FLASH for Astrophysics, High-Energy-Density Physics, and more...

Dongwook Lee
The Flash Center at the University of Chicago

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Outline

Applications

Numerical algorithms

B.C. (Before Computation)

Why do we need numerical simulations?

What does it take to make a simulation?

What do we expect to learn from simulations?

A.D. (After Decision)

Your checklist should include:

1. Timescales

$$\Delta t_{\rm adv} \sim \frac{\Delta x}{\lambda_{\rm max}}\ , \quad \Delta t_{\rm dff} \sim \frac{\Delta x^2}{\eta}\ , \quad \Delta t_{\rm rad} \sim \frac{p}{\Lambda_{\rm cool}}$$

2. Length scales (Fluid vs. Kinetic; Resolutions)

3. Parameters (non-dimensional; numerical)

4. Time for shopping!

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Code Shopping List:
✓ Hydro, MHD, multi-physics
✓ Shock-capturing schemes
✓ Explicit (or implicit?) AMR
✓ Do I want to write my own code? hmmm...
Or, can I get one from somewhere?

What you can get from the FLASH Store

What you can get from the FLASH Store

1. Something to play with: FLASH code

- publicly available, modular, portable, massively-parallel scientific application code http://www.flash.uchicago.edu
- 700 scientists from around the world have co-authored roughly 400 research papers using FLASH
- compressible astrophysics, cosmology, high-energy-density physics
- incompressible Navier-Stokes (GWU)

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2. Something to read: extensive User's guide

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4. Someone to talk to: FLASH team

FLASH Capabilities

Astrophysics

- hydrodynamics, MHD, RHD, cosmology, hybrid PIC
- EoS:
  gamma laws, multi-gamma, Helmholtz
- nuclear physics and other source terms
- external gravity, self-gravity
- active and passive particles
- material properties

HEDP

- multi-temperature (1T, 2T, & 3T) in hydrodynamics and MHD
- implicit thermal conduction
- flux-limited multigroup approxmiation for diffusion radiative transfer
- multi-material support:
  EoS and opacity (tabular & analytic)
- laser ray tracing for energy deposition
- rigid body structures

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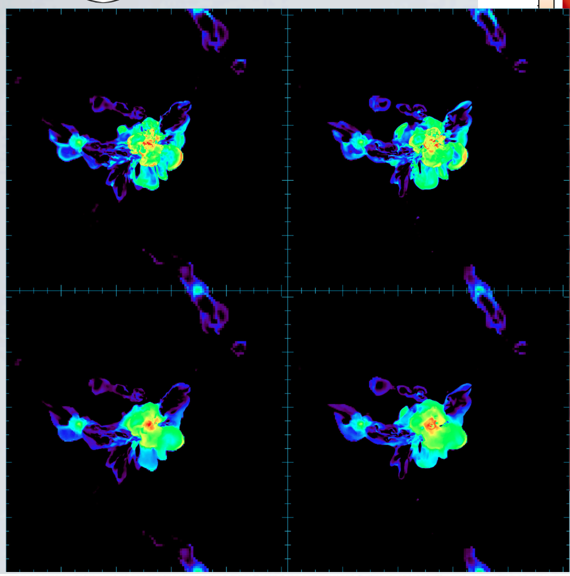
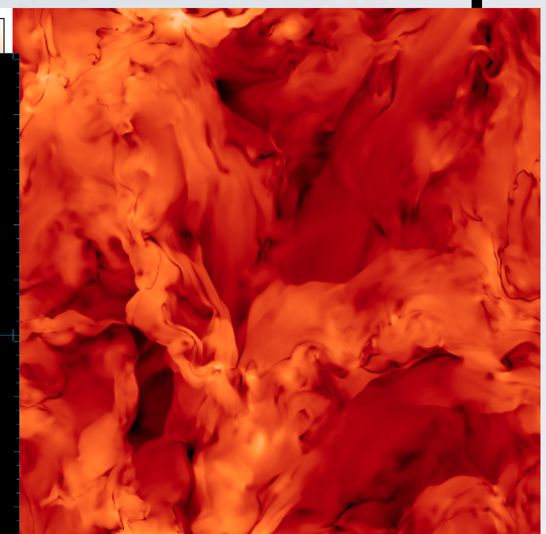
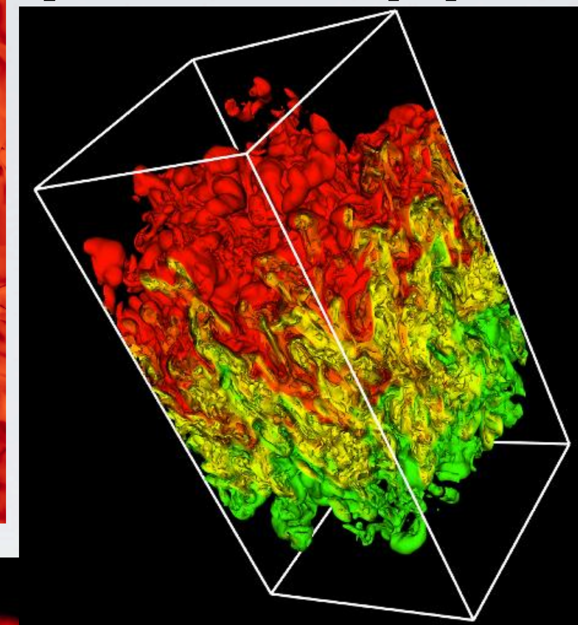
✔ Fortran, C, Python ~ 1.2 million lines (25% comments!)
✔ scalable to tens of thousand processors

