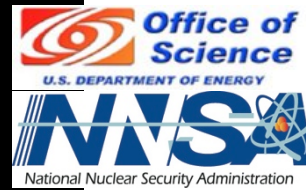




The Flash Center for Computational Science



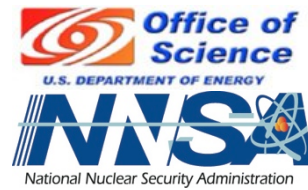
A New CT-MHD Algorithm in FLASH & FLASH's Applications to HEDP

ICM

Dongwook Lee
Flash Center for Computational Science,
The University of Chicago



Outline



□ *Part 1: Applications*

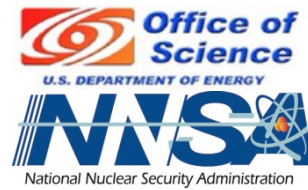
- Applications of new physics in FLASH
- High-Energy-Density Laboratory experiments: LULI/RAL
- FLASH code validation and predictive science

□ *Part 2: Algorithms*

- 3D Unsplit Staggered Mesh (USM) MHD Scheme
- A new upwind biased constrained-transport (CT) scheme (Lee, JCP, 2012, under review)
- Small angle weakly magnetized field loop advection tests



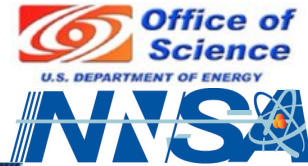
Part 1



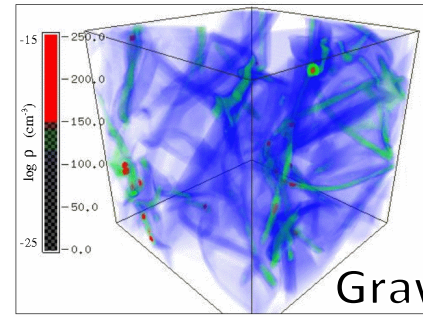
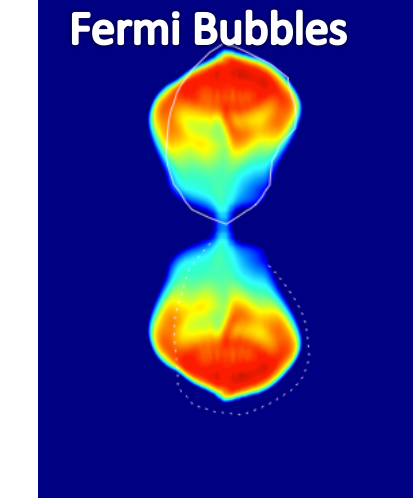
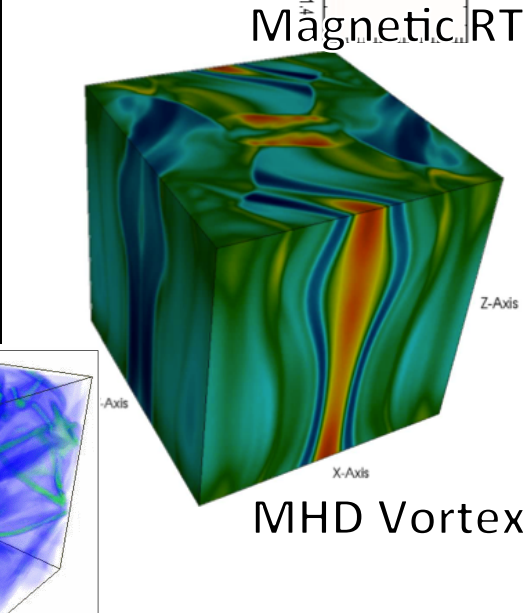
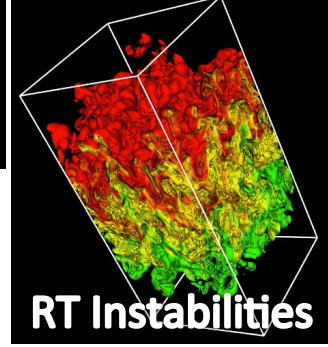
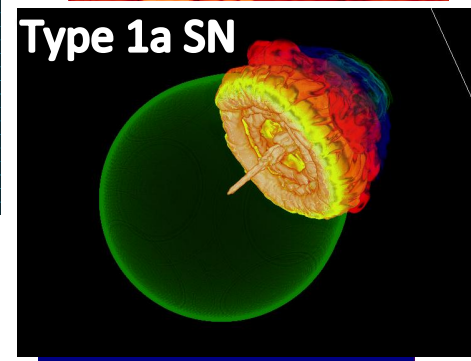
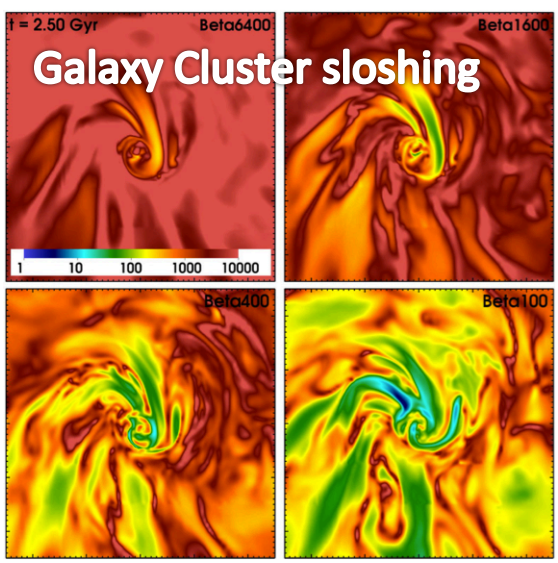
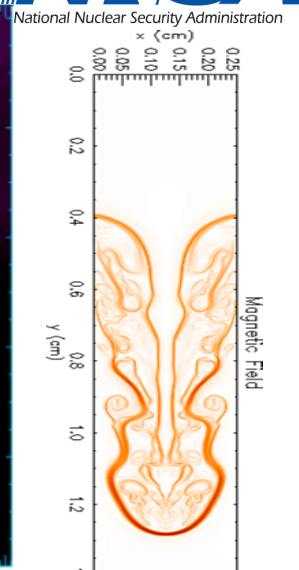
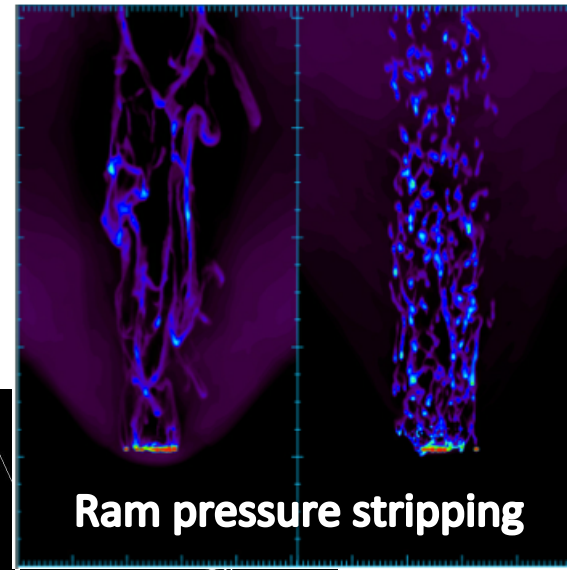
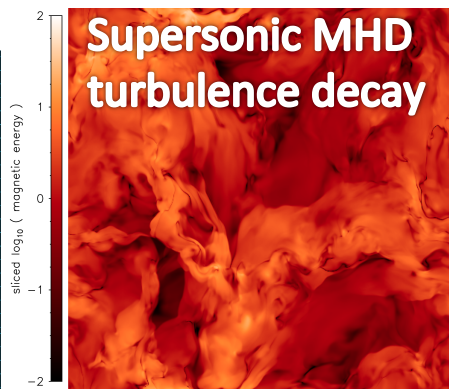
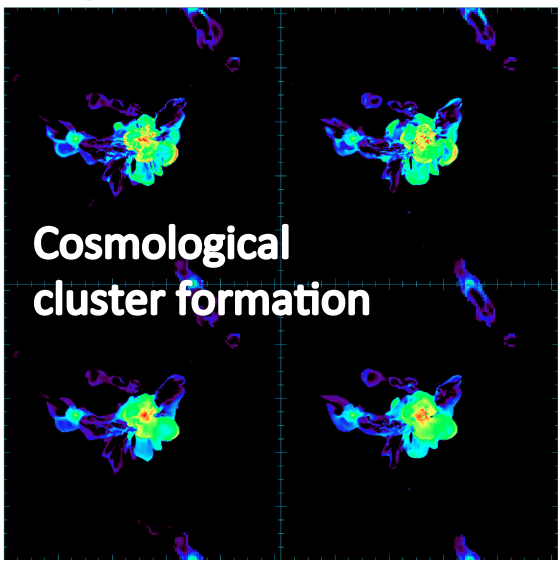
Applications: FLASH Simulations of Astrophysics & Validations of HEDP



