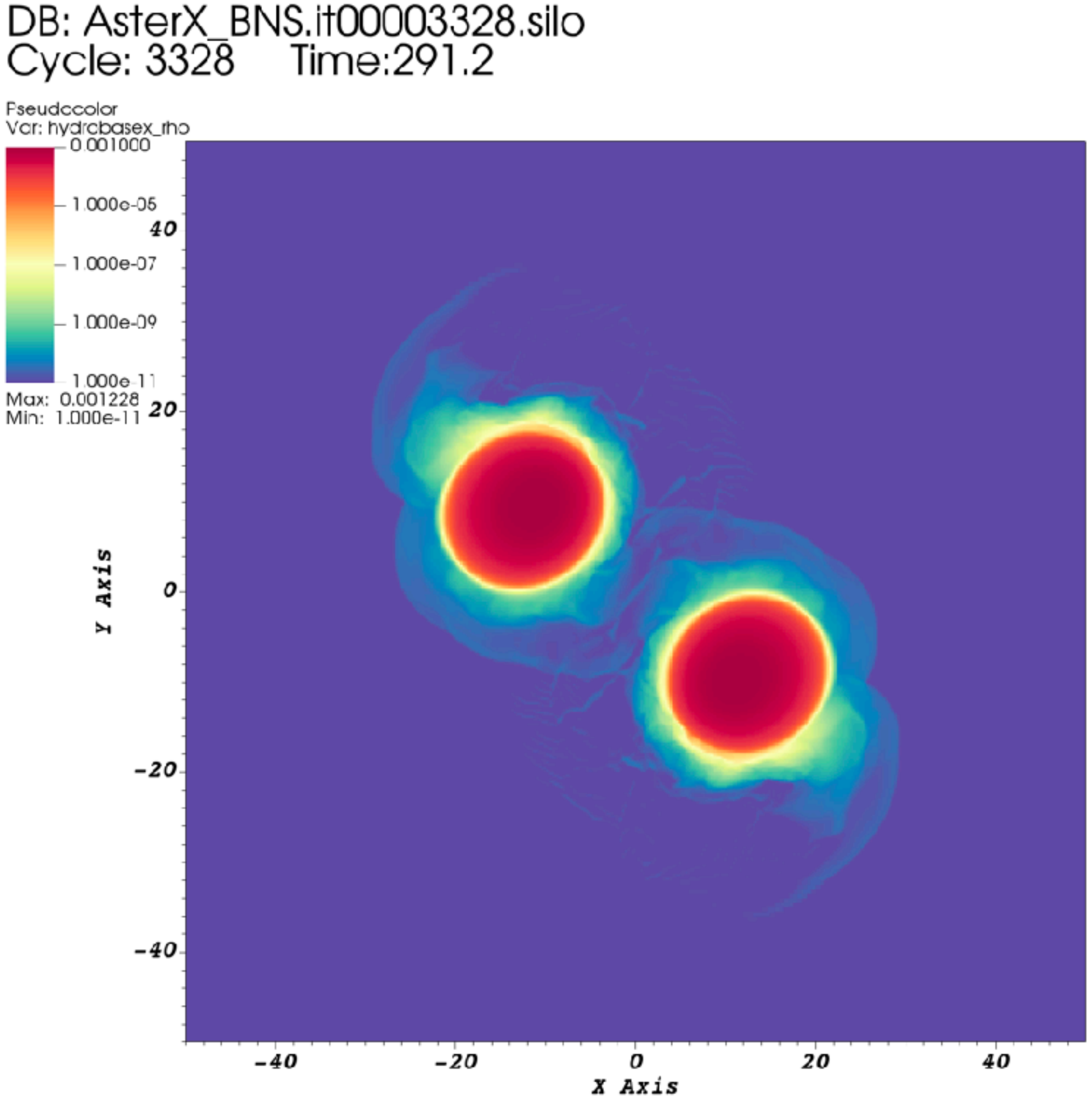
Photon leakage + FM disk simulations

Michail Chabanov



BNS simulations

FUKA ID + Importer Samuel Tootle



Work in Progress

- Extension of EOSX and Con2PrimFactory
- Code optimization
- M1 neutrino transport
- BNS & SMBBH merger simulations!

Thank you for your attention!