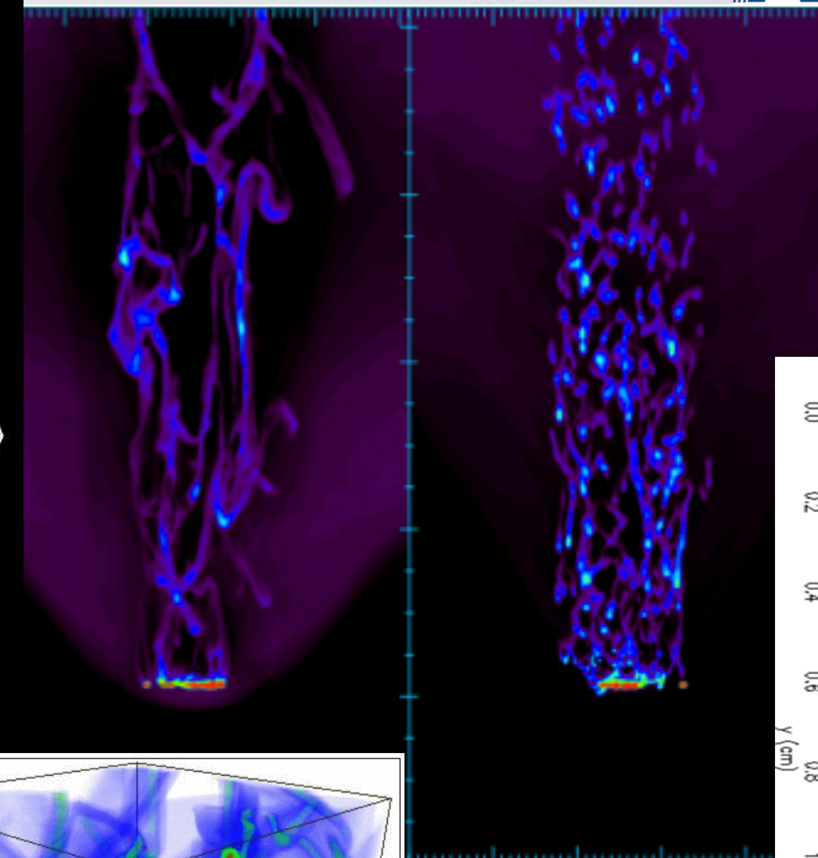
Astrophysical Applications

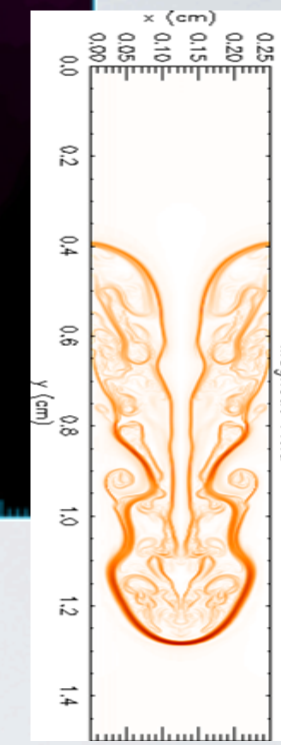
Astrophysical Applications

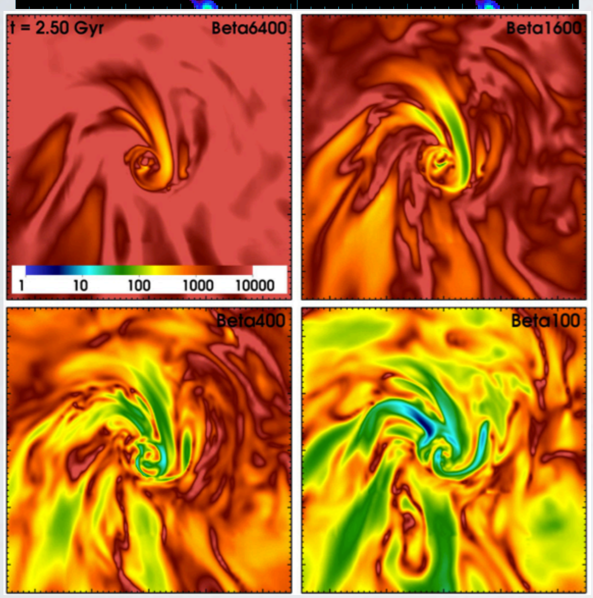


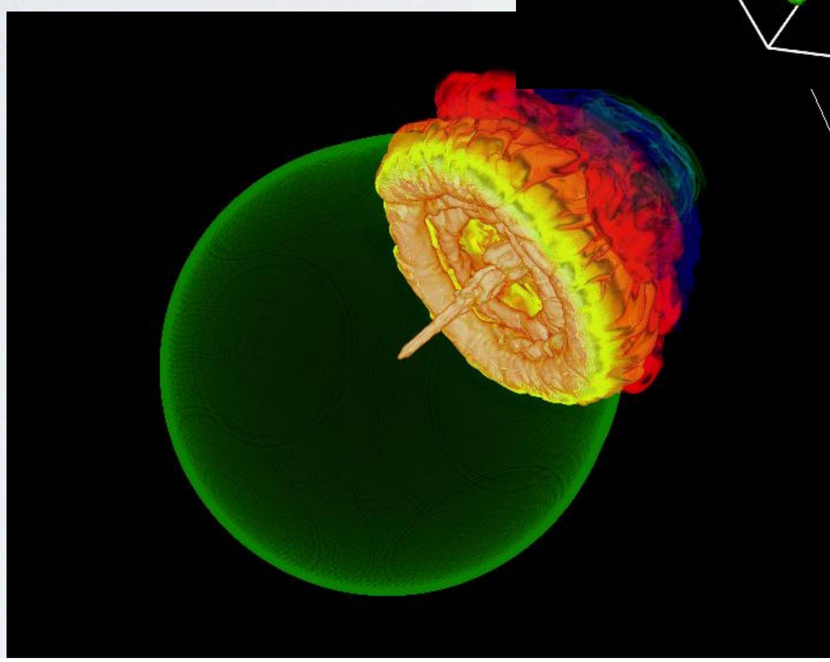


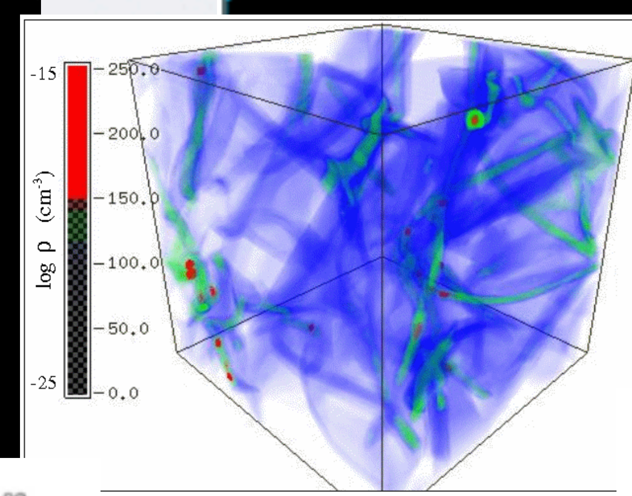


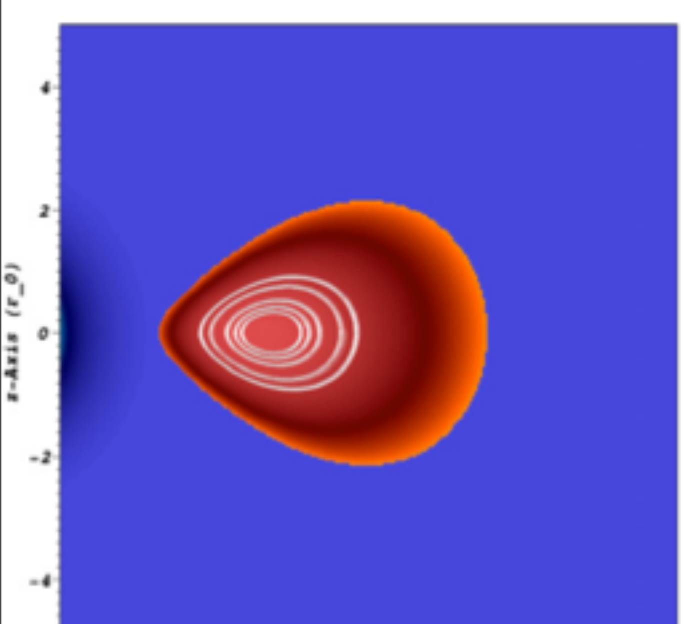


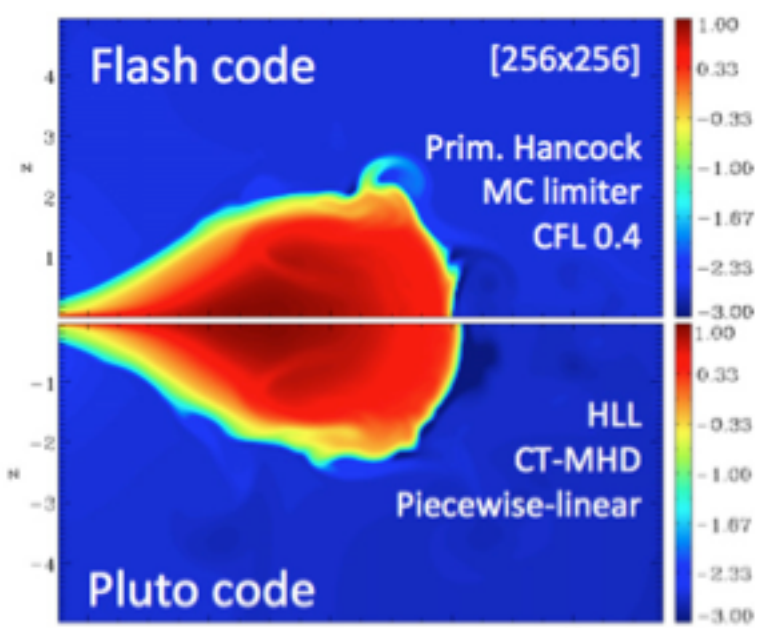


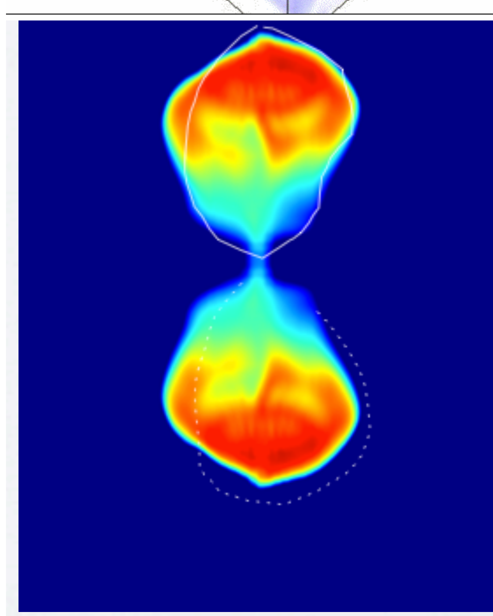


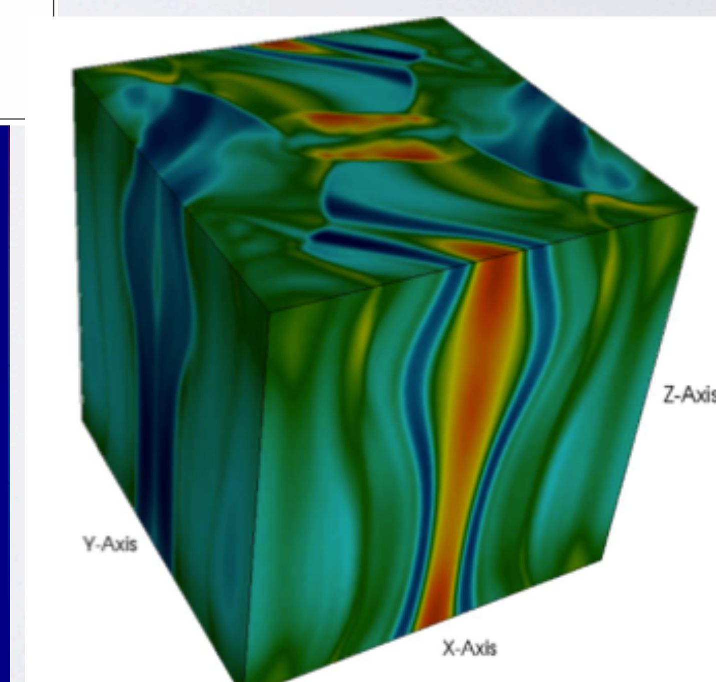




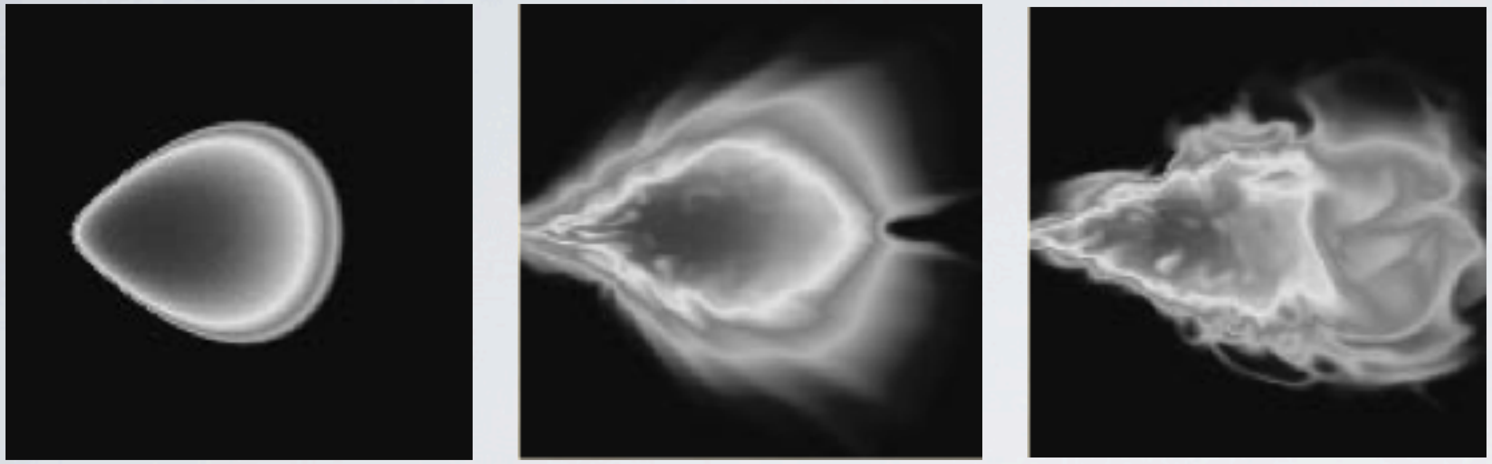


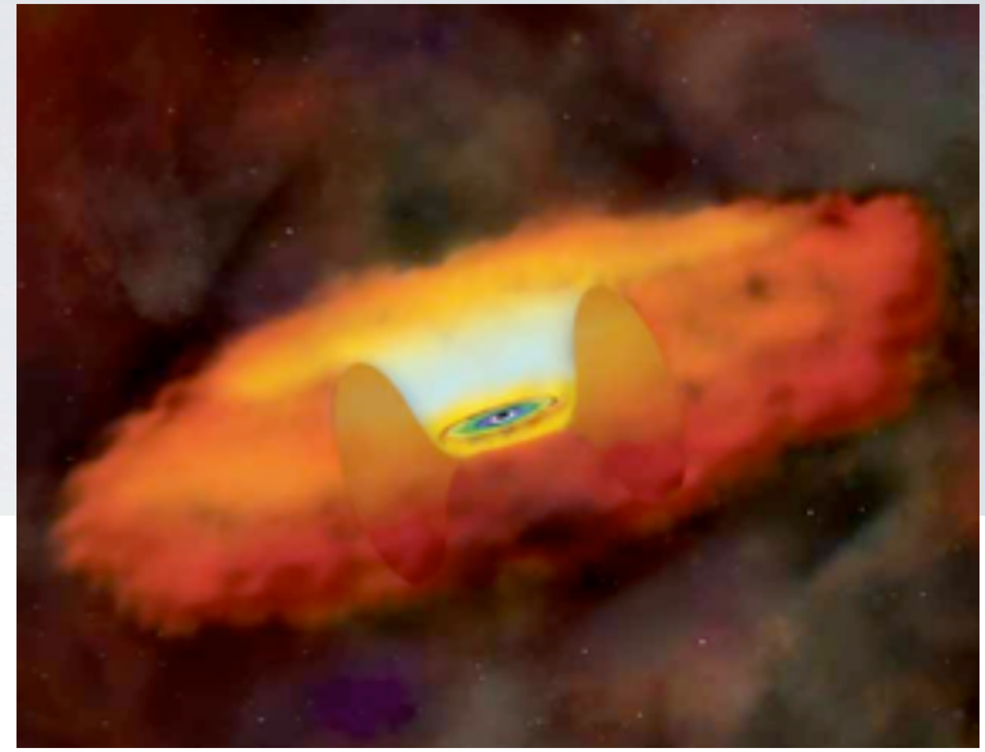






Astrophysical Accretion Torus





The Astrophysical Journal, 528:462–479, 2000 January 1

GLOBAL MAGNETOHYDRODYNAMICAL SIMULATIONS OF ACCRETION TORI

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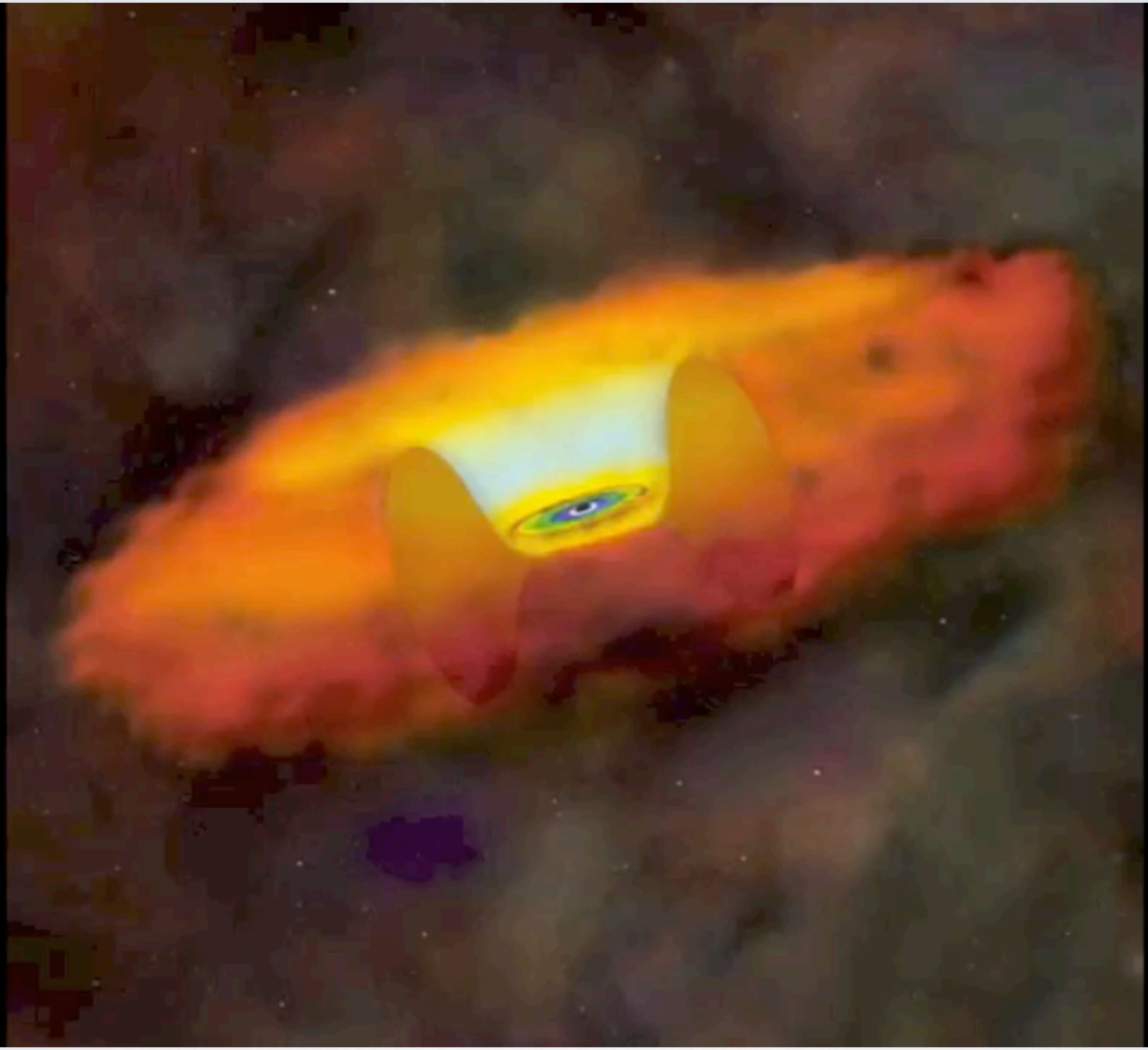
ABSTRACT

Global time-dependent simulations provide a means to investigate time-dependent dynamic evolution in accretion disks. This paper seeks to extend previous local simulations by beginning a systematic effort

- ✓constant angular momentum
- ✓psedo-Newtonian gravity potential
- ✓initial magnetic fields in poloidal direction

Astrophysical Accretion Torus



HEDP Applications

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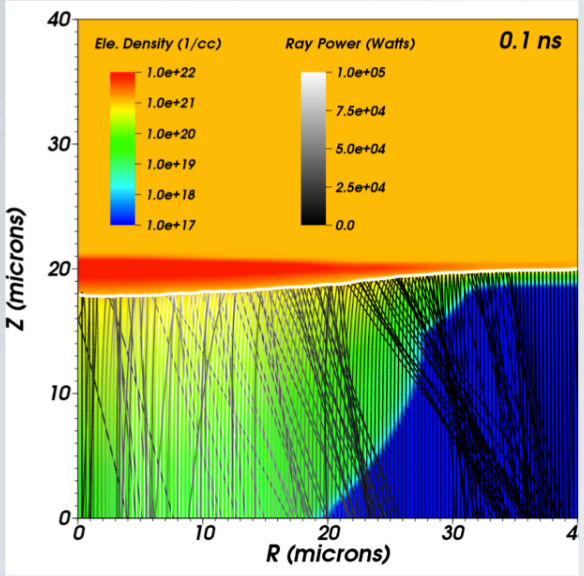
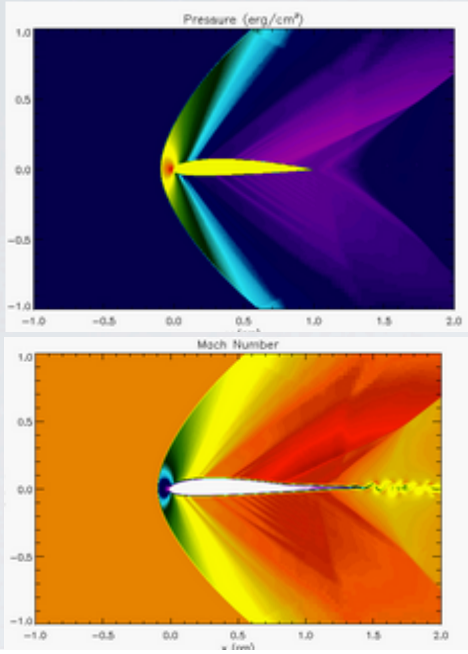
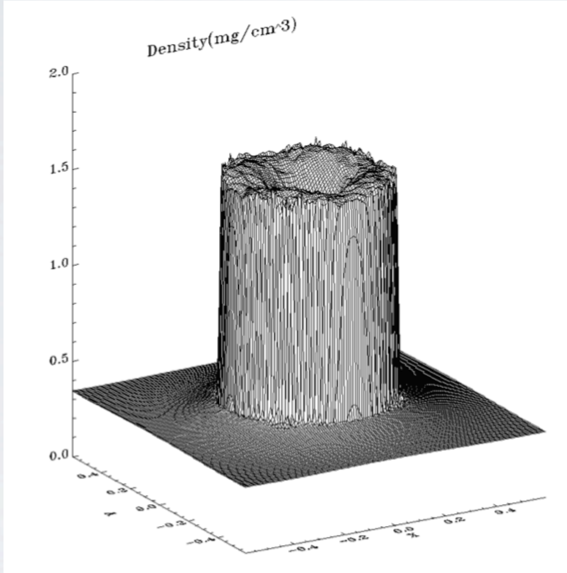
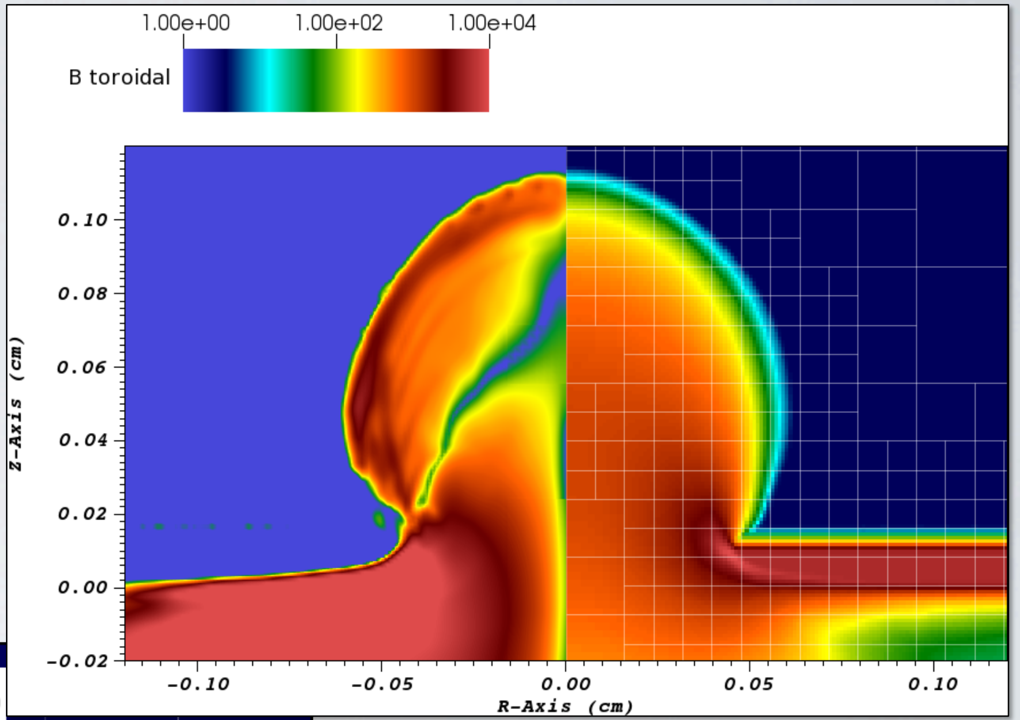
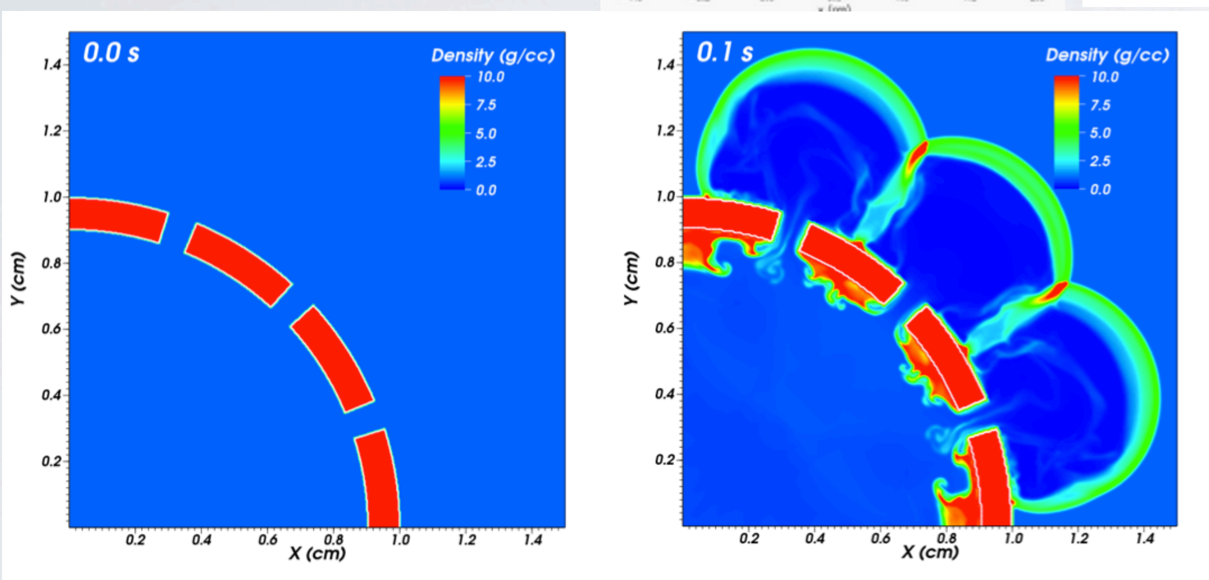
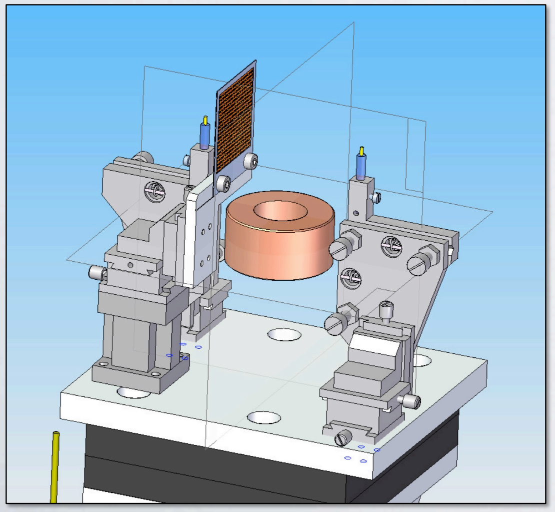