Astrophysical Applications

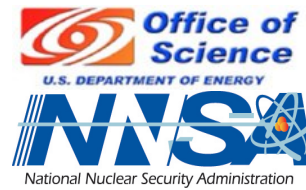


National Nuclear Security Administration





FLASH Basics



- An application code, composed of units/modules

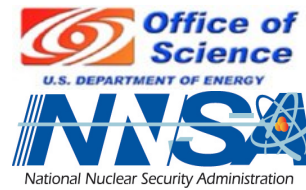
- Particular modules are set up together to run different physics problems
 - Astrophysics
 - High-energy-density physics
 - Incompressible Navier-Stokes (GWU)

- Fortran, C, Python, ...
 - More than 1.2 million lines of code, 75% code, 25% comments

- Very portable, scales to tens of thousand processors



FLASH Capabilities



Astrophysics

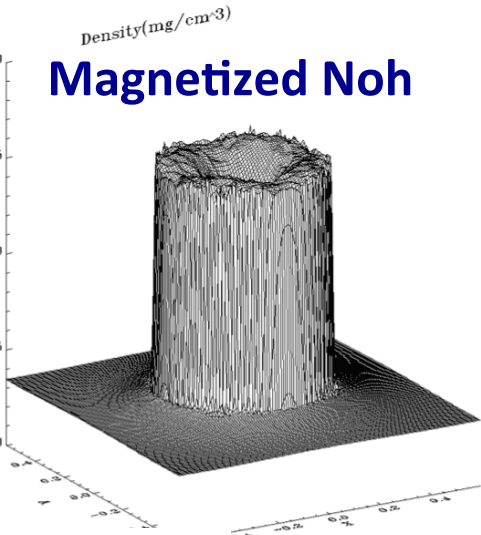
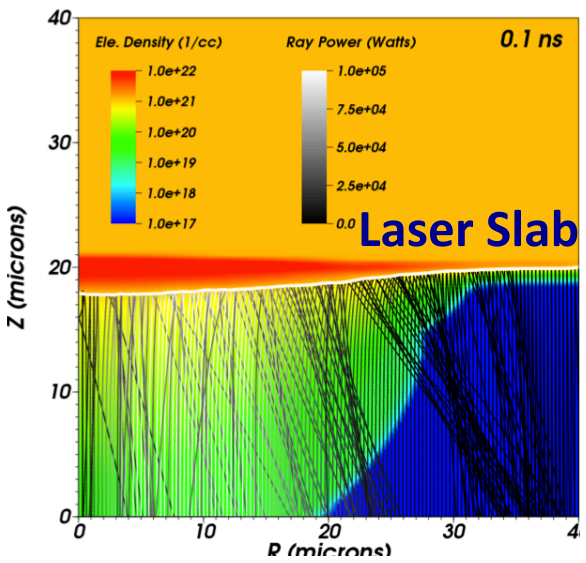
- ❑ Hydrodynamics, MHD, RHD, hybrid PIC
- ❑ Equation of States (Gamma laws, multigamma, Helmholtz)
- ❑ Nuclear Physics and other local source terms
- ❑ External gravity, Self-gravity
- ❑ Particles: active and passive
- ❑ Material Properties
- ❑ Cosmology

HEDP

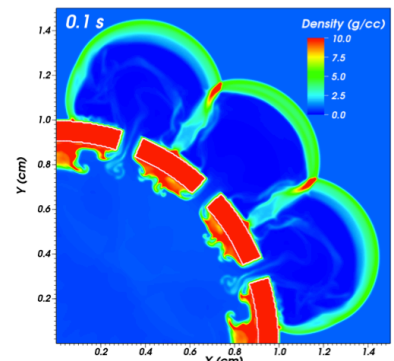
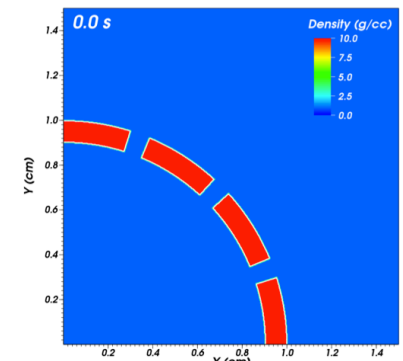
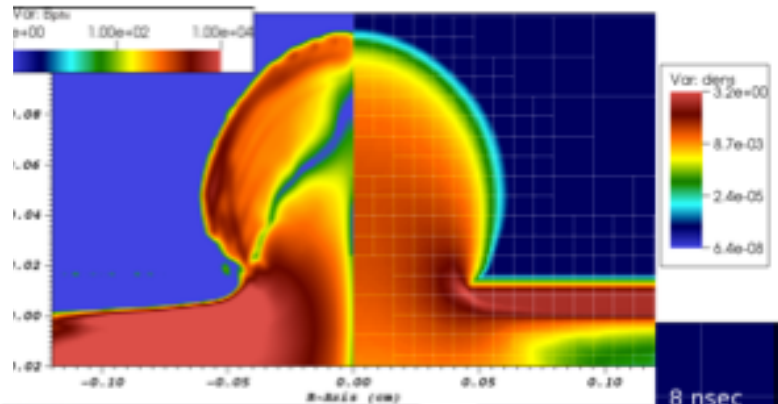
- ❑ Advancing 1T (single temperature), 2T (distinct ion + electron), and 3T (ion+ electron + radiation temperatures) in HD and MHD
- ❑ Implicit thermal conduction and flux limited multi-group radiation diffusion with HYPRE
- ❑ Multi-material support: EOS and opacities can combine tabular and analytic models for different materials
- ❑ Laser Ray Tracing for energy deposition
- ❑ Preliminary hybrid particle-in-cell capability (only in uniform grid)
- ❑ Ability to represent rigid bodies inside the flow



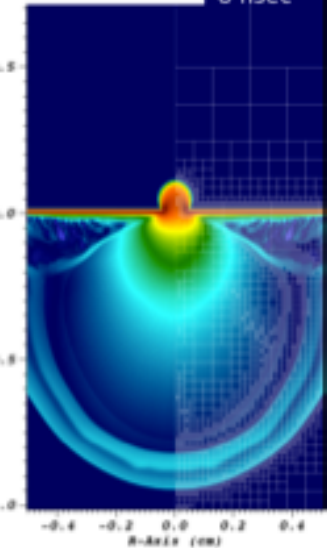
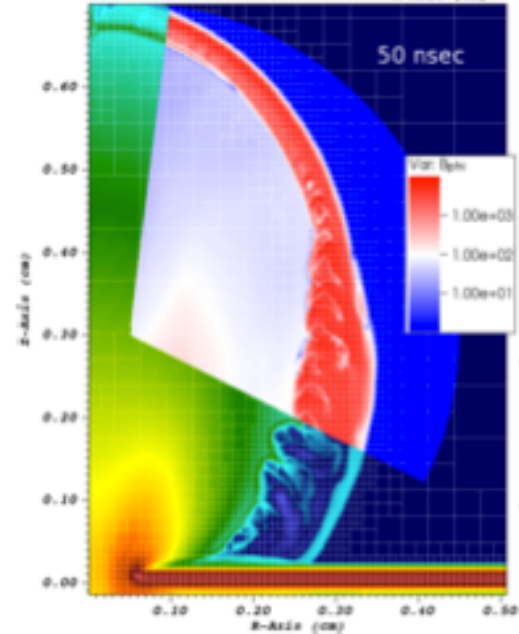
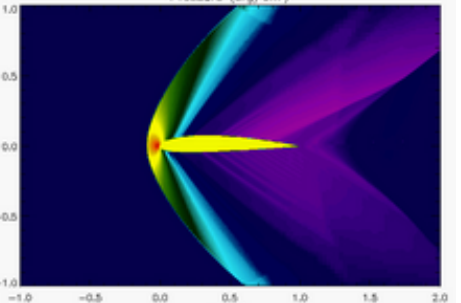
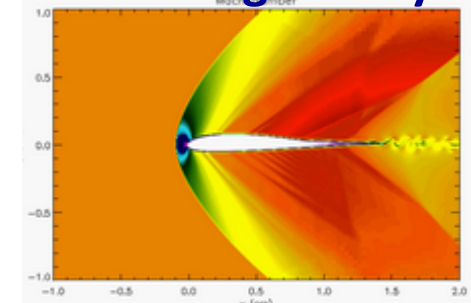
HEDP Applications