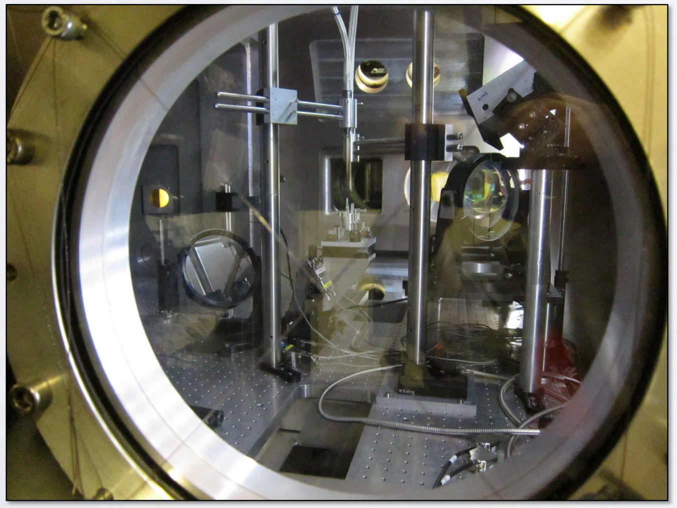


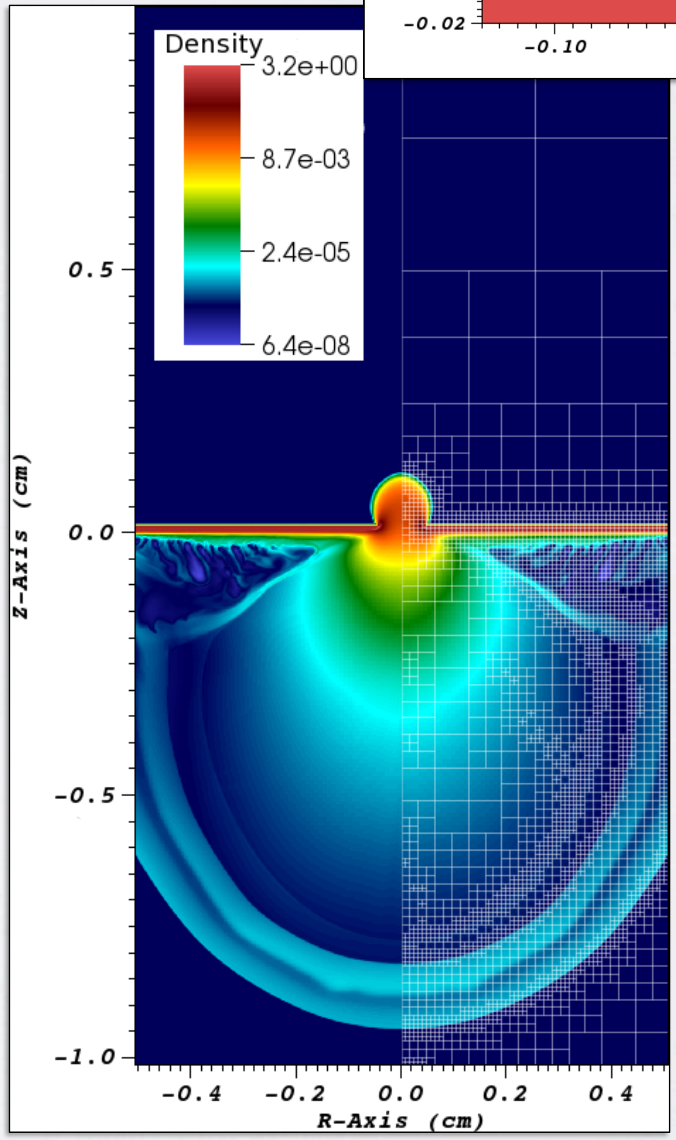


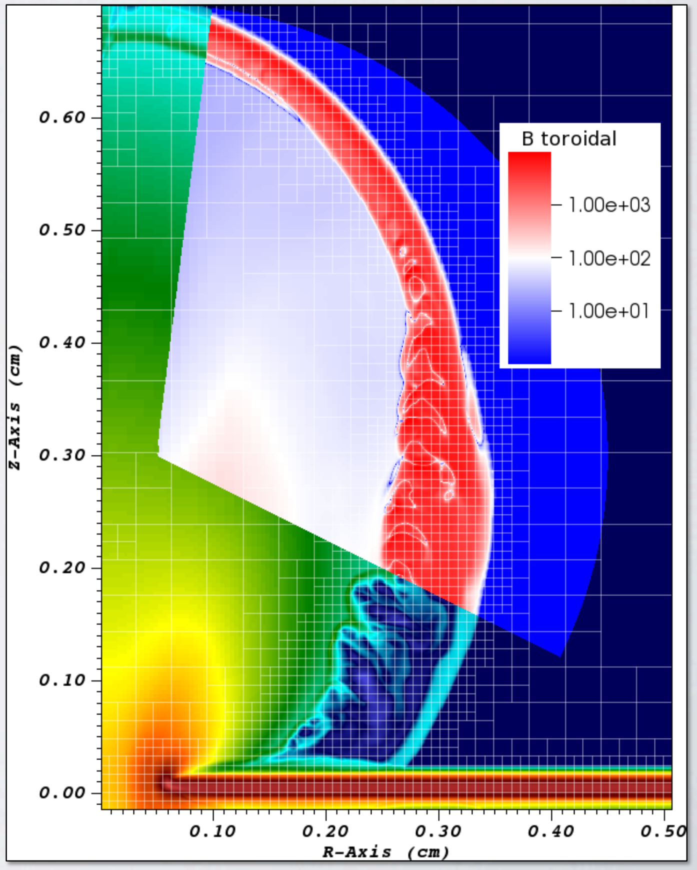




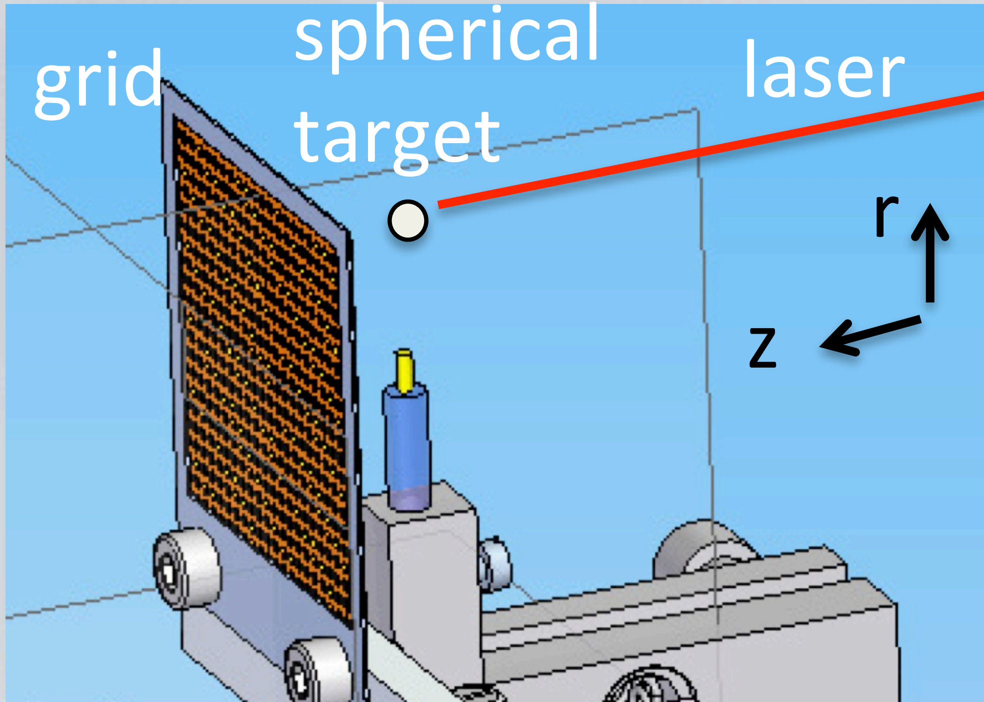


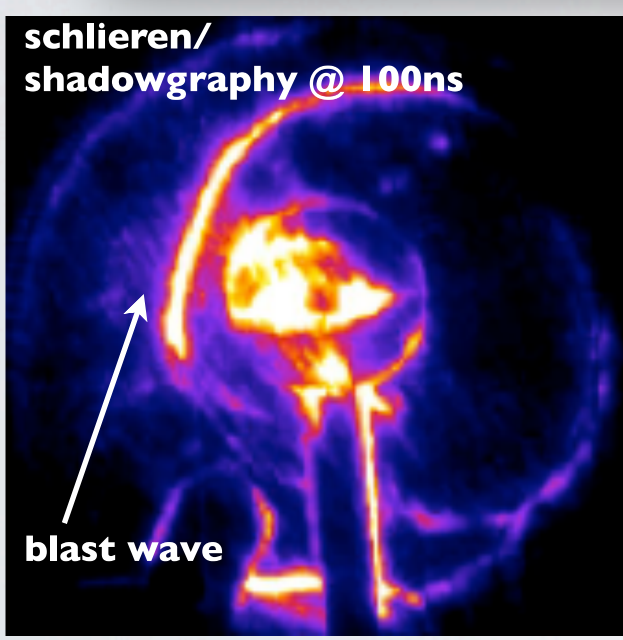




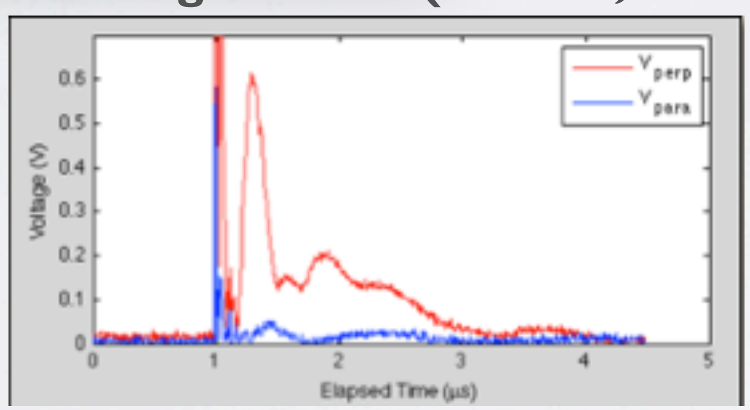


LULI/Vulcan Experiments

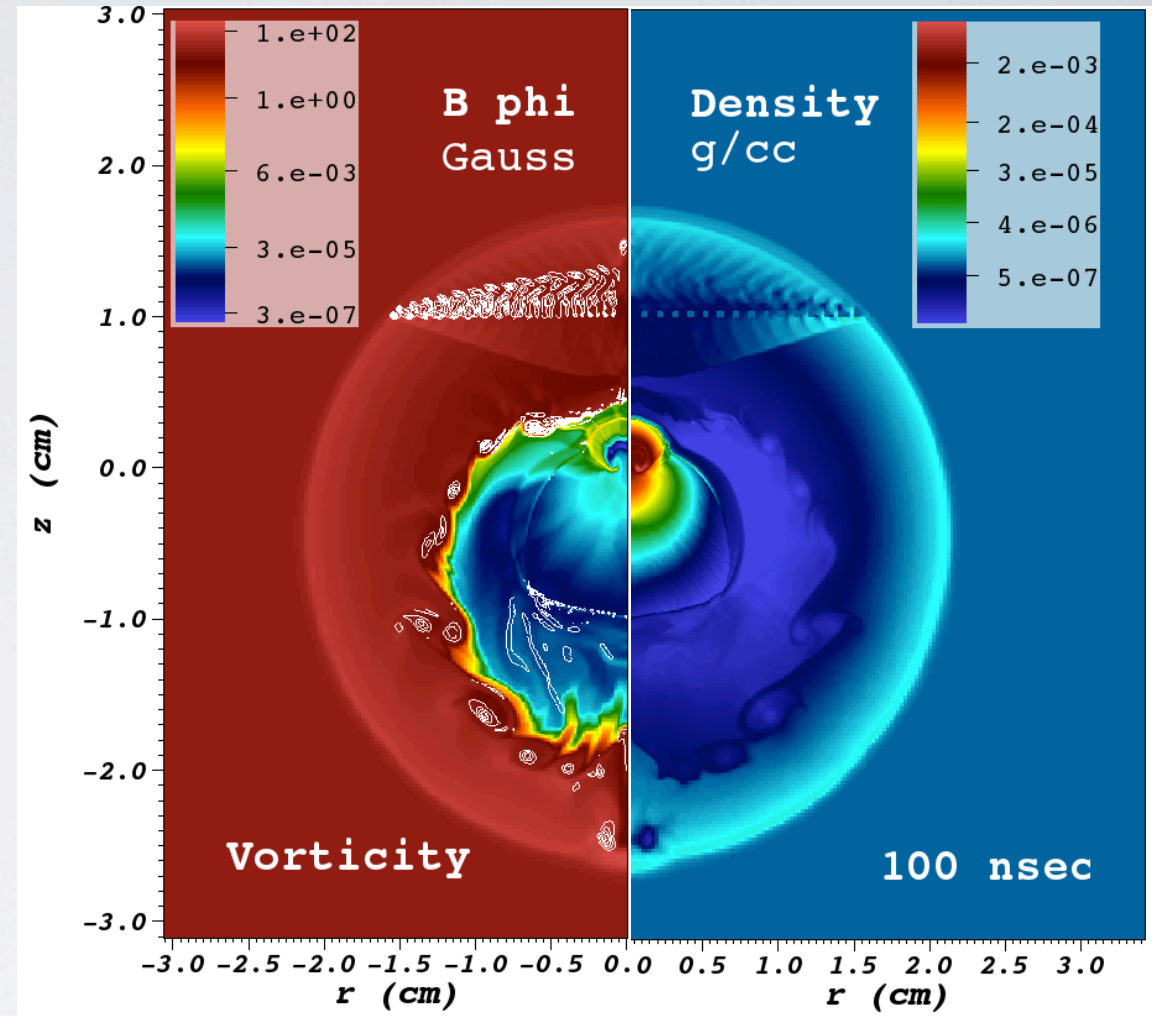




G. Gregori et al. (Nature, 2012)



measured Bdot probes



Fatenajad et al. (2012);
Scopatz et al. (2012);
Tzeferacos et al. (2012)

$$\frac{\partial \mathbf{B}}{\partial t} \sim \frac{\nabla P_e \times \nabla n_e}{e n_e^2}$$

✓ Las ... his HEDLA group at U of Oxfor...

✓ See ... ery mechanism in laser driven ...

✓ FL... understanding underlying physics, assist in future experimental design

500 micro meter plastic sphere
0.5 mbar Argon filled chamber
400J, 2 omega, 1.5ns square pulse laser
ablation and shock front creation
Quantitative measurements of magnetic field generations

Numerical Algorithms

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My code already works well and perfect!

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It's been producing good results for me for many years!

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I trust numerical schemes should provides physically meaningful answers!

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Really?

Improving MHD Algorithms

An unsplit staggered mesh scheme for multidimensional magnetohydrodynamics

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A R T I C L E I N F O

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Magnetohydrodynamics
Constrained transport
Corner transport upwind
Unsplit scheme
Staggered mesh
High-order Godunov method

A B S T R A C T

We introduce an unsplit staggered mesh scheme (USM) for multidimensional magnetohydrodynamics (MHD) that uses a constrained transport (CT) method with high-order Godunov fluxes and incorporates a new data reconstruction–evolution algorithm for second-order MHD interface states. In this new algorithm, the USM scheme includes so-called "multidimensional MHD terms", proportional to $\nabla \cdot \mathbf{B}$, in a dimensionally-unsplit way in a single update. This data reconstruction–evolution step, extended from the corner transport upwind (CTU) approach of Colella, maintains in-plane dynamics very well, as shown by the advection of a very weak magnetic field loop in 2D. This data reconstruction–evolution algorithm is also of advantage in its consistency and simplicity when extended to 3D. The scheme maintains the $\nabla \cdot \mathbf{B} = 0$ constraint by solving a set of discrete induction equations using the standard CT approach, where the accuracy of the computed electric field directly influences the quality of the magnetic field solution. We address the lack of proper dissipative behavior in the simple electric field averaging scheme and present a new modified electric field construction (MEC) that includes multidimensional derivative information and enhances solution accuracy. A series of comparison studies demonstrates the excellent performance of the full USM–MEC scheme for many stringent multidimensional MHD test problems chosen from the literature. The scheme is implemented and currently freely available in the University of Chicago ASC FLASH Center's FLASH3 release.

2D MHD, JCP, 2009

A Solution Accurate, Efficient and Stable Unsplit Staggered Mesh Scheme for Three Dimensional Magnetohydrodynamics

Dongwook Lee

The Flash Center for Computational Science, University of Chicago, 5747 S. Ellis, Chicago, IL 60637

Abstract

In this paper, we extend the unsplit staggered mesh scheme (USM) for 2D magnetohydrodynamics (MHD) [D. Lee, A. Deane, An Unsplit Staggered Mesh Scheme for Multidimensional Magnetohydrodynamics, J. Comput. Phys. 228 (2009) 952–975] to a full 3D MHD scheme. The 3D scheme uses the same set of fundamental algorithmic ideas that have been developed in the 2D USM scheme. The scheme is a finite-volume Godunov method consisting of (1) a constrained transport (CT) method for preserving the solenoidal magnetic field evolution on a staggered grid, and (2) an efficient and accurate single-step, directionally unsplit multidimensional data reconstruction-evolution algorithm, which extends Colella's original 2D corner transport upwind (CTU) method [P. Colella, Multidimensional Upwind Methods for Hyperbolic Conservation Laws, J. Comput. Phys. 87 (1990) 446–466]. We present two types of data reconstruction-evolution algorithms for 3D: a reduced CTU scheme and a full CTU scheme. The reduced 3D CTU scheme is a variant of a direct 3D extension of Collela's 2D CTU method, whereas our full 3D CTU approach is a variant of the 3D unsplit CTU method by Saltzman [J. Saltzman, An unsplit 3D upwind method for hyperbolic conservation laws, J. Comput. Phys. 115 (1994) 153–168] for hyperbolic conservation laws. The key novelty in our algorithms is a new approach to account for transverse fluxes that stabilize an unsplit hyperbolic system *without* solving intermediate Riemann problems. The two schemes use multidimensional characteristic tracing to account for the stabilizing effects provided by incorporating the transverse fluxes in CTU. The proposed algorithms are simple and efficient especially when including multidimensional MHD source terms that maintain in-plane magnetic field dynamics. We also introduce a new CT scheme that makes use of proper upwind information in taking an average of electric fields. This method enhances numerical accuracy in solving the induction equations using the third-order spatially accurate modified electric field construction (MEC) scheme developed in 2D USM. We show that the new 3D USM-MHD algorithm provides a full CFL stability limit (CFL number ≤ 1) in most of the MHD test problems available in the literature, only requiring three Riemann problems (except for the extra three Riemann solves for the intermediate magnetic field update) per zone per time step in 3D. Our 3D USM schemes can be easily combined with various reconstruction methods (e.g., first-order Godunov, second-order MUSCL-Hancock, third-order PPM and fifth-order WENO), and a wide choice of Riemann solvers (e.g., local Lax-Friedrichs, HLLE, HLLC, HLLD, and Roe). The 3D USM-MHD solver is available in the University of Chicago Flash Center's official FLASH release.

Key words: MHD; Magnetohydrodynamics; Constrained Transport; Corner Transport Upwind; Unsplit Scheme; Staggered Mesh; High-Order Godunov Method; Large CFL Number.

3D MHD, JCP, 2012
(under revision)

Constrained Transport (CT) MHD

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Solves induction equations on staggered grid

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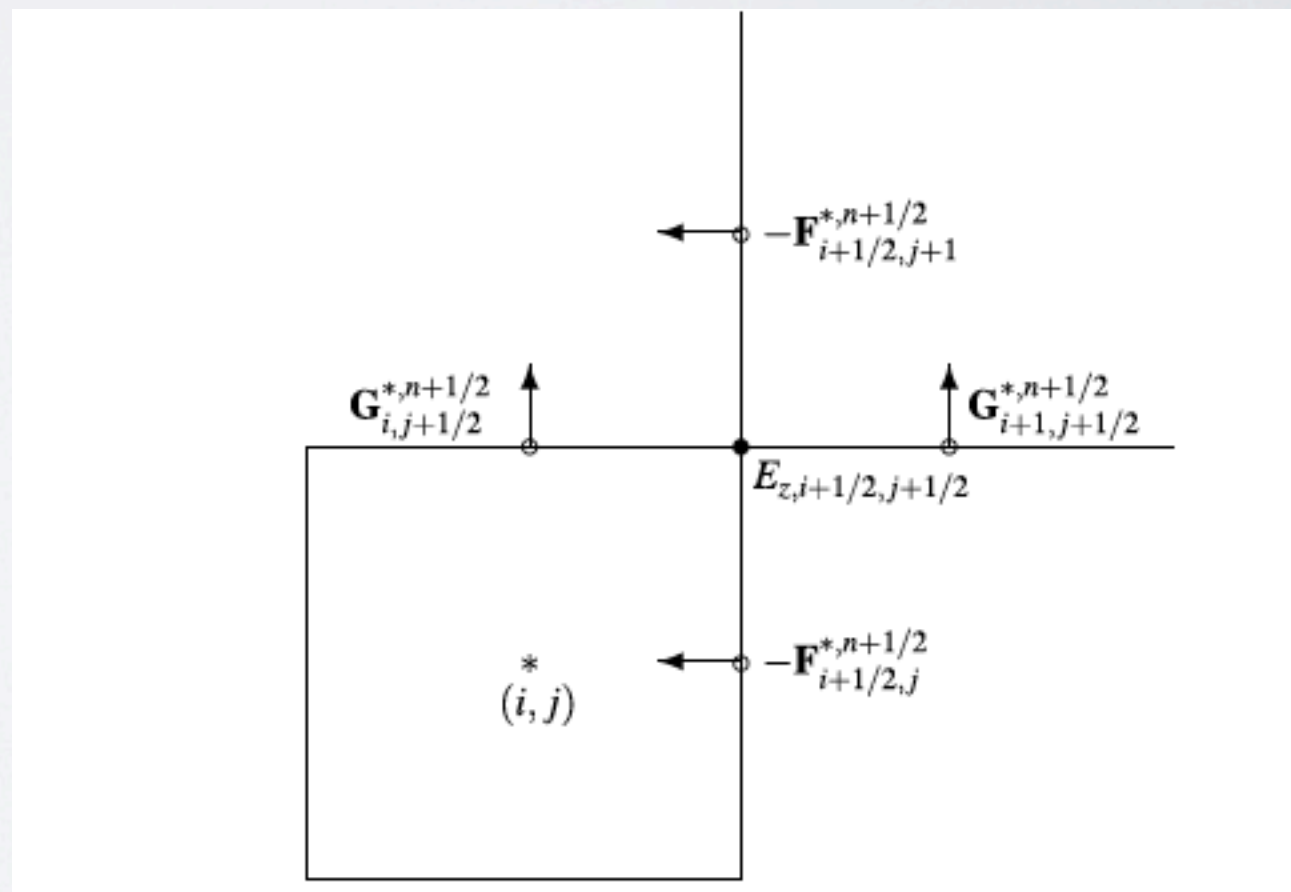
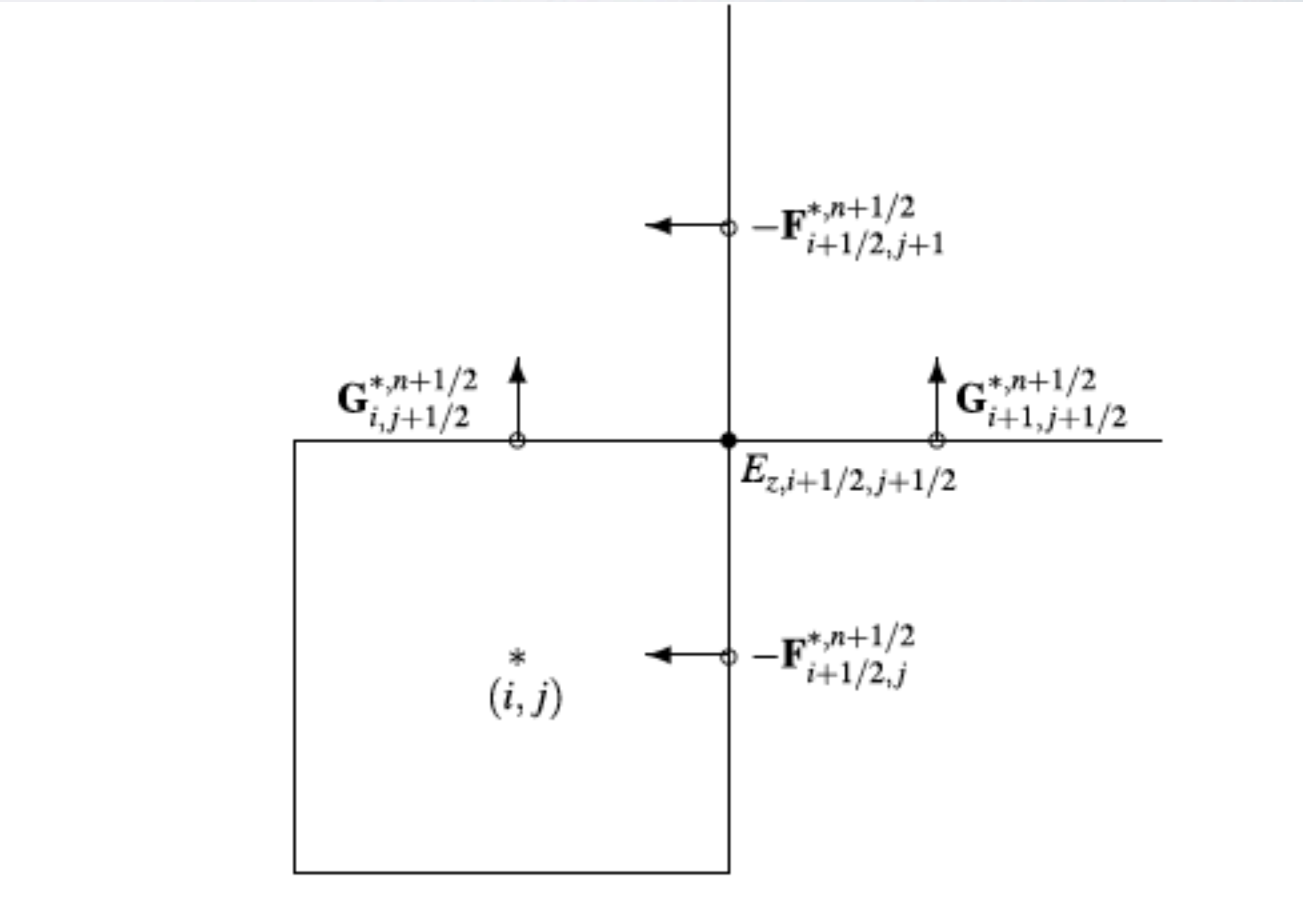
Solves induction equations on staggered grid