LULI/Vulcan experiments: B field generation/ amplification

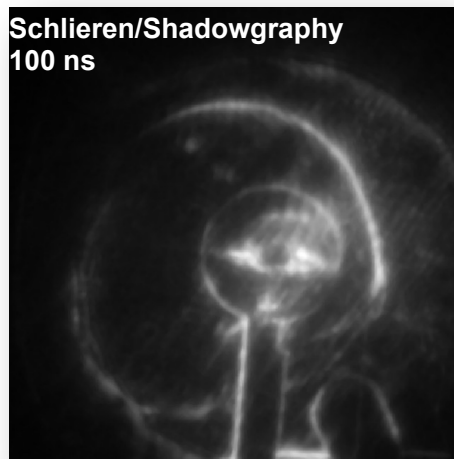


Rigid body structures

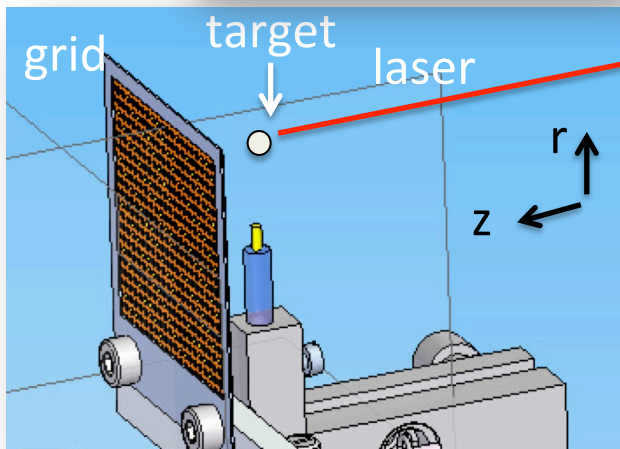




B Field Generation Experiments at LULI

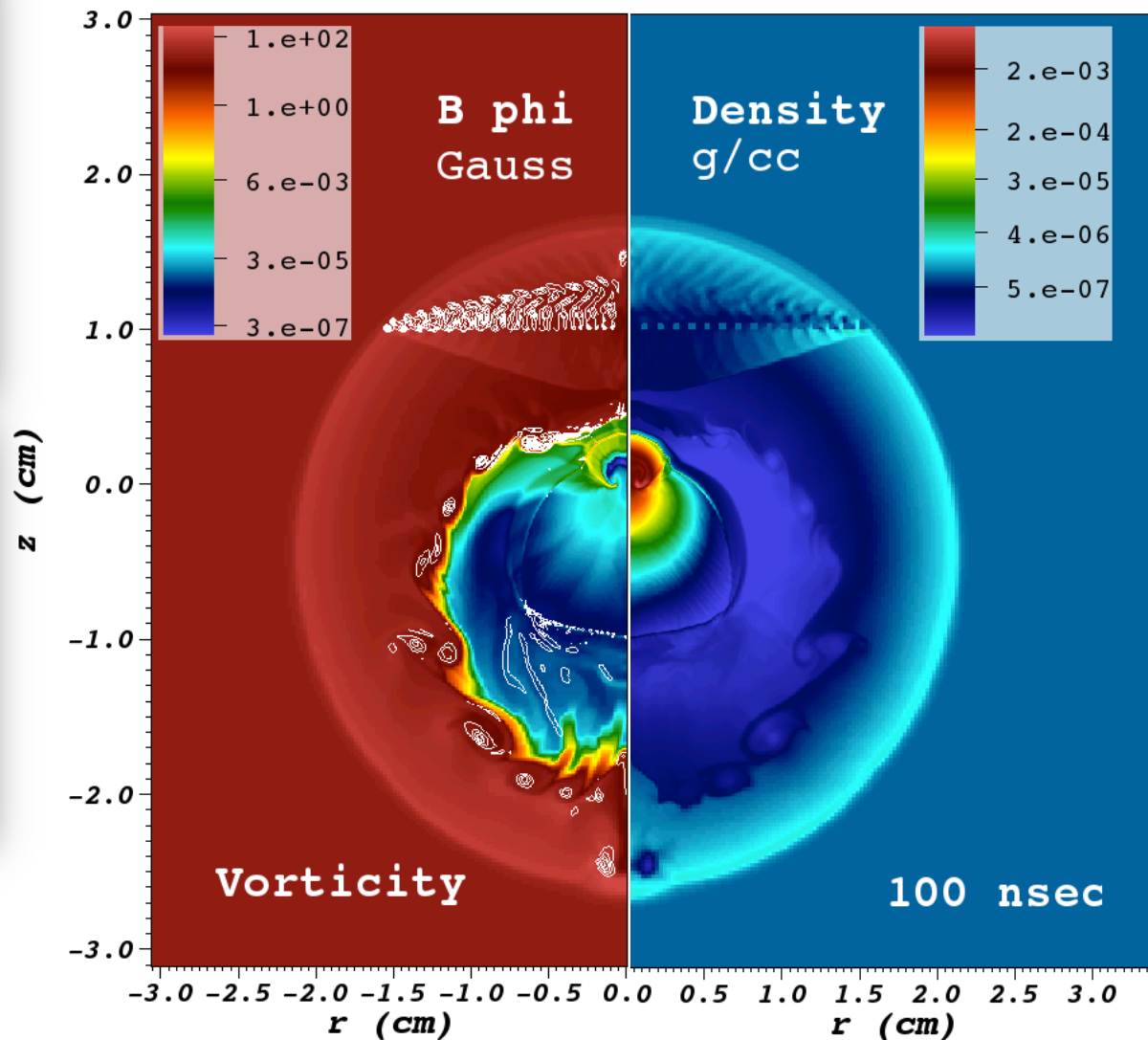


Schlieren/Shadowgraphy
100 ns



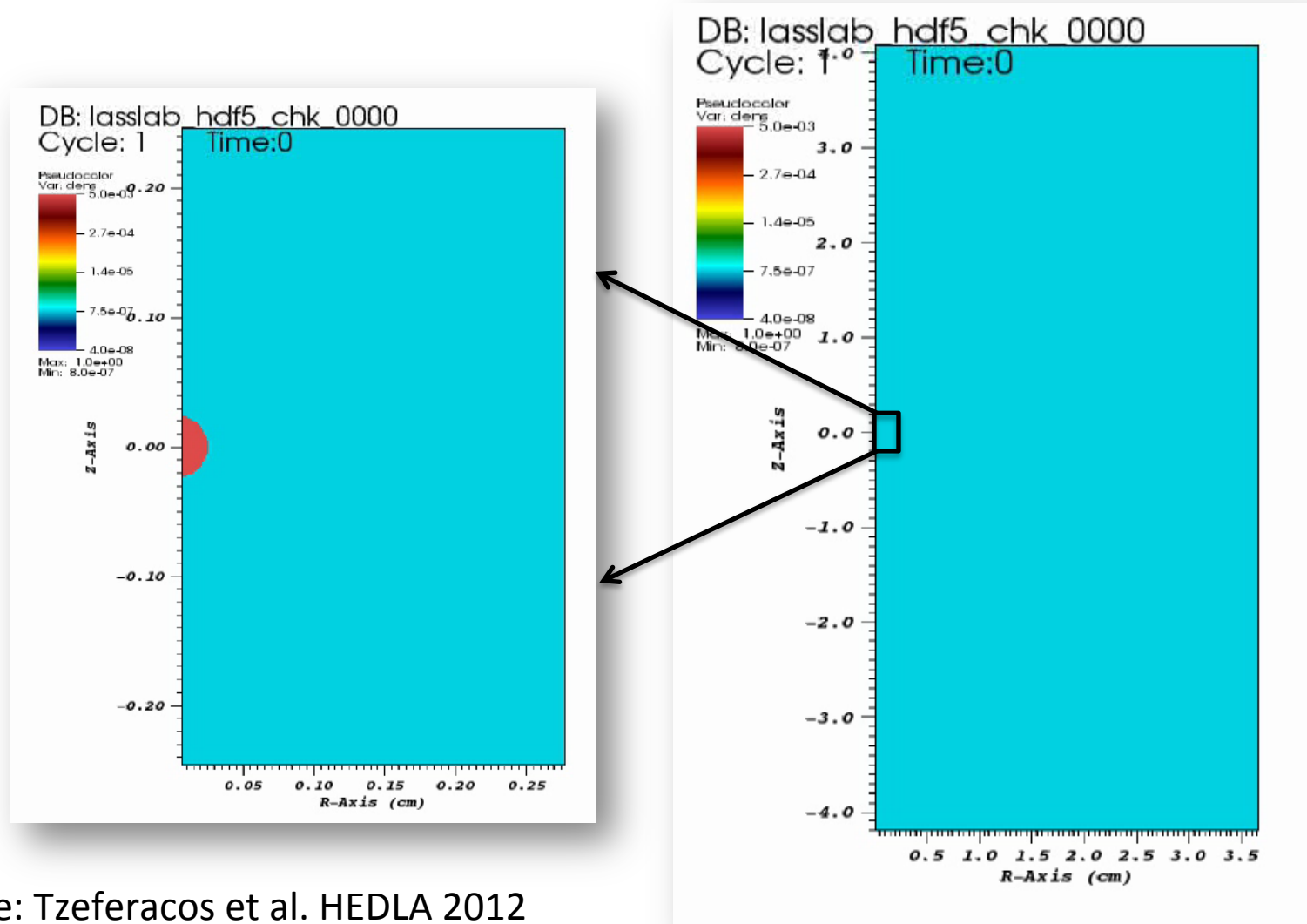
Sources:

- Gregori et al. Nature 2012
- Fatenejad et al. HEDLA 2012,
- Tzeferacos et al. HEDLA 2012





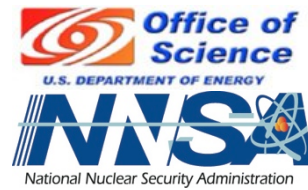
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Source: Tzeferacos et al. HEDLA 2012



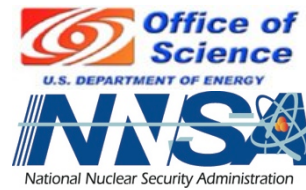
Part 2



Divergence-Free Fields: A New Upwind Constrained Transport (CT)-MHD Algorithm



Four (Three + One) CT Methods



- ❑ CT scheme by Balsara and Spicer, JCP, 1999:

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

- ❑ \mathcal{E}_z^c CT scheme by Gardiner and Stone, JCP, 2005

- ❑ MEC (modified electric field construction) scheme by Lee and Deane, JCP, 2009

→ These three CT approaches ALL fail for a special case of field loop advection!!!

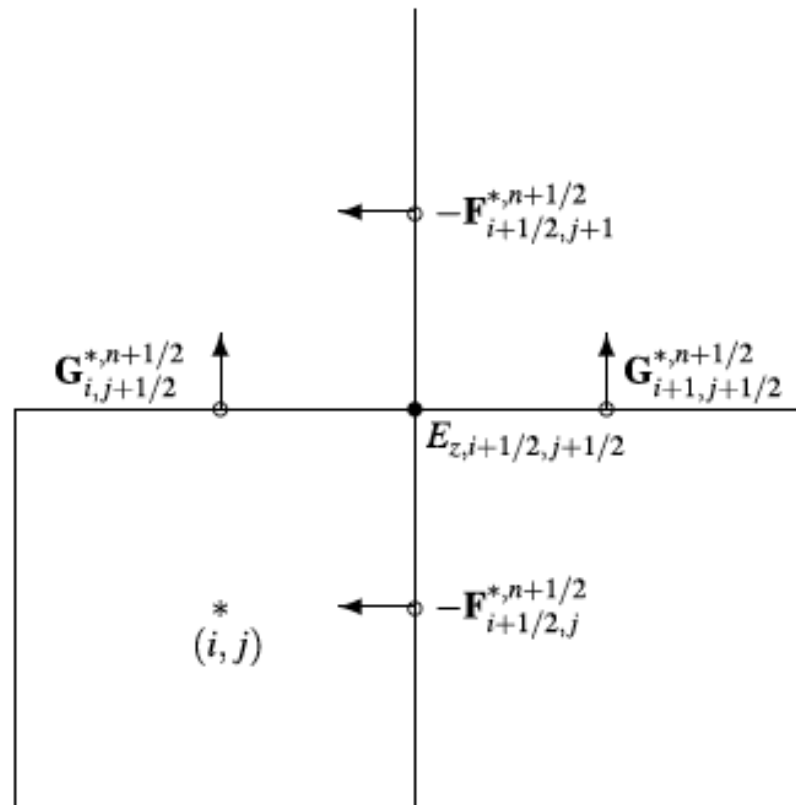
- ❑ ... and a new upwind biased MEC scheme, Lee, JCP, 2012, submitted



1. CT by Balsara & Spicer (BSCT)

- CT scheme by Balsara and Spicer, JCP, 1999:

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



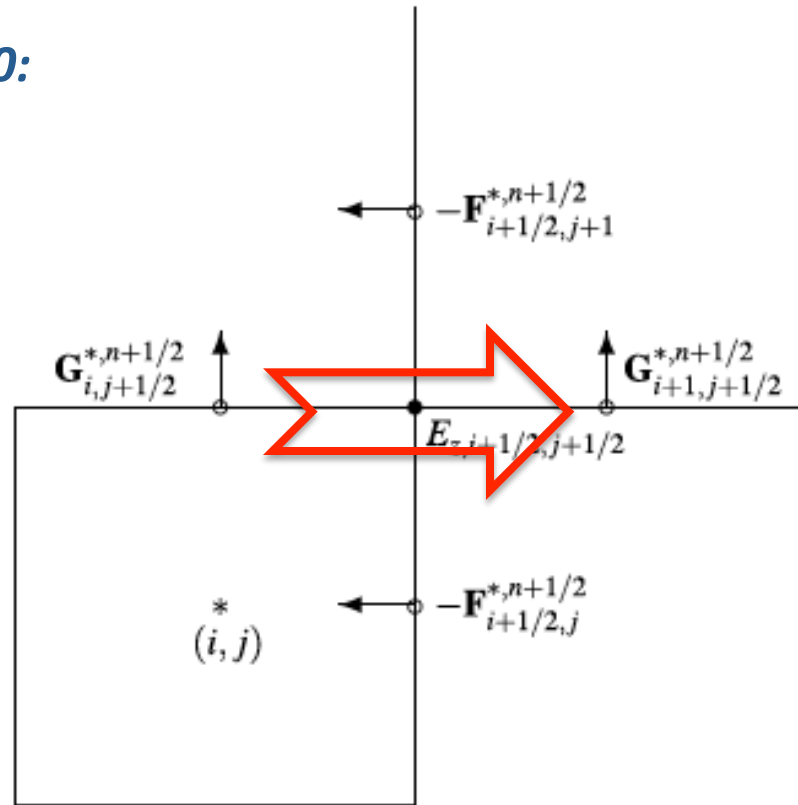


Lack of Upwind Consideration in BSCT

- ❑ CT scheme by Balsara and Spicer, 1998:

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

- ❑ Consider $u > 0, v \rightarrow 0$:





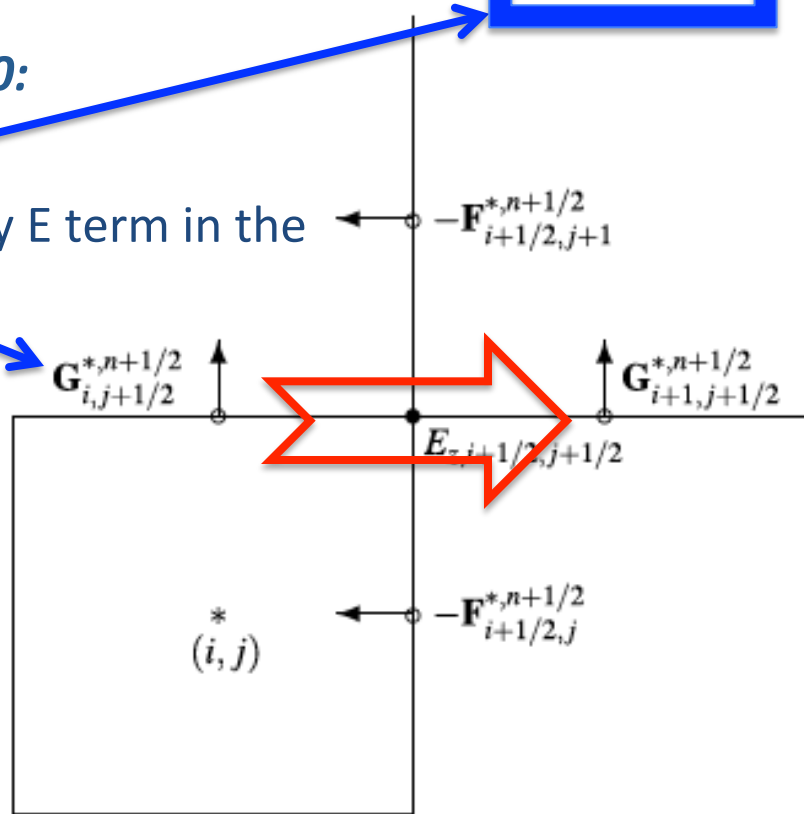
Lack of Upwind Consideration in BSCT

- CT scheme by Balsara and Spicer, 1998:

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- Consider $u > 0, v \rightarrow 0$:

- $E_{z,i,j+1/2,k}^{*,n+1/2}$ is the only E term in the upwind direction!





Lack of Upwind Consideration in BSCT



- CT scheme by Balsara and Spicer, 1998:

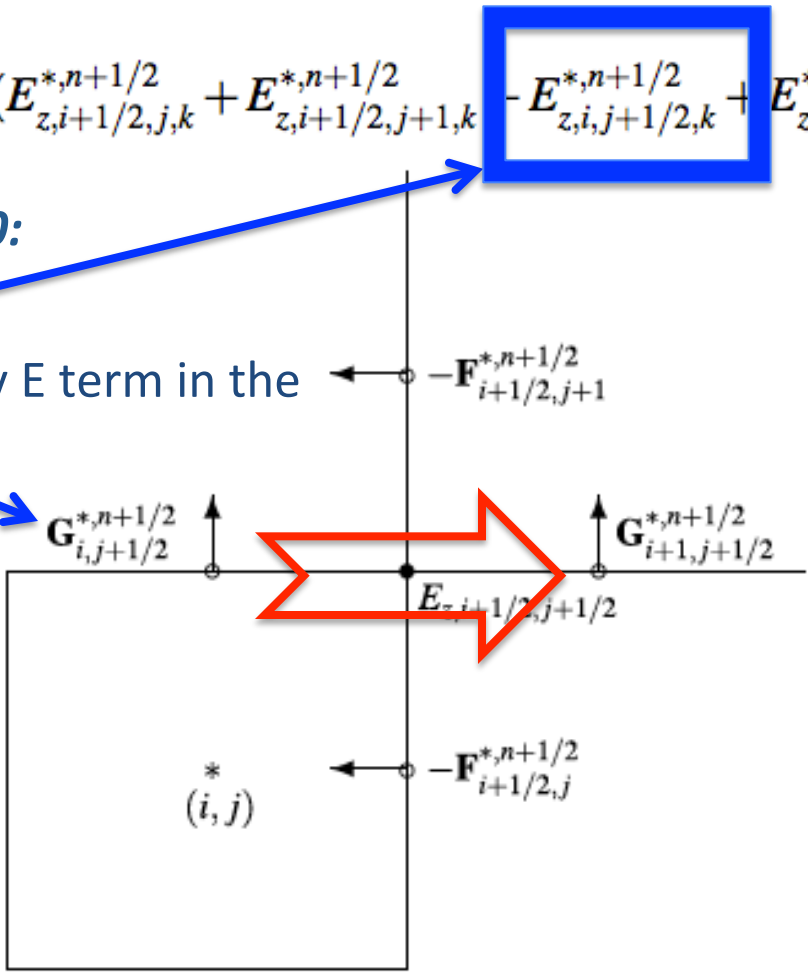
$$E_{z,i+1/2,j+1/2,k}^{n+1/2} = \frac{1}{4} (E_{z,i+1/2,j,k}^{*,n+1/2} + E_{z,i+1/2,j+1,k}^{*,n+1/2} - E_{z,i,j+1/2,k}^{*,n+1/2} + E_{z,i+1,j+1/2,k}^{*,n+1/2})$$

- Consider $u > 0, v \rightarrow 0$:

- $E_{z,i,j+1/2,k}^{*,n+1/2}$ is the only E term in the upwind direction!

Numerical Oscillations!

This is true in most CT schemes!





2. Gardiner & Stone's CT (GSCT)

- The method is consistent for plane-parallel, grid-aligned flows:

$$\begin{aligned} \tilde{E}_{z,i+1/2,j+1/2,k}^{n+1/2} = & \frac{1}{4} \left(E_{z,i+1/2,j,k}^{*,n+1/2} + E_{z,i+1/2,j+1,k}^{*,n+1/2} + E_{z,i,j+1/2,k}^{*,n+1/2} + E_{z,i+1,j+1/2,k}^{*,n+1/2} \right) \\ & + \frac{\Delta y}{8} \left(\left. \frac{\partial E_z^{*,n+1/2}}{\partial y} \right|_{i+1/2,j+1/4,k} - \left. \frac{\partial E_z^{*,n+1/2}}{\partial y} \right|_{i+1/2,j+3/4,k} \right) \\ & + \frac{\Delta x}{8} \left(\left. \frac{\partial E_z^{*,n+1/2}}{\partial x} \right|_{i+1/4,j+1/2,k} - \left. \frac{\partial E_z^{*,n+1/2}}{\partial x} \right|_{i+3/4,j+1/2,k} \right) \end{aligned}$$



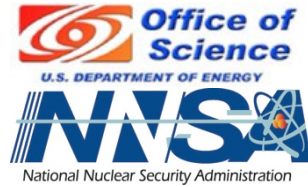
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 &= \frac{1}{4} (E_{z,i+1/2,j,k}^{*,n+1/2} + E_{z,i+1/2,j+1,k}^{*,n+1/2} + E_{z,i,j+1/2,k}^{*,n+1/2} + E_{z,i+1,j+1/2,k}^{*,n+1/2}) \\
 &\quad + \frac{1}{4} (E_{z,i,j+1/2,k}^{*,n+1/2} - E_{z,i,j,k}^{*,n+1/2} - E_{z,i,j+1,k}^{*,n+1/2} + E_{z,i,j+1/2,k}^{*,n+1/2}) \\
 &\quad + \frac{1}{8} (E_{z,i+1/2,j,k}^{*,n+1/2} - E_{z,i,j,k}^{*,n+1/2} + E_{z,i+1/2,j+1,k}^{*,n+1/2} - E_{z,i,j+1,k}^{*,n+1/2}) \\
 &\quad - \frac{1}{8} (E_{z,i+1,j,k}^{*,n+1/2} - E_{z,i+1/2,j,k}^{*,n+1/2} + E_{z,i+1,j+1,k}^{*,n+1/2} - E_{z,i+1/2,j+1,k}^{*,n+1/2}).
 \end{aligned}$$