Constrained Transport (CT) MHD

Solves induction equations on staggered grid

Divergence of magnetic fields ~ machine accuracy



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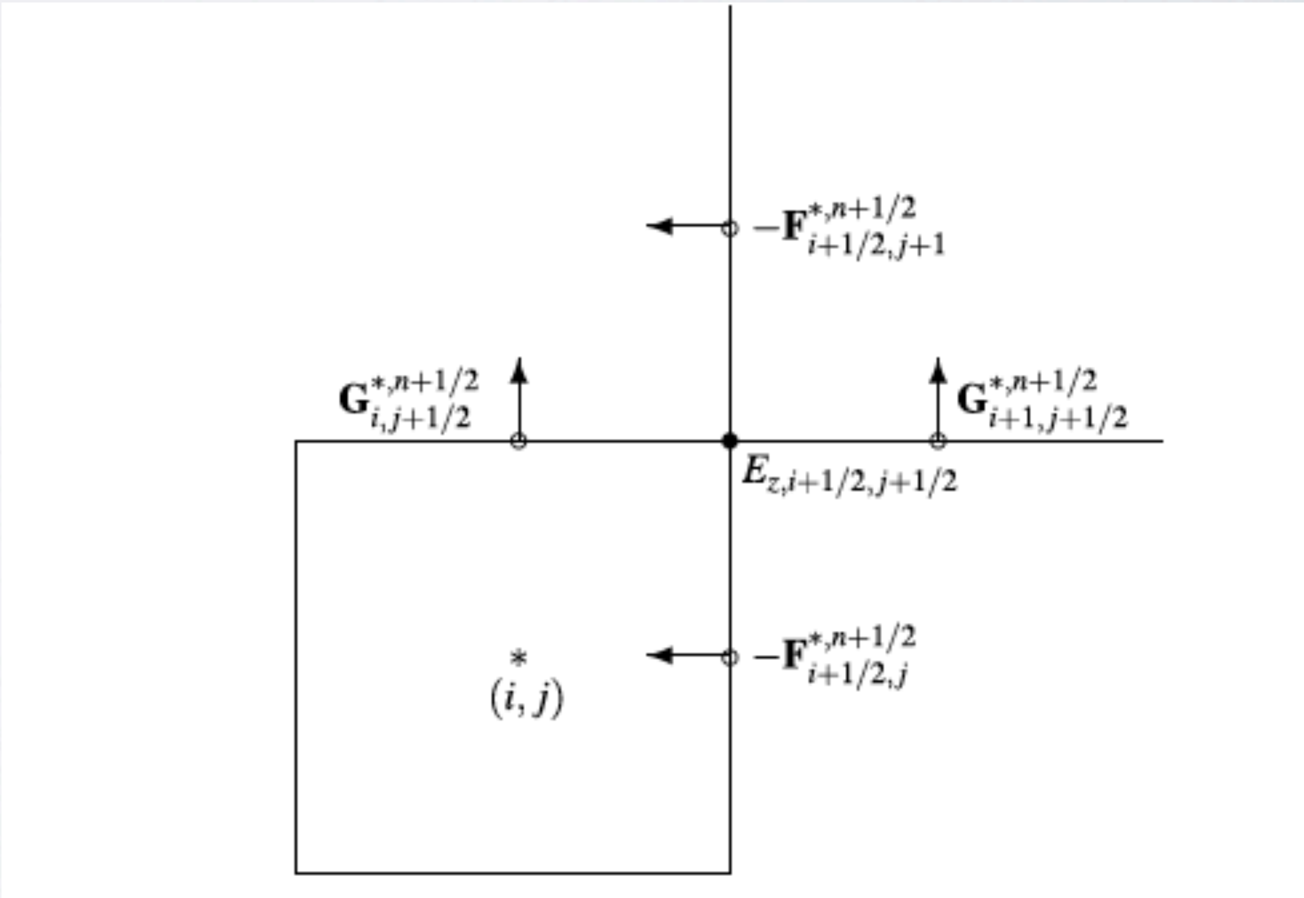
Divergence of magnetic fields ~ machine accuracy

Finite volume Godunov algorithms gives electric fields at face centers



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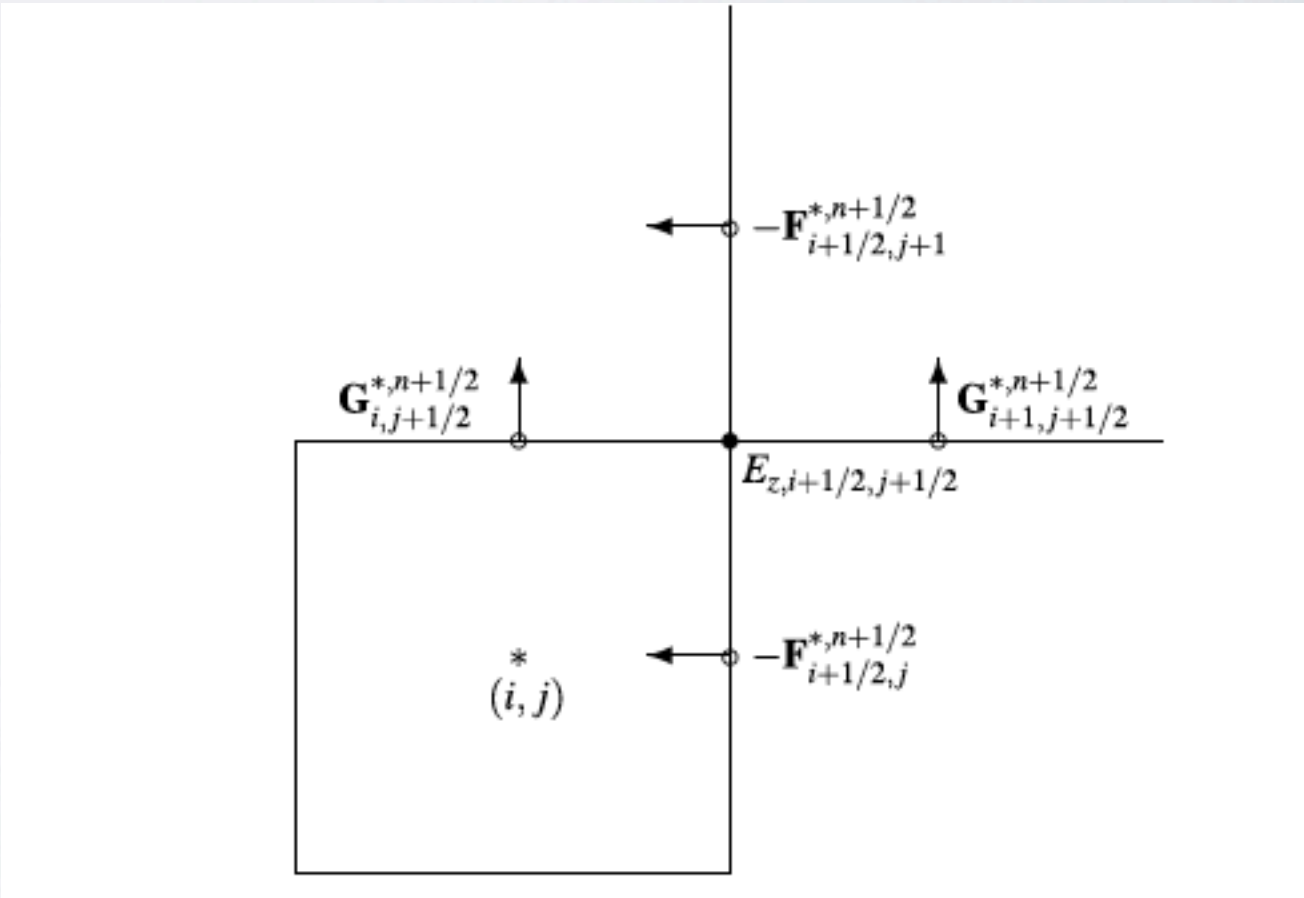
2. plane-parallel, grid-aligned reconstruction (Gardiner & Stone, 2005)
3. high-order interpolation (Lee & Deane, 2009)



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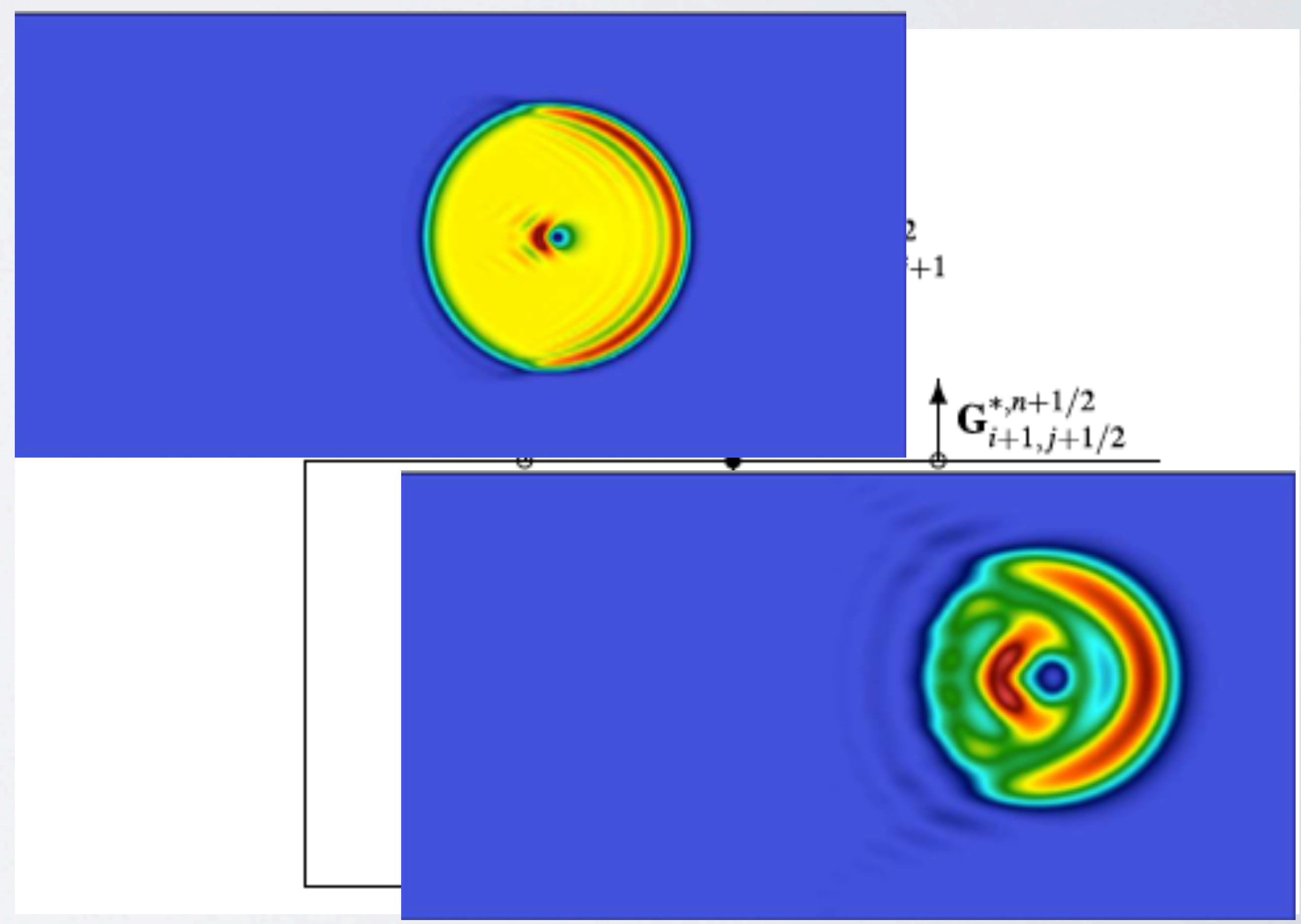

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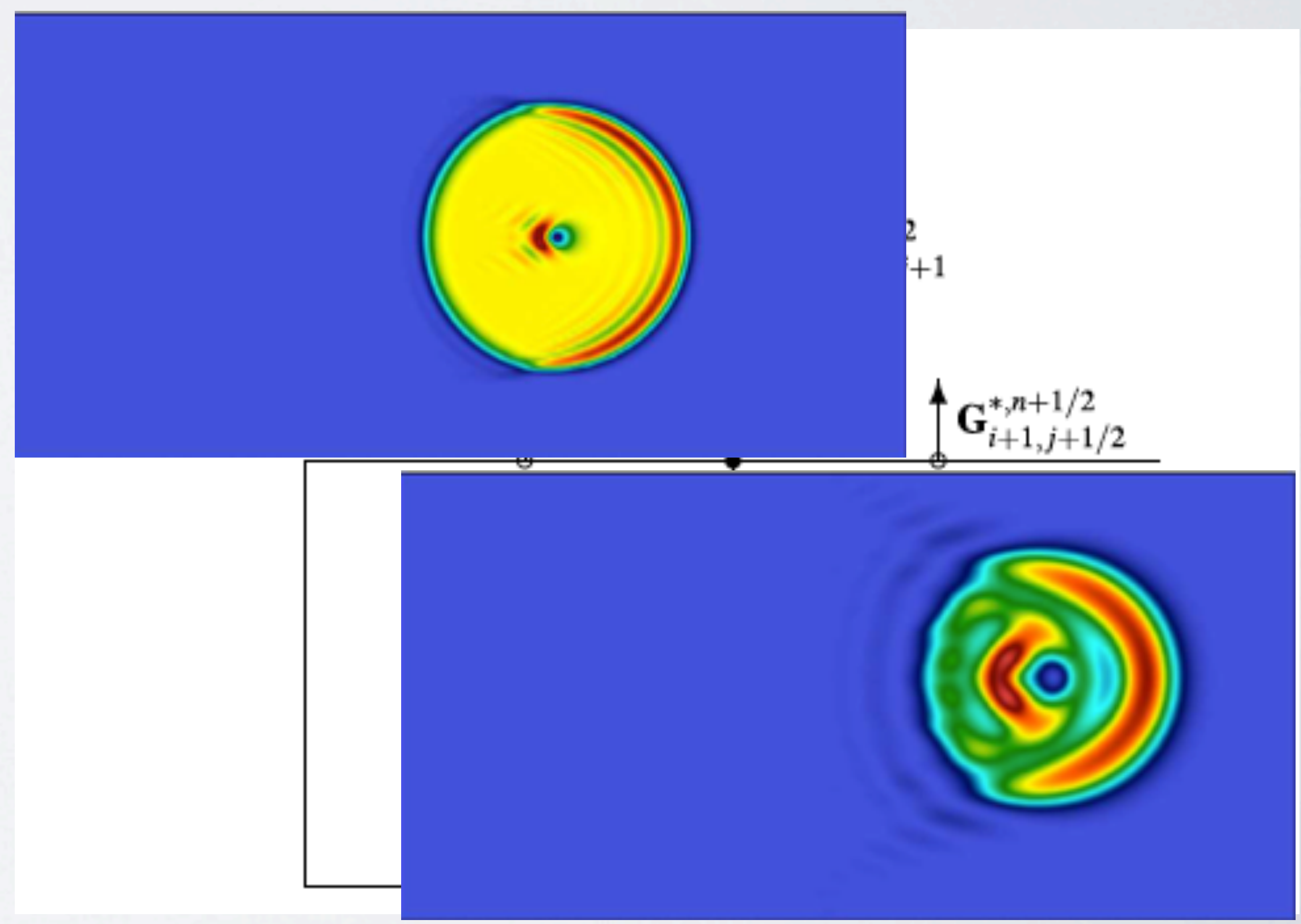
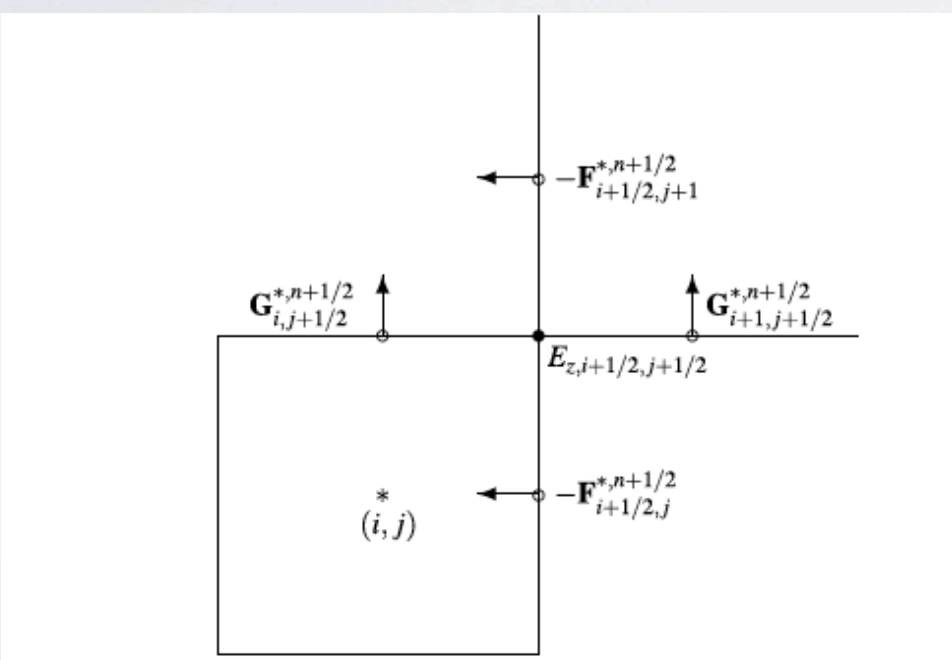


Arithmetic averaging by Balsara & Spicer

$$E^{n+1/2}_{z,i+1/2,j+1/2,k} = \frac{1}{4}(E^{*,n+1/2}_{z,i+1/2,j,k} + E^{*,n+1/2}_{z,i+1/2,j+1,k} + E^{*,n+1/2}_{z,i,j+1/2,k} + E^{*,n+1/2}_{z,i+1,j+1/2,k})$$



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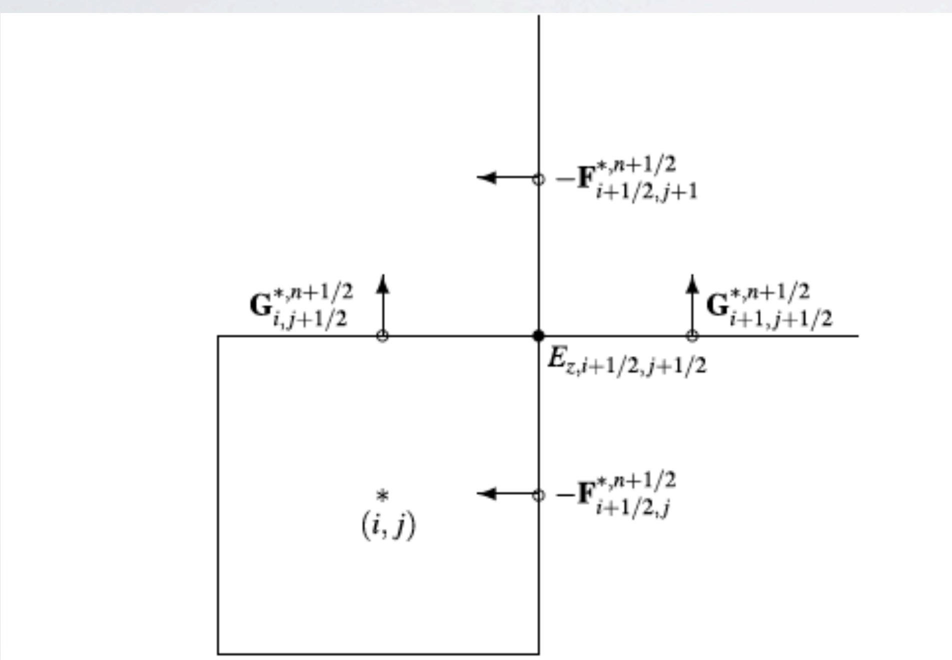
Consider u>0; v→0



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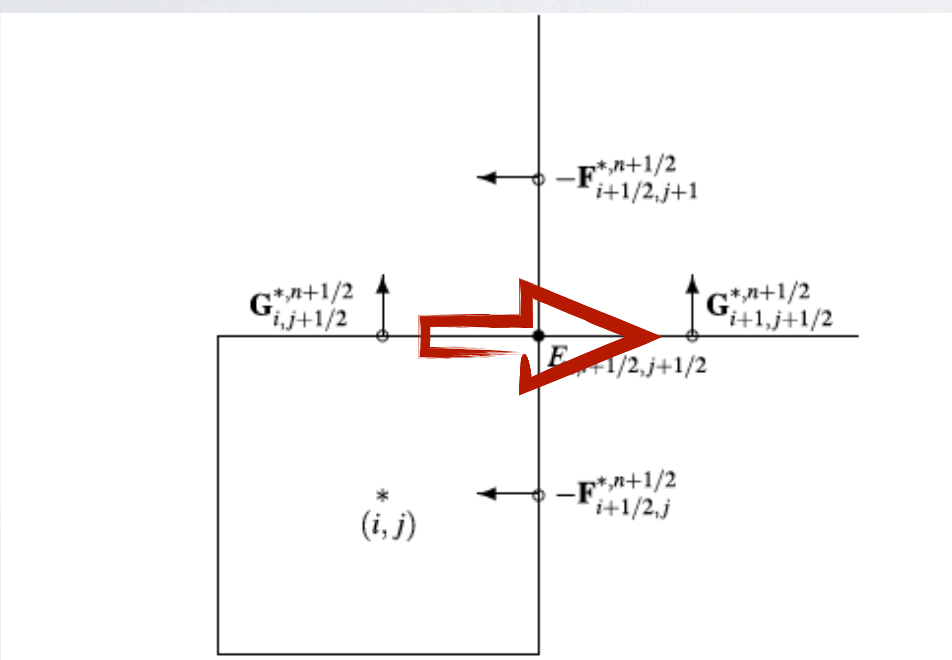

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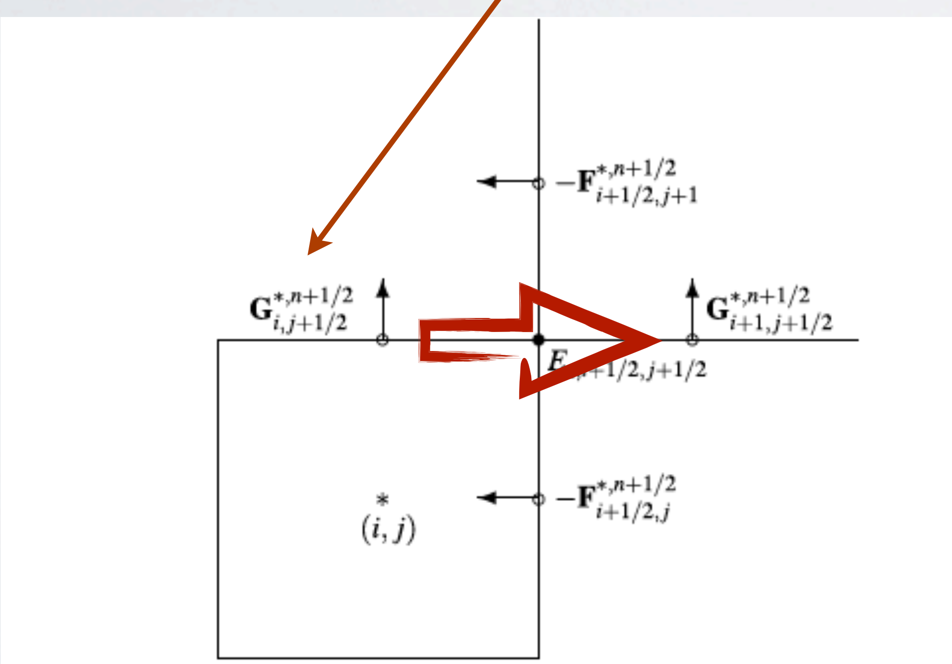


Arithmetic averaging by Balsara & Spicer

$$E^{n+1/2}_{z,i+1/2,j+1/2,k} = \frac{1}{4}\left(E^{*,n+1/2}_{z,i+1/2,j,k} + E^{*,n+1/2}_{z,i+1/2,j+1,k} + E^{*,n+1/2}_{z,i,j+1/2,k} + E^{*,n+1/2}_{z,i+1,j+1/2,k}\right)$$

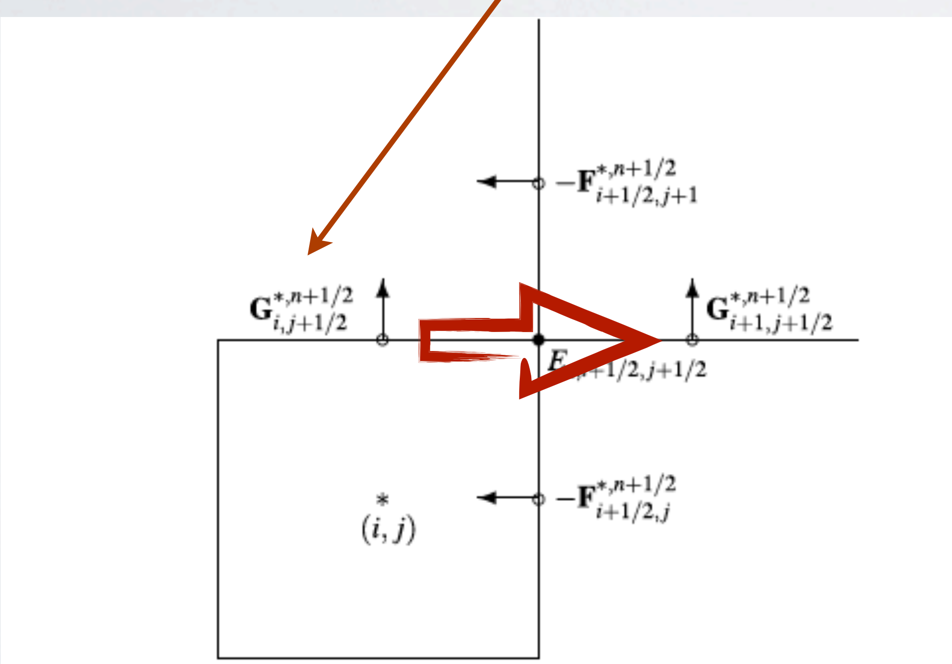
Consider u>0; v→0

Weakly magnetized field loop advection test

Gardiner & Stone (2005);

Lee & Deane (2009);

Lee (2012) for small angle advection



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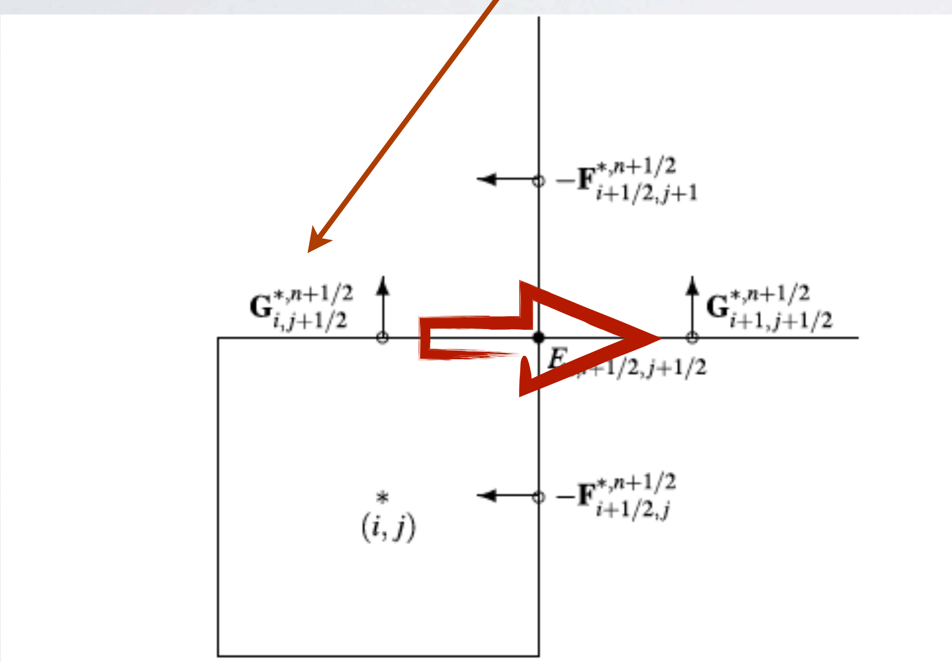
Consider u>0; v→0



DB: FL_mcBalsaraRoe_hdf5_chk_0000
Cycle: 1 Time:0

Weakly magnetized field loop advection test

Gardiner & Stone (2005);
Lee & Deane (2009);
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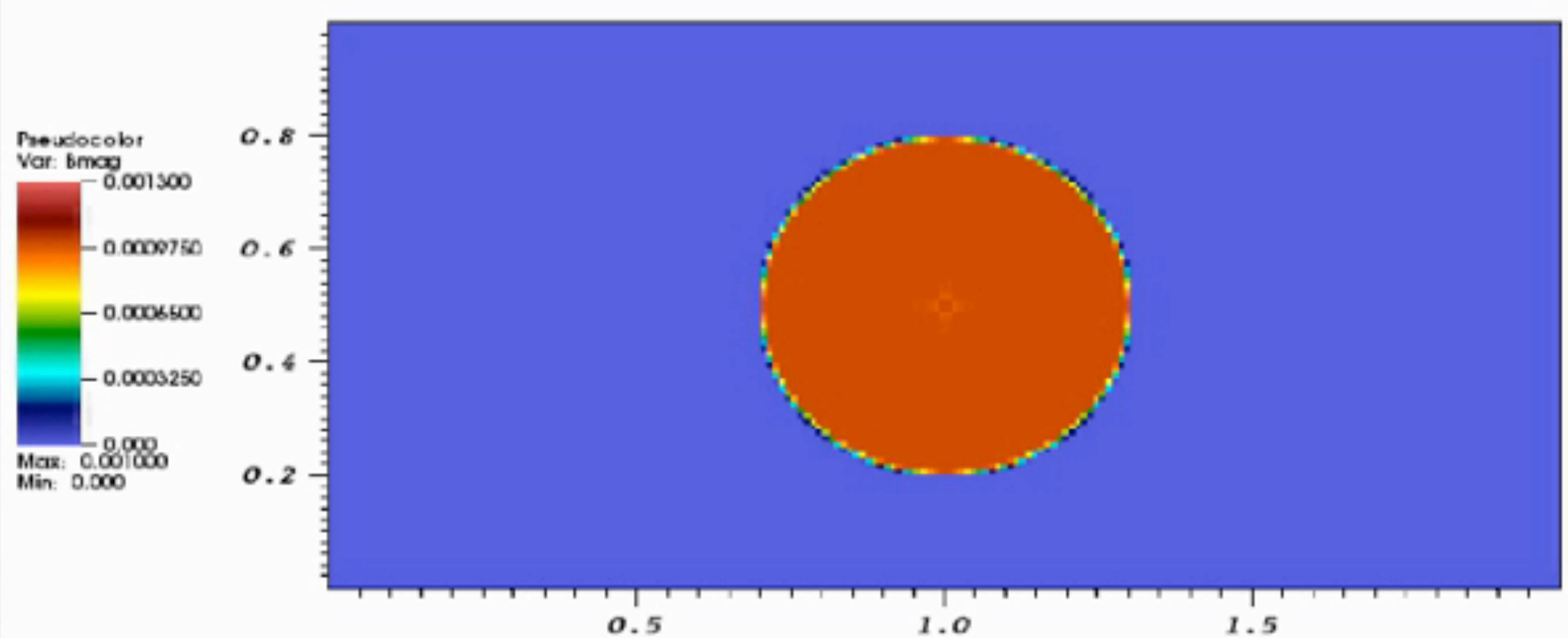
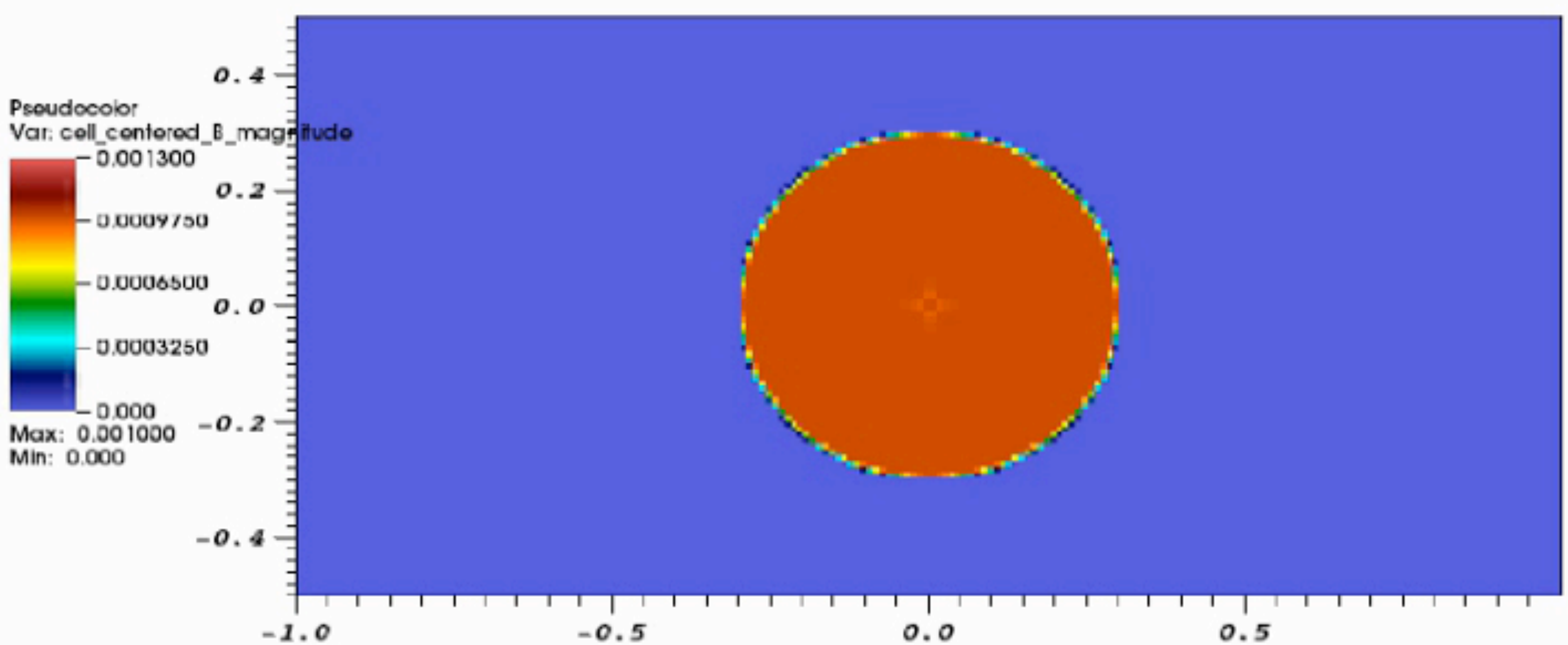


Lack of Upwinding

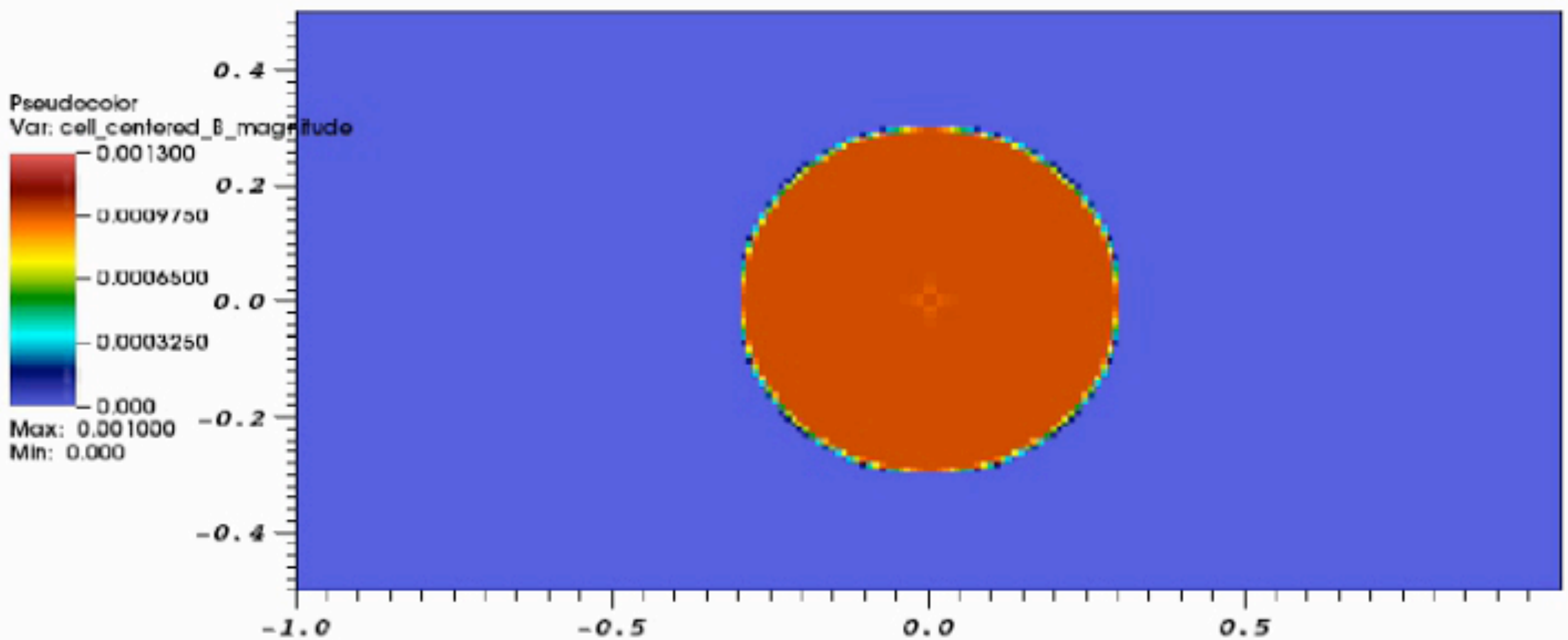
Gardiner & Stone (2005)