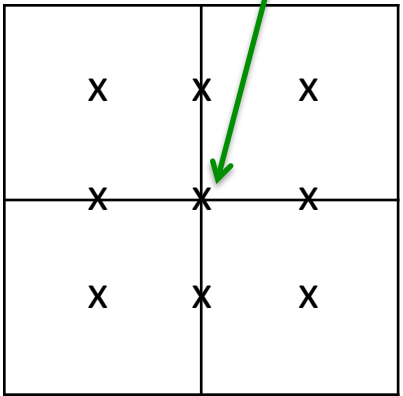


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 &+ \frac{\Delta y}{8} \left(\left. \frac{\partial E_z^{*,n+1/2}}{\partial y} \right|_{i+1/2,j+1/4,k} - \left. \frac{\partial E_z^{*,n+1/2}}{\partial y} \right|_{i+1/2,j+3/4,k} \right) \\
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 &= \frac{1}{4} (E_{z,i+1/2,j,k}^{*,n+1/2} + E_{z,i+1/2,j+1,k}^{*,n+1/2} + E_{z,i,j+1/2,k}^{*,n+1/2} + E_{z,i+1,j+1/2,k}^{*,n+1/2}) \\
 &+ \frac{1}{4} (E_{z,i,j+1/2,k}^{*,n+1/2} - E_{z,i,j,k}^{*,n+1/2} - E_{z,i,j+1,k}^{*,n+1/2} + E_{z,i,j+1/2,k}^{*,n+1/2}) \\
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 &- \frac{1}{8} (E_{z,i+1,j,k}^{*,n+1/2} - E_{z,i+1/2,j,k}^{*,n+1/2} + E_{z,i+1,j+1,k}^{*,n+1/2} - E_{z,i+1/2,j+1,k}^{*,n+1/2}).
 \end{aligned}$$



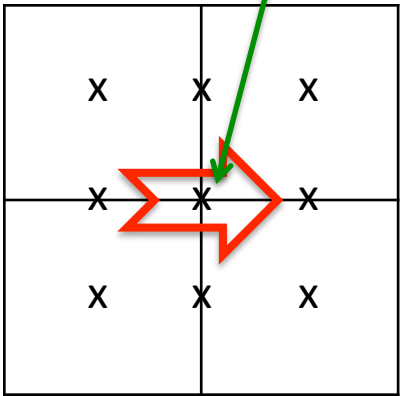


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 &+ \frac{\Delta y}{8} \left(\left. \frac{\partial E_z^{*,n+1/2}}{\partial y} \right|_{i+1/2,j+1/4,k} - \left. \frac{\partial E_z^{*,n+1/2}}{\partial y} \right|_{i+1/2,j+3/4,k} \right) \\
 &+ \frac{\Delta x}{8} \left(\left. \frac{\partial E_z^{*,n+1/2}}{\partial x} \right|_{i+1/4,j+1/2,k} - \left. \frac{\partial E_z^{*,n+1/2}}{\partial x} \right|_{i+3/4,j+1/2,k} \right) \\
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 &+ \frac{1}{4} (E_{z,i,j+1/2,k}^{*,n+1/2} - E_{z,i,j,k}^{*,n+1/2} - E_{z,i,j+1,k}^{*,n+1/2} + E_{z,i,j+1/2,k}^{*,n+1/2}) \\
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 &- \frac{1}{8} (E_{z,i+1,j,k}^{*,n+1/2} - E_{z,i+1/2,j,k}^{*,n+1/2} + E_{z,i+1,j+1,k}^{*,n+1/2} - E_{z,i+1/2,j+1,k}^{*,n+1/2}).
 \end{aligned}$$





2. Gardiner & Stone's CT (GSCT)



- The method is consistent for plane-parallel, grid-aligned flows:

↑ ↔
upwind downwind

$$\begin{aligned}
 \bar{E}_{z,i+1/2,j+1/2,k}^{n+1/2} &= \frac{1}{4} \left(E_{z,i+1/2,j,k}^{*,n+1/2} + E_{z,i+1/2,j+1,k}^{*,n+1/2} + E_{z,i,j+1/2,k}^{*,n+1/2} + E_{z,i+1,j+1/2,k}^{*,n+1/2} \right) \\
 &+ \frac{\Delta y}{8} \left(\left. \frac{\partial E_z^{*,n+1/2}}{\partial y} \right|_{i+1/2,j+1/4,k} - \left. \frac{\partial E_z^{*,n+1/2}}{\partial y} \right|_{i+1/2,j+3/4,k} \right) \\
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 &= \frac{1}{4} (E_{z,i+1/2,j,k}^{*,n+1/2} + E_{z,i+1/2,j+1,k}^{*,n+1/2} + E_{z,i,j+1/2,k}^{*,n+1/2} + E_{z,i+1,j+1/2,k}^{*,n+1/2}) \\
 &+ \frac{1}{4} (E_{z,i,j+1/2,k}^{*,n+1/2} - E_{z,i,j,k}^{*,n+1/2} - E_{z,i,j+1,k}^{*,n+1/2} + E_{z,i,j+1/2,k}^{*,n+1/2}) \\
 &+ \frac{1}{8} (E_{z,i+1/2,j,k}^{*,n+1/2} - E_{z,i,j,k}^{*,n+1/2} + E_{z,i+1/2,j+1,k}^{*,n+1/2} - E_{z,i,j+1,k}^{*,n+1/2}) \\
 &- \frac{1}{8} (E_{z,i+1,j,k}^{*,n+1/2} - E_{z,i+1/2,j,k}^{*,n+1/2} + E_{z,i+1,j+1,k}^{*,n+1/2} - E_{z,i+1/2,j+1,k}^{*,n+1/2}).
 \end{aligned}$$