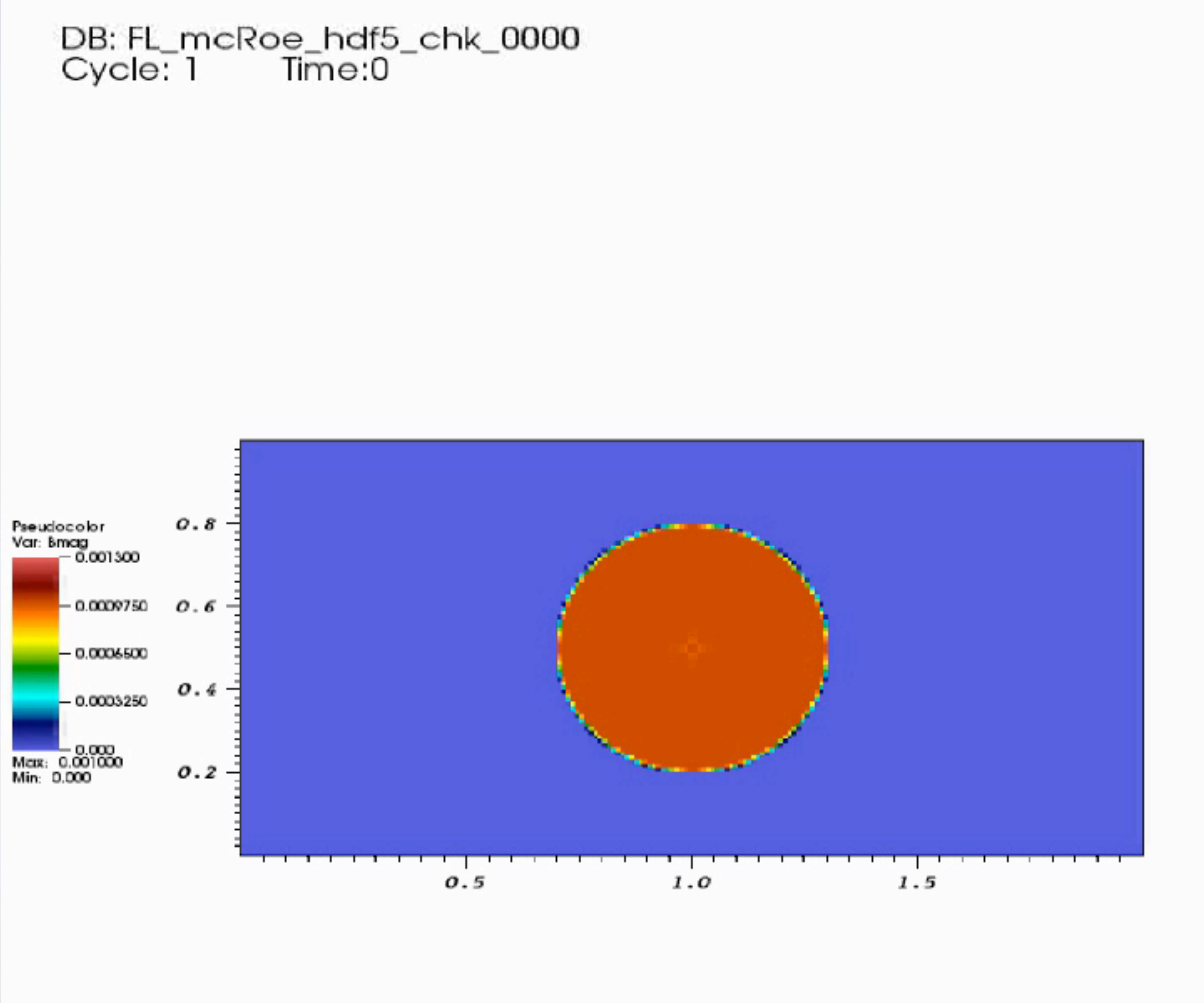
Lack of Upwinding

Gardiner & Stone (2005)

Similar oscillations in Lee & Deane (2009)



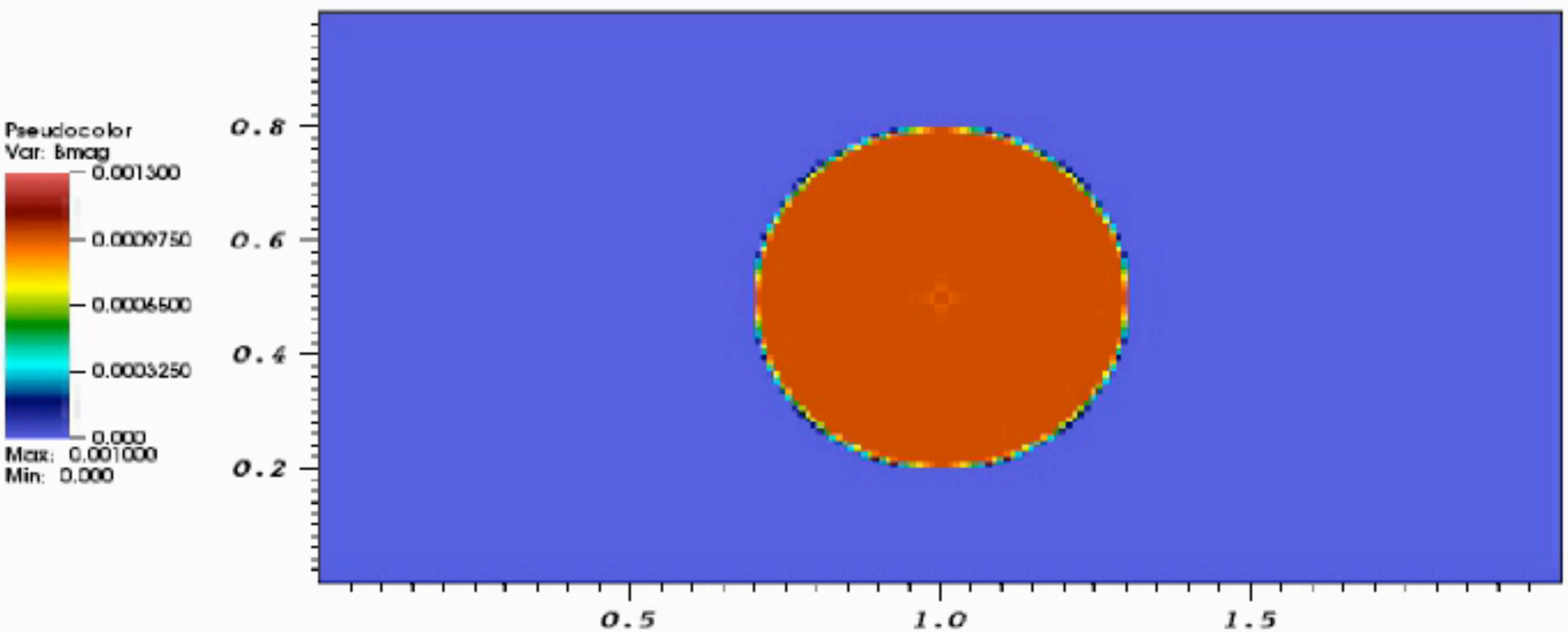
Improved Upwind CT



Improved Upwind CT

DB: FL_mcRoe_hdf5_chk_0000
Cycle: 1 Time:0

Upwind-biased scheme improves numerical stability in FL advection (Lee, 2012)



Improved Upwind CT

DB: FL_mcRoe_hdf5_chk_0000
Cycle: 1 Time:0

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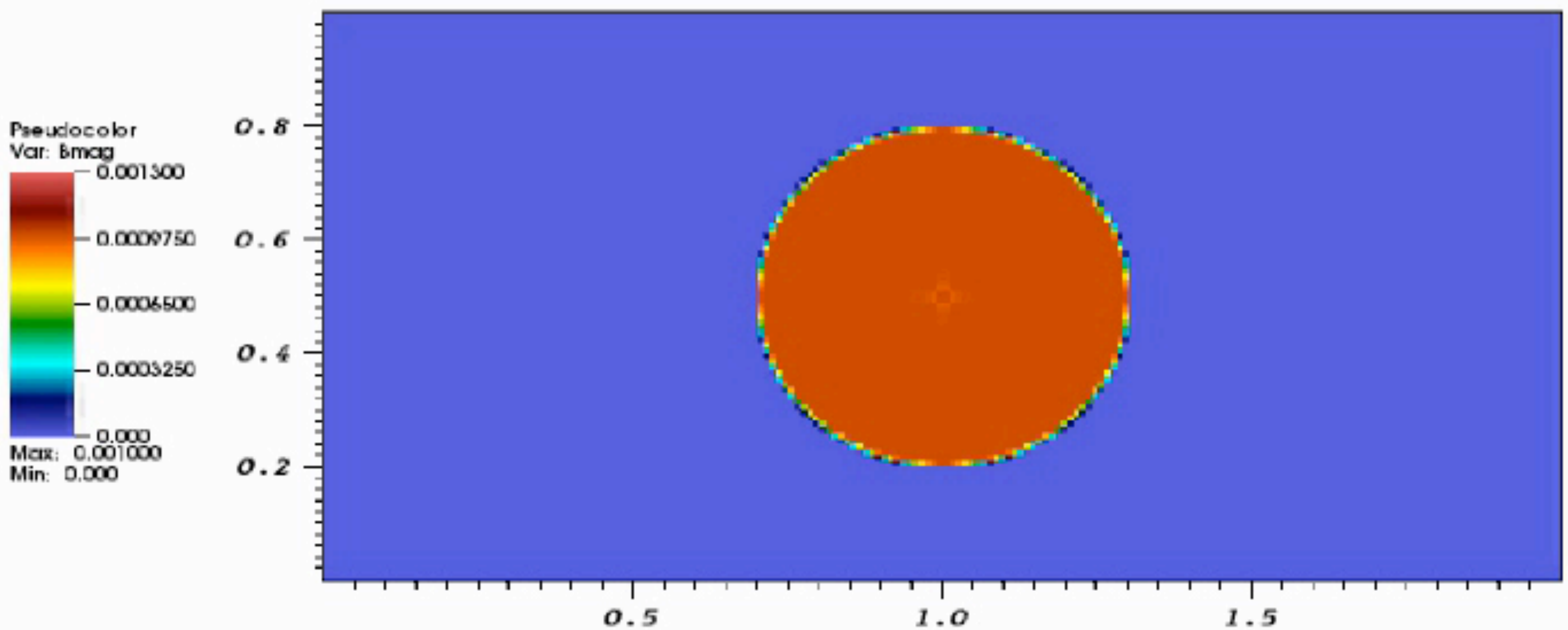
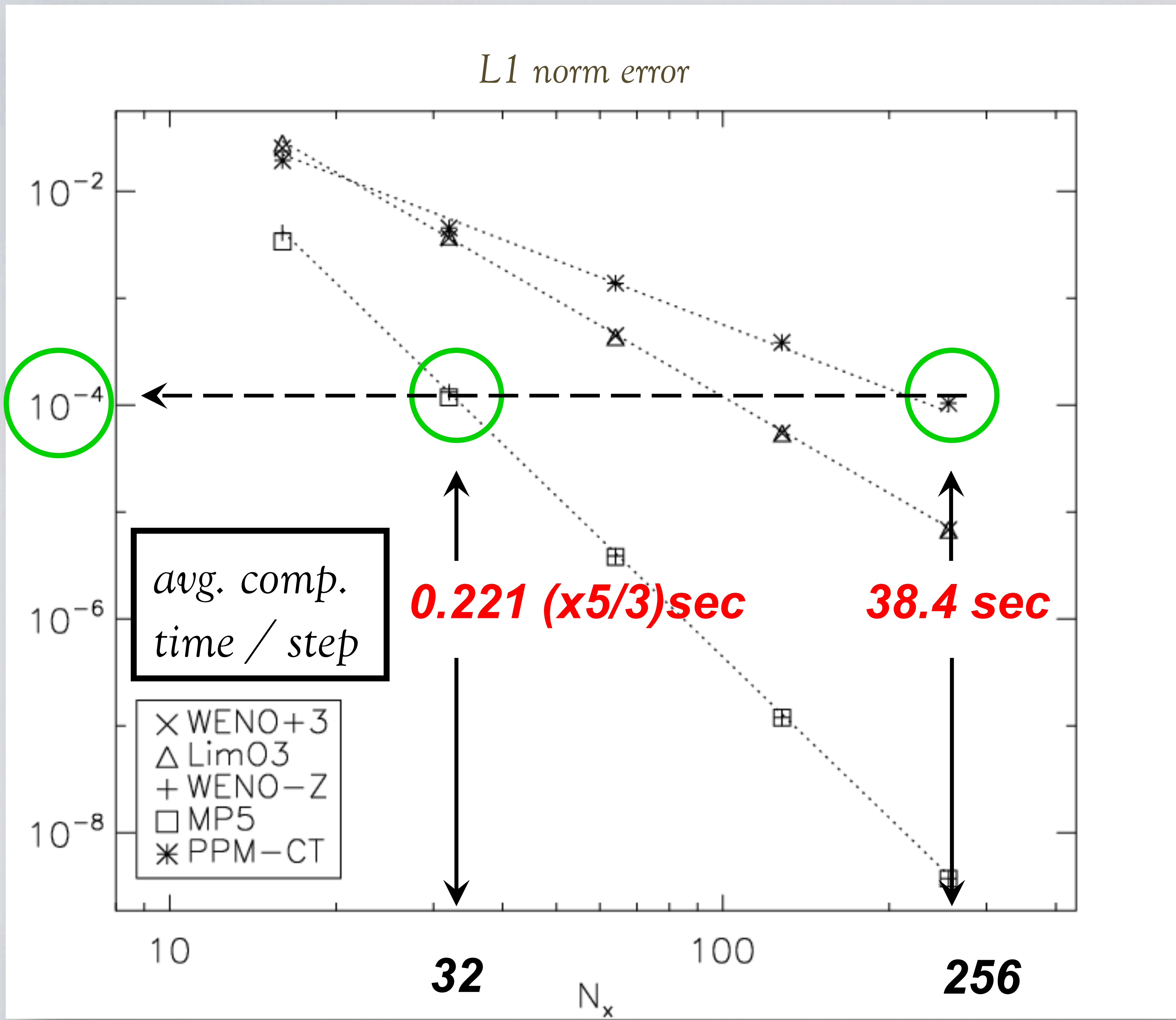
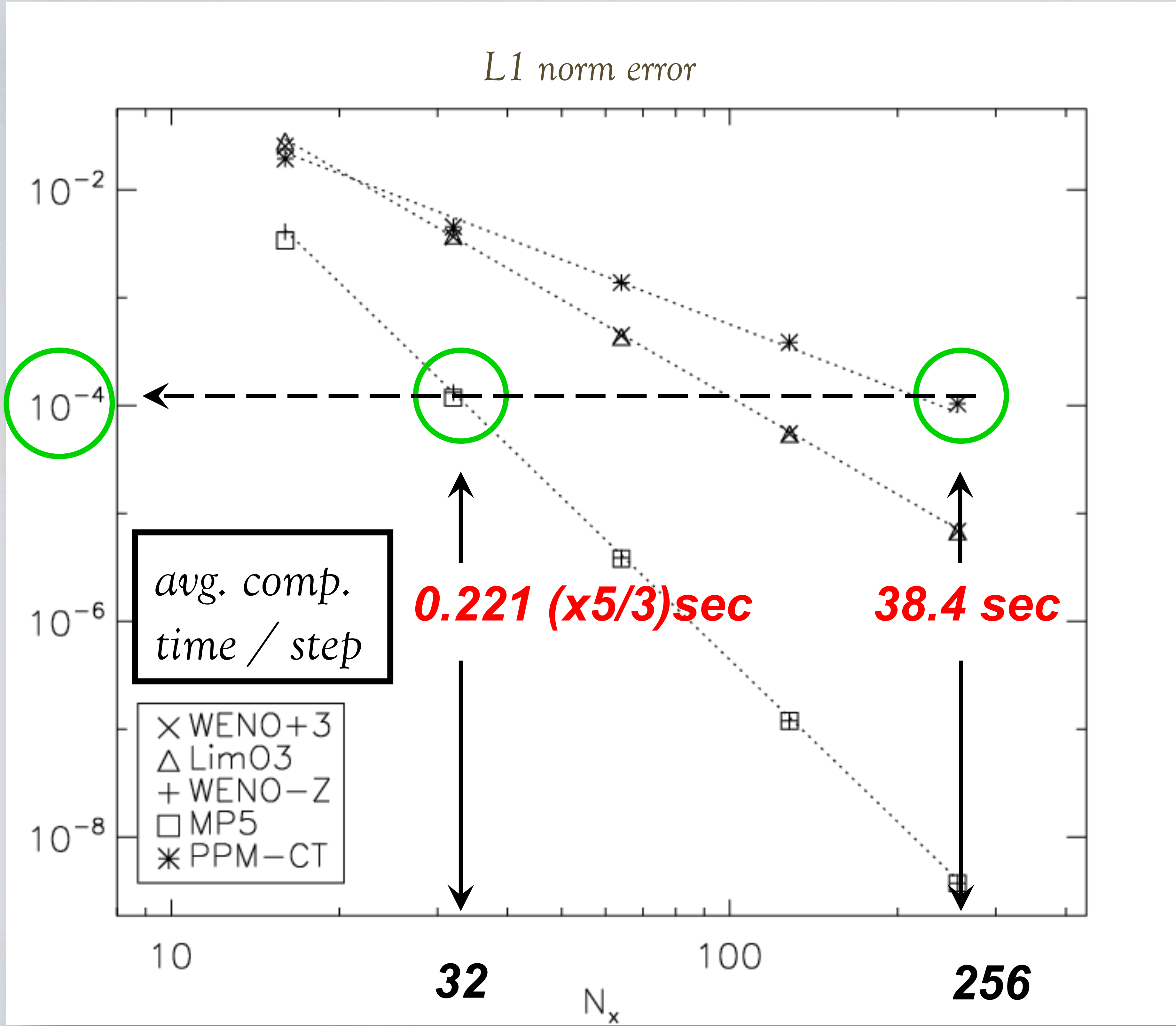


High-Order methods



Source: Mignone & Tzeferacos (2010)

High-Order methods



Source: Mignone & Tzeferacos (2010)

High-order schemes provides high-order convergence

They are extremely cost effective than increasing resolutions in smooth flows

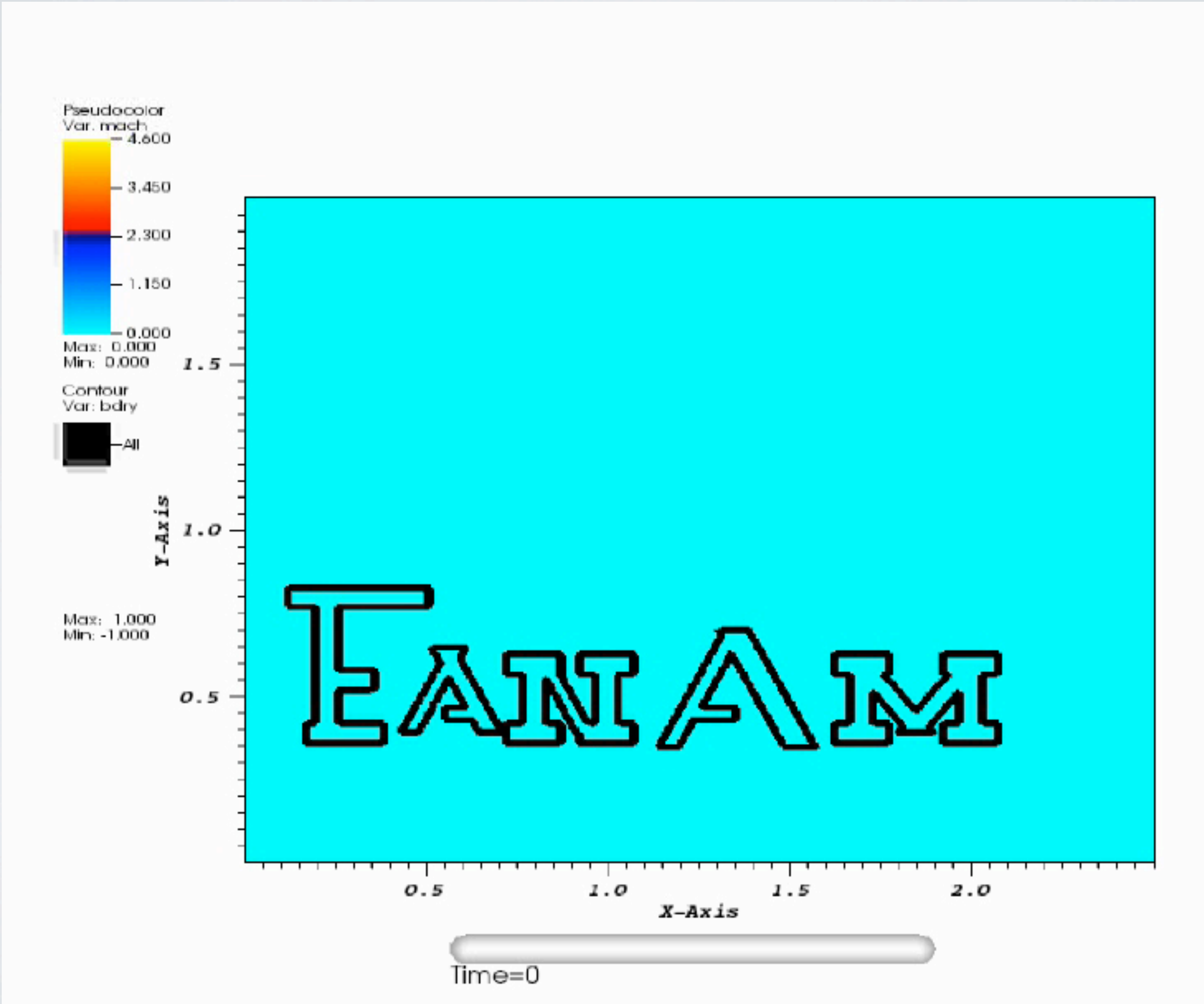
High-orders schemes are better in preserving solution accuracy on AMR

More computational work is needed

Numerics are mostly 1st order near shocks

Care should be taken in choosing what you want to simulate

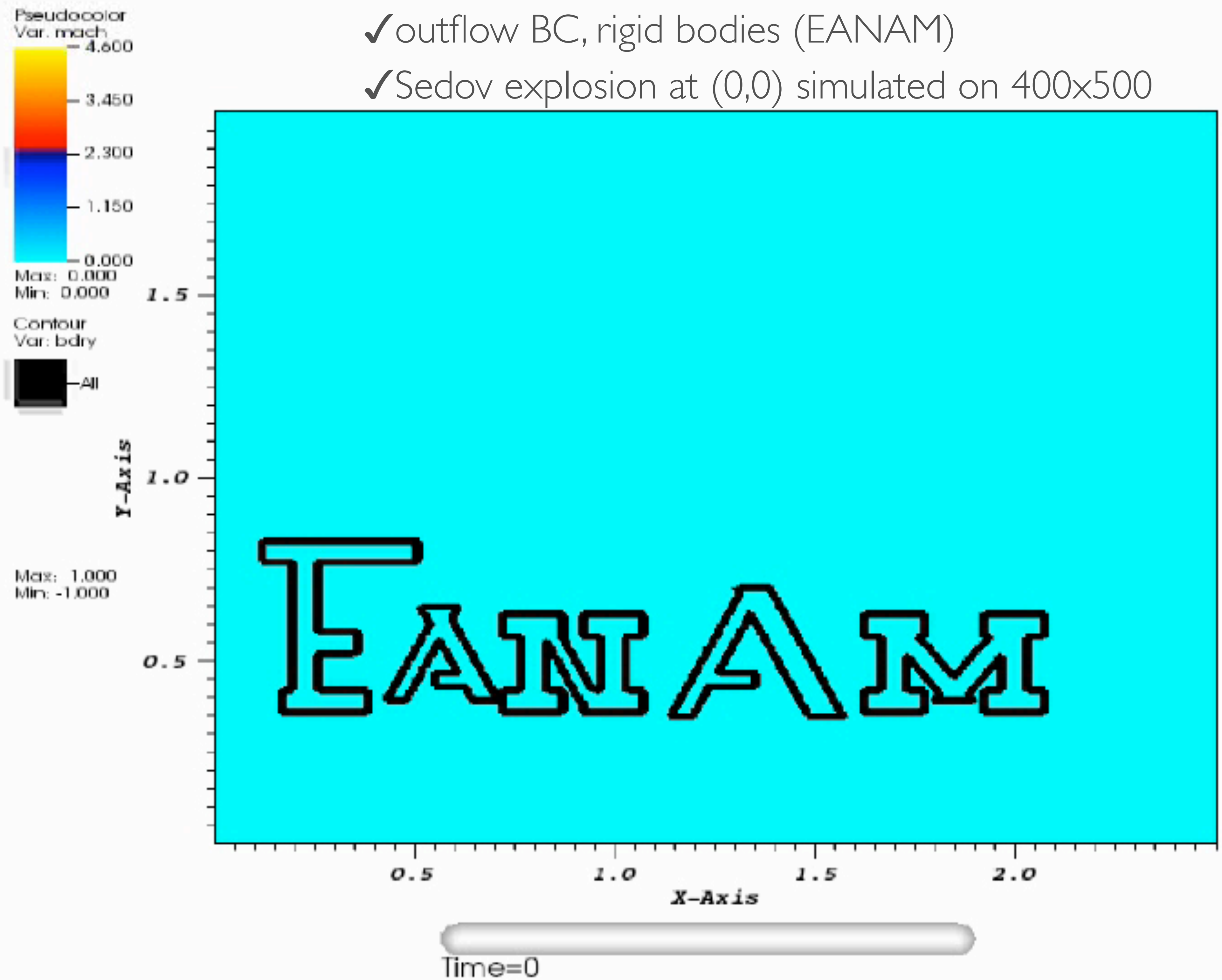
EANAM in Supersonic Turbulence!



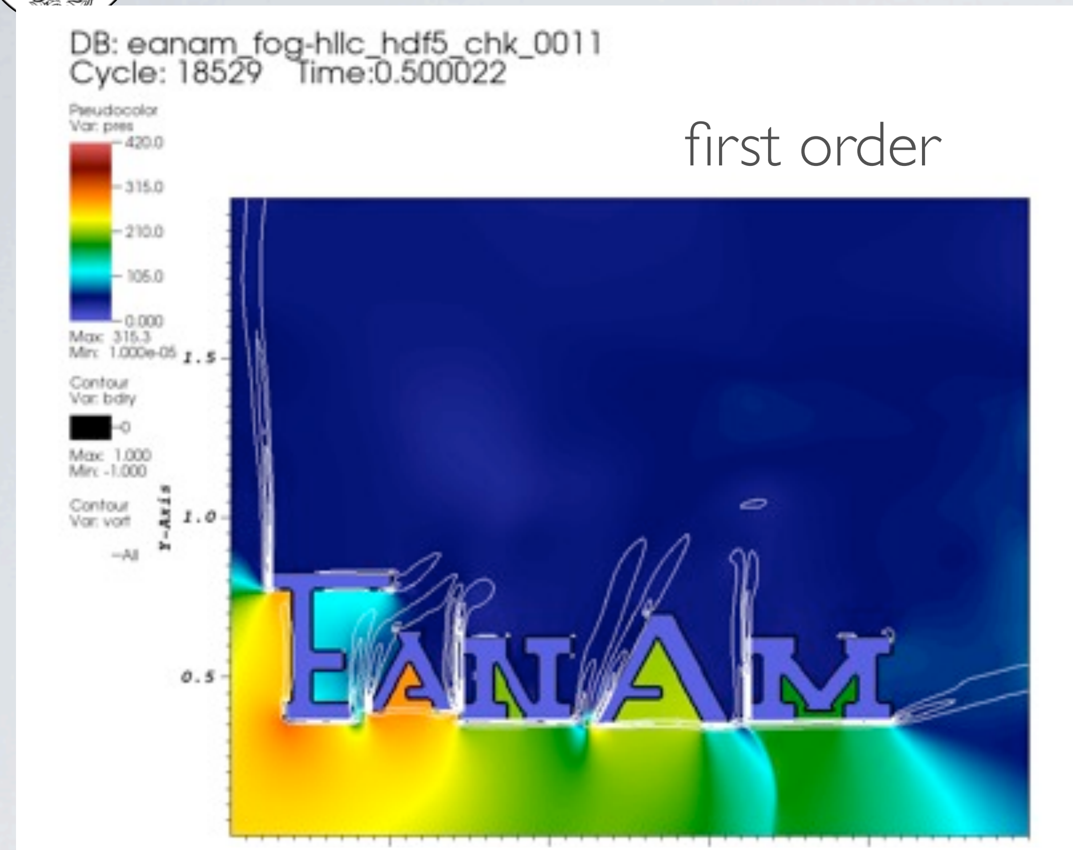
EANAM in Supersonic Turbulence!

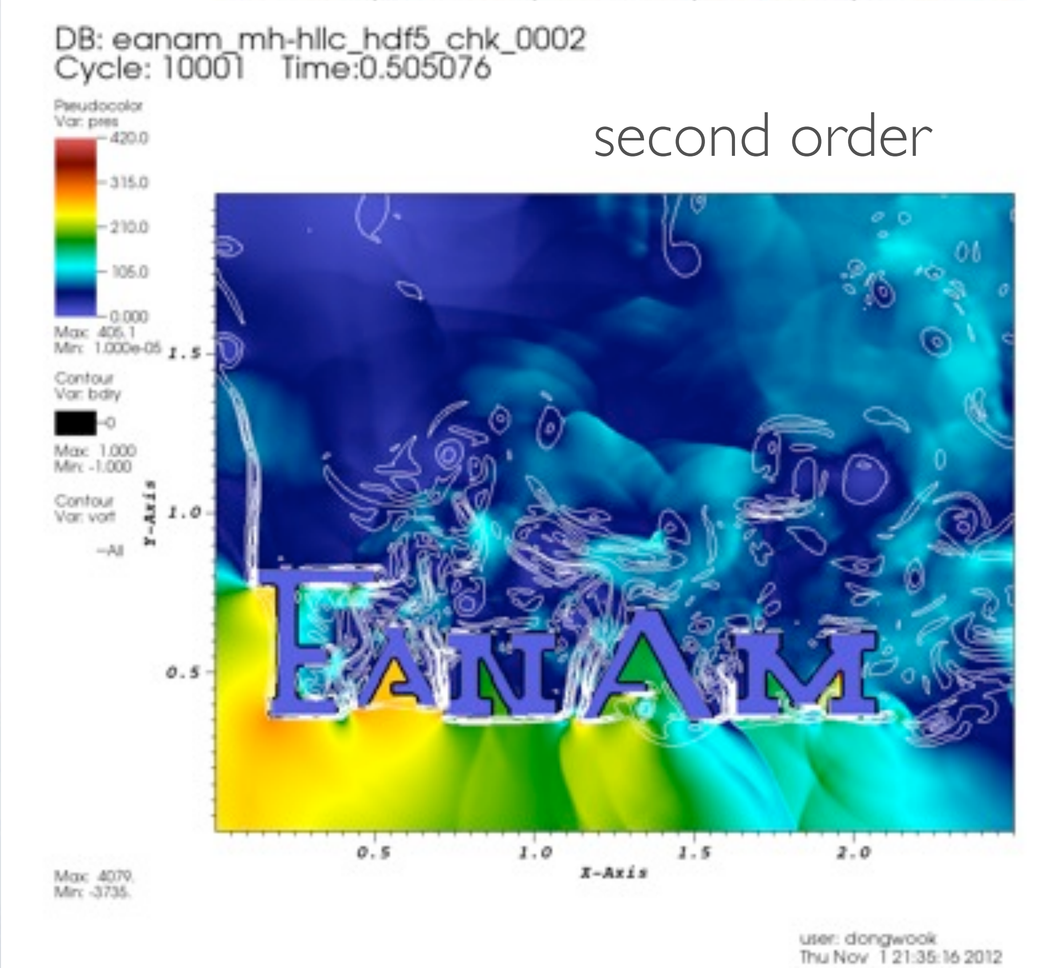
Unsplit hydrodynamics solver in FLASH using

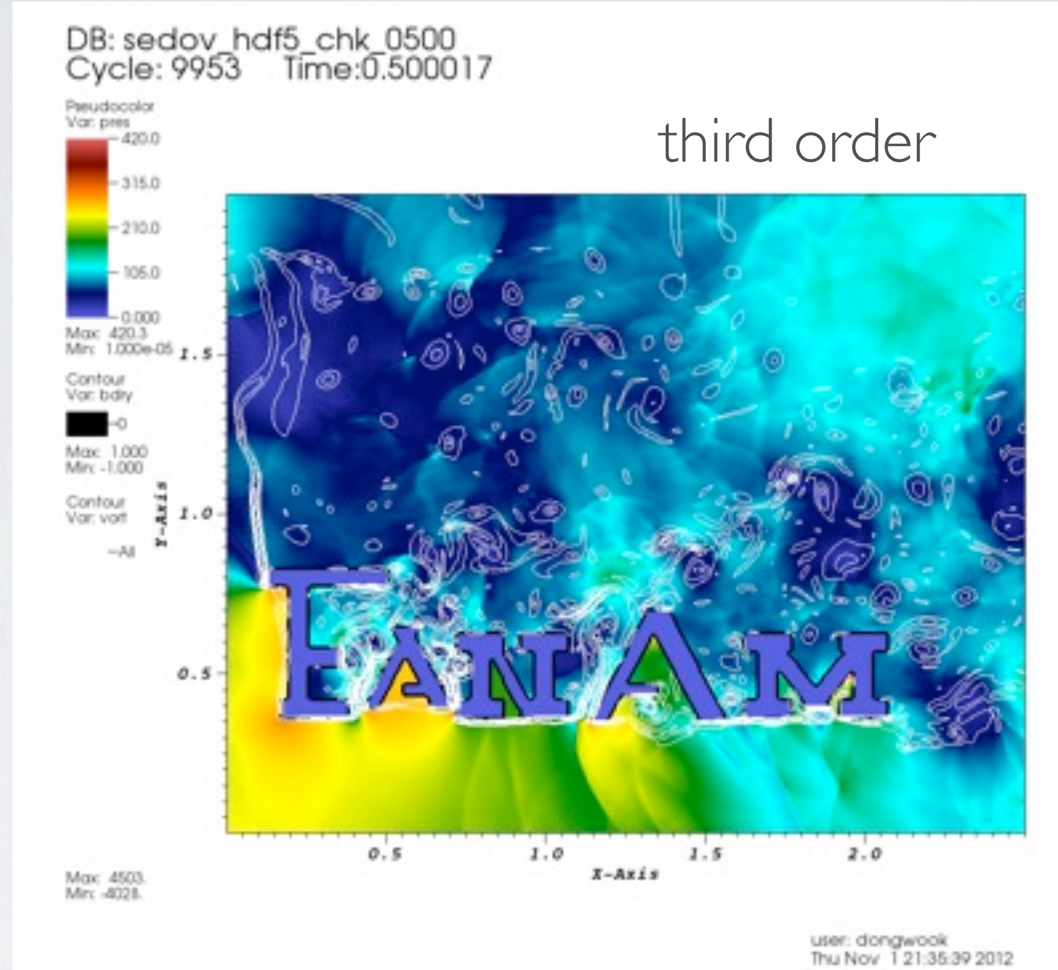
- ✓PPM, MC slope limiter, HLLC
- ✓outflow BC, rigid bodies (EANAM)
- ✓Sedov explosion at (0,0) simulated on 400x500



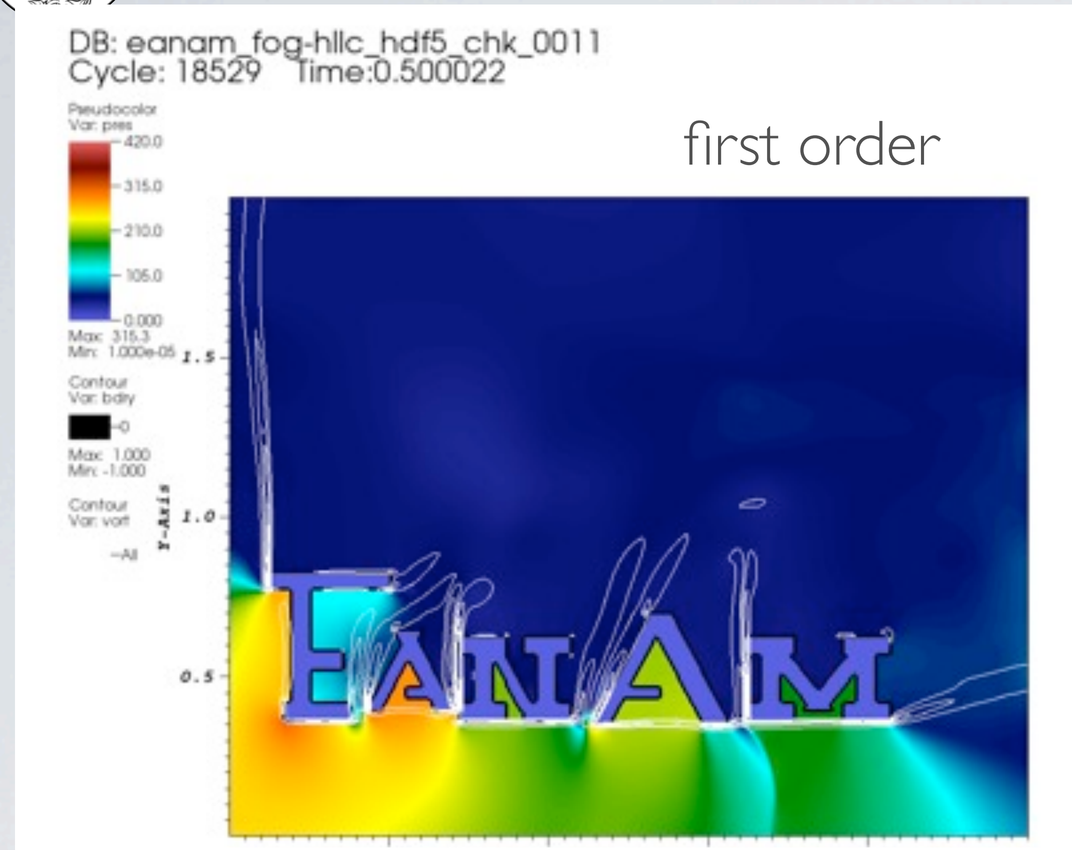
EANAM in Different Numerics

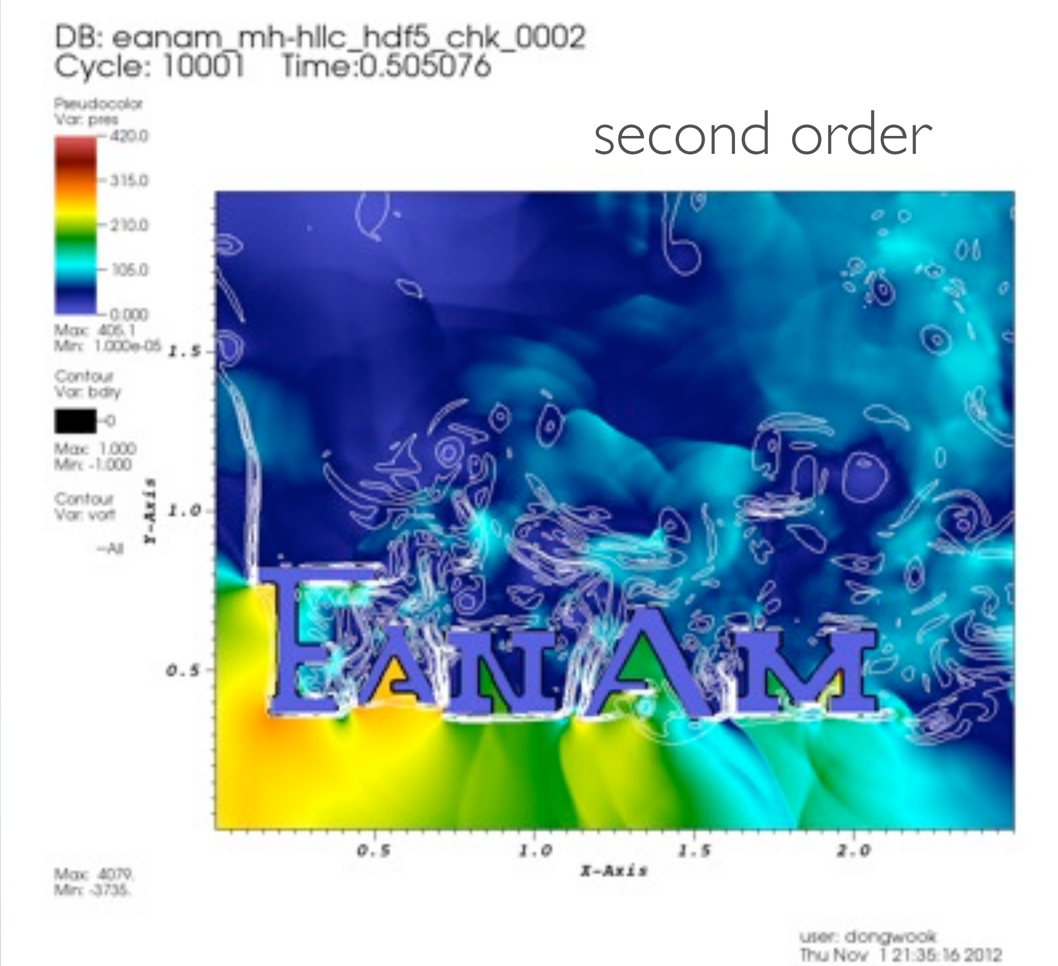


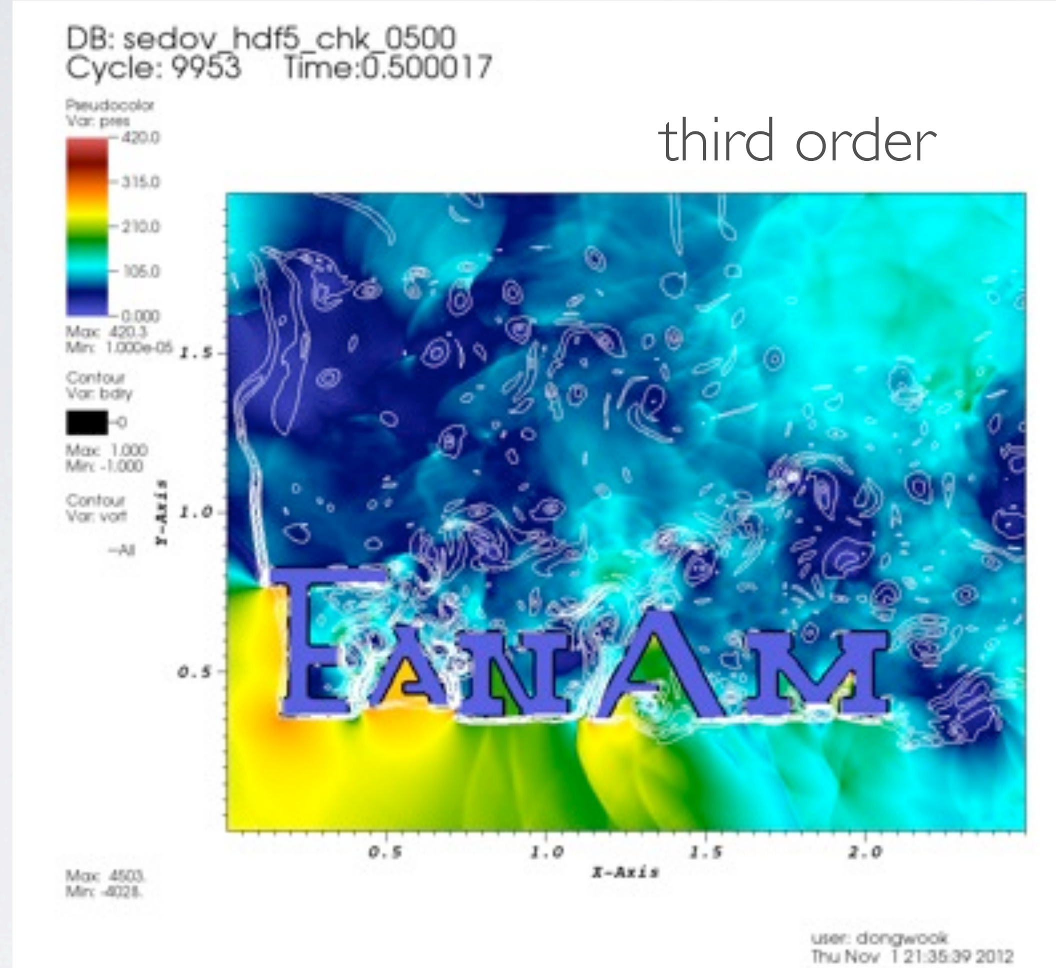




EANAM in Different Numerics







Small scales are more captured in higher order schemes

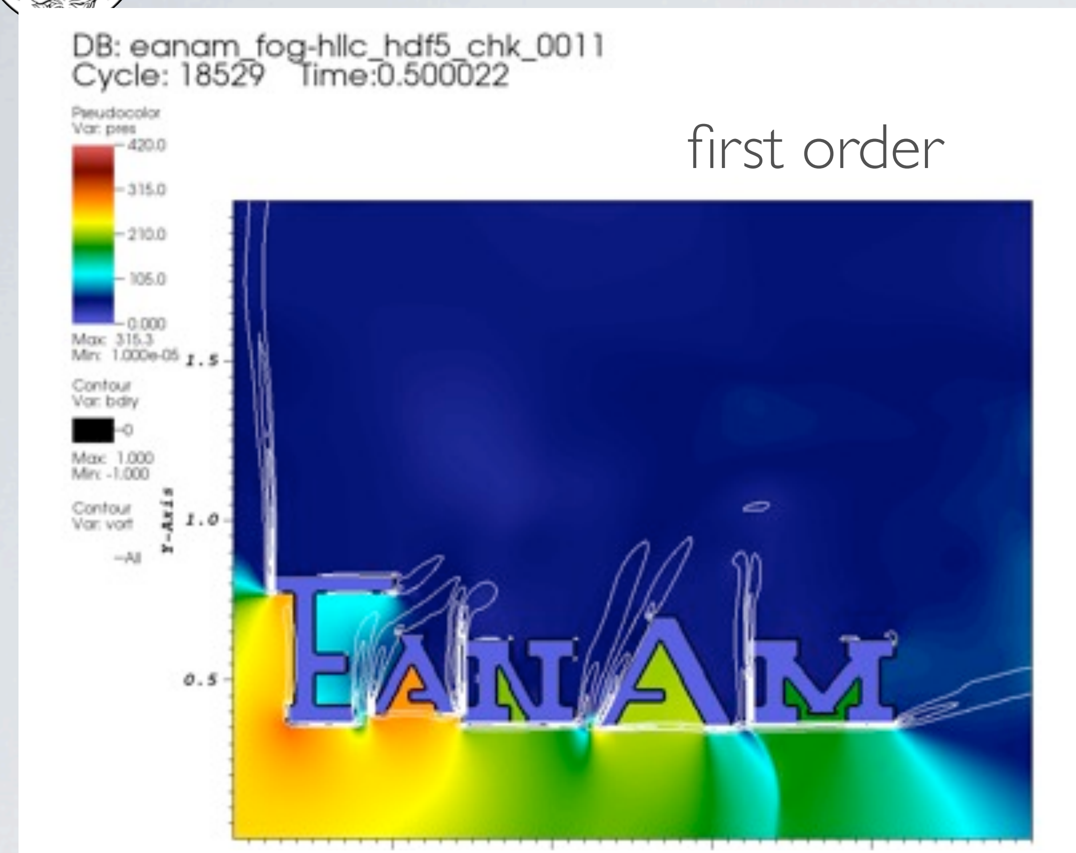
Shocks are resolved in fewer zones in higher order

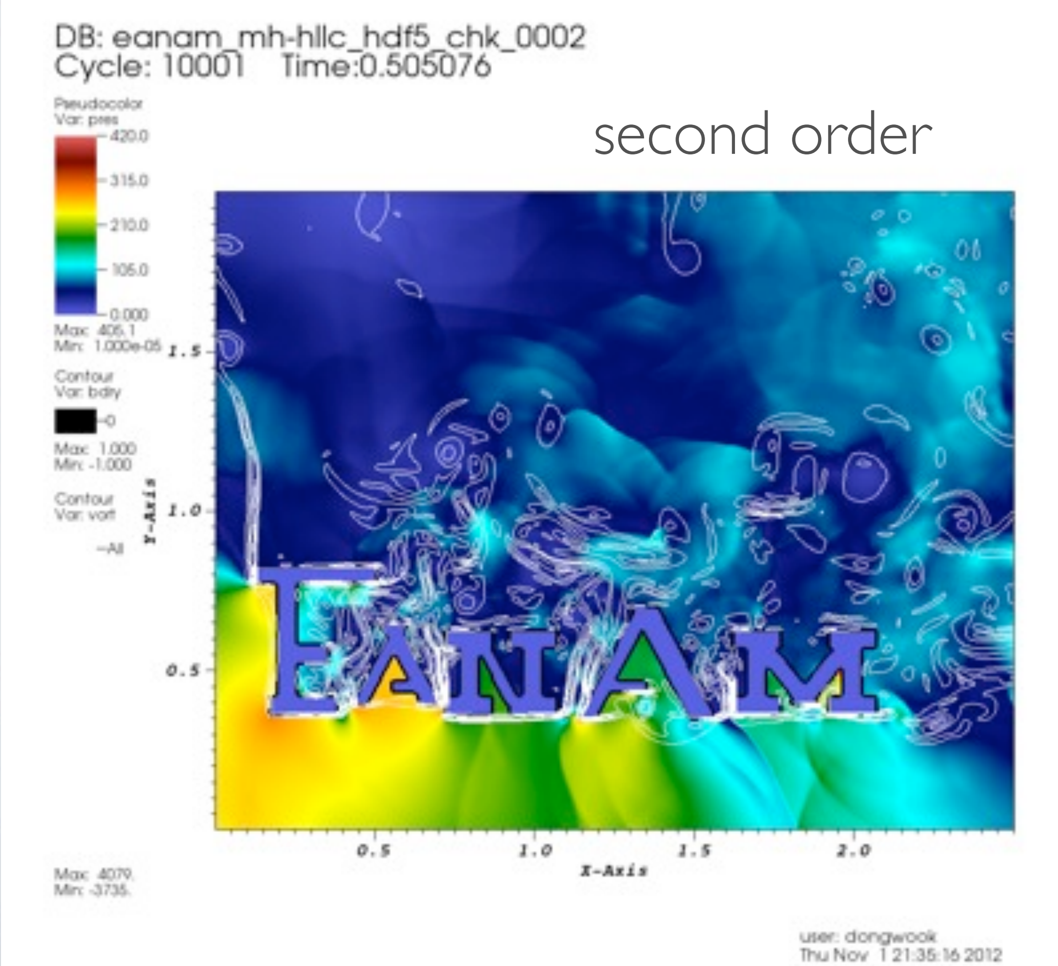
Numerical instability vs. accuracy

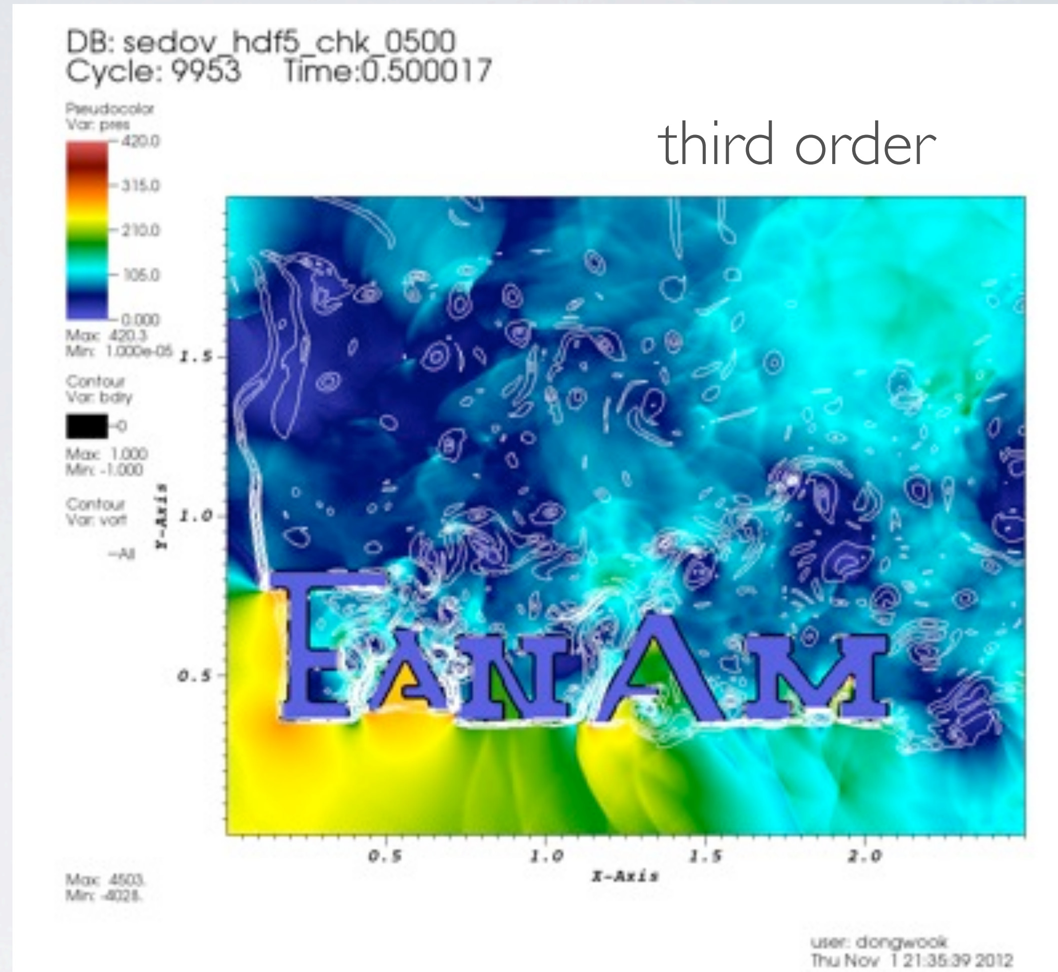
Need extensive studies on convergence, reproducibility, verification, validation, etc.

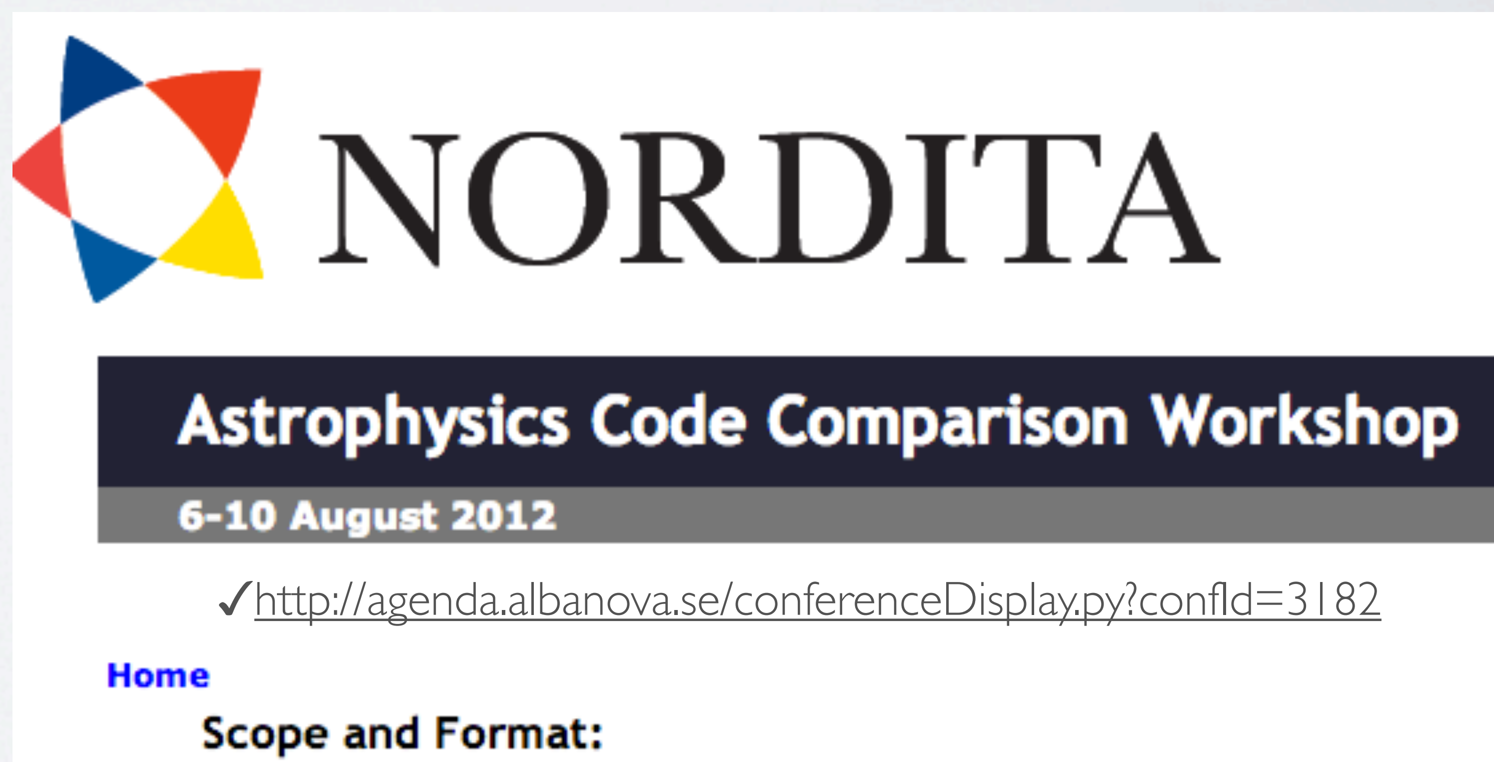
- ✓NORDITA Code Comparison Workshop
- ✓http://agenda.albanova.se/conferenceDisplay.py?confId=3182

EANAM in Different Numerics



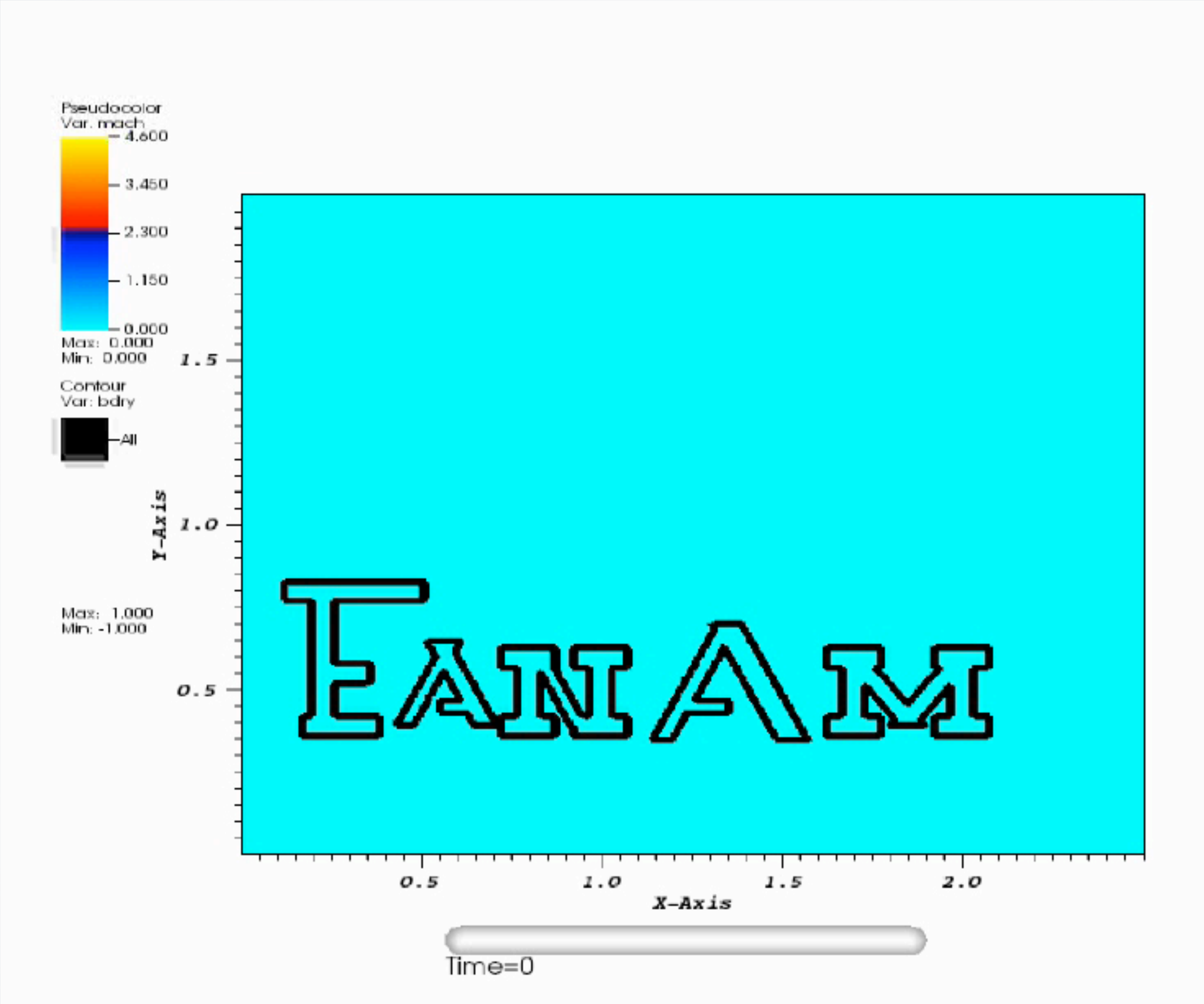






✓http://agenda.albanova.se/conferenceDisplay.py?confId=3182

Thank you



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2.300
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Max: 0.000
Min: 0.000
Contour
Var: bdry
All
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Min: -1.000
Y-Axis
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1.0
0.5
0.5
1.0
1.5
2.0
X-Axis
Time=0

Thank you