3. Standard-MEC (LD-MEC)



3rd order modified electric field construction (standard-MEC), Lee & Deane, JCP, 2009:

$$E_{z,i+1/2,j+1/2,k}^{n+1/2} = \left[\begin{aligned} &\left(E_{z,i+1/2,j,k}^{*,n+1/2} + \frac{\Delta y}{2} \frac{\partial E_{z,i+1/2,j,k}^{*,n+1/2}}{\partial y} + \frac{\Delta y^2}{8} \frac{\partial^2 E_{z,i+1/2,j,k}^{*,n+1/2}}{\partial y^2} \right) + \\ &\left(E_{z,i+1/2,j+1,k}^{*,n+1/2} - \frac{\Delta y}{2} \frac{\partial E_{z,i+1/2,j+1,k}^{*,n+1/2}}{\partial y} + \frac{\Delta y^2}{8} \frac{\partial^2 E_{z,i+1/2,j+1,k}^{*,n+1/2}}{\partial y^2} \right) + \\ &\left(E_{z,i,j+1/2,k}^{*,n+1/2} + \frac{\Delta x}{2} \frac{\partial E_{z,i,j+1/2,k}^{*,n+1/2}}{\partial x} + \frac{\Delta x^2}{8} \frac{\partial^2 E_{z,i,j+1/2,k}^{*,n+1/2}}{\partial x^2} \right) + \\ &\left(E_{z,i+1,j+1/2,k}^{*,n+1/2} - \frac{\Delta x}{2} \frac{\partial E_{z,i+1,j+1/2,k}^{*,n+1/2}}{\partial x} + \frac{\Delta x^2}{8} \frac{\partial^2 E_{z,i+1,j+1/2,k}^{*,n+1/2}}{\partial x^2} \right) \end{aligned} \right].$$



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Only upwind term!



4. New Upwind-MEC (U-MEC)



❑ New upwind biased modified electric field construction(upwind-MEC), Lee, JCP, submitted, 2012

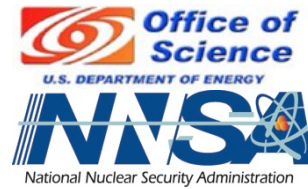
$$E_{z,i+1/2,j+1/2,k}^{n+1/2} = \alpha \left[v_P \left(E_{z,i+1/2,j,k}^{*,n+1/2} + \frac{\Delta y}{2} \frac{\partial E_{z,i+1/2,j,k}^{*,n+1/2}}{\partial y} + \frac{\Delta y^2}{8} \frac{\partial^2 E_{z,i+1/2,j,k}^{*,n+1/2}}{\partial y^2} \right) + \right. \\ v_N \left(E_{z,i+1/2,j+1,k}^{*,n+1/2} - \frac{\Delta y}{2} \frac{\partial E_{z,i+1/2,j+1,k}^{*,n+1/2}}{\partial y} + \frac{\Delta y^2}{8} \frac{\partial^2 E_{z,i+1/2,j+1,k}^{*,n+1/2}}{\partial y^2} \right) + \\ u_P \left(E_{z,i,j+1/2,k}^{*,n+1/2} + \frac{\Delta x}{2} \frac{\partial E_{z,i,j+1/2,k}^{*,n+1/2}}{\partial x} + \frac{\Delta x^2}{8} \frac{\partial^2 E_{z,i,j+1/2,k}^{*,n+1/2}}{\partial x^2} \right) + \\ \left. u_N \left(E_{z,i+1,j+1/2,k}^{*,n+1/2} - \frac{\Delta x}{2} \frac{\partial E_{z,i+1,j+1/2,k}^{*,n+1/2}}{\partial x} + \frac{\Delta x^2}{8} \frac{\partial^2 E_{z,i+1,j+1/2,k}^{*,n+1/2}}{\partial x^2} \right) \right].$$

$$u_P = \frac{1}{2}(1 + \text{sign}(u_{i+1/2,j+1/2}))|\text{sign}(u_{i+1/2,j+1/2})|, \\ u_N = \frac{1}{2}(1 - \text{sign}(u_{i+1/2,j+1/2}))|\text{sign}(u_{i+1/2,j+1/2})| \\ v_P = \frac{1}{2}(1 + \text{sign}(v_{i+1/2,j+1/2}))|\text{sign}(v_{i+1/2,j+1/2})| \\ v_N = \frac{1}{2}(1 - \text{sign}(v_{i+1/2,j+1/2}))|\text{sign}(v_{i+1/2,j+1/2})|,$$

$$\text{sign}(x) = \begin{cases} 1 & \text{if } x > 0, \\ 0 & \text{if } x = 0, \\ -1 & \text{if } x < 0. \end{cases}$$



4. New Upwind-MEC (U-MEC)



- New upwind biased modified electric field construction (upwind-MEC), Lee, JCP, submitted, 2012

$$E_{z,i+1/2,j+1/2,k}^{n+1/2} = \alpha \left[\begin{array}{l} v_P \left(E_{z,i+1/2,j,k}^{*,n+1/2} + \frac{\Delta y}{2} \frac{\partial E_{z,i+1/2,j,k}^{*,n+1/2}}{\partial y} + \frac{\Delta y^2}{8} \frac{\partial^2 E_{z,i+1/2,j,k}^{*,n+1/2}}{\partial y^2} \right) + \\ v_N \left(E_{z,i+1/2,j+1,k}^{*,n+1/2} - \frac{\Delta y}{2} \frac{\partial E_{z,i+1/2,j+1,k}^{*,n+1/2}}{\partial y} + \frac{\Delta y^2}{8} \frac{\partial^2 E_{z,i+1/2,j+1,k}^{*,n+1/2}}{\partial y^2} \right) + \\ u_P \left(E_{z,i,j+1/2,k}^{*,n+1/2} + \frac{\Delta x}{2} \frac{\partial E_{z,i,j+1/2,k}^{*,n+1/2}}{\partial x} + \frac{\Delta x^2}{8} \frac{\partial^2 E_{z,i,j+1/2,k}^{*,n+1/2}}{\partial x^2} \right) + \\ u_N \left(E_{z,i+1,j+1/2,k}^{*,n+1/2} - \frac{\Delta x}{2} \frac{\partial E_{z,i+1,j+1/2,k}^{*,n+1/2}}{\partial x} + \frac{\Delta x^2}{8} \frac{\partial^2 E_{z,i+1,j+1/2,k}^{*,n+1/2}}{\partial x^2} \right) \end{array} \right].$$



$$u_P = \frac{1}{2}(1 + \text{sign}(u_{i+1/2,j+1/2}))|\text{sign}(u_{i+1/2,j+1/2})|,$$

$$u_N = \frac{1}{2}(1 - \text{sign}(u_{i+1/2,j+1/2}))|\text{sign}(u_{i+1/2,j+1/2})|$$

$$v_P = \frac{1}{2}(1 + \text{sign}(v_{i+1/2,j+1/2}))|\text{sign}(v_{i+1/2,j+1/2})|$$

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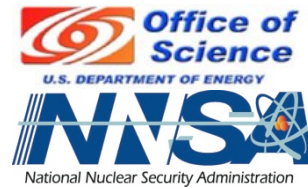
$$v_P = \frac{1}{2} (1 + \text{sign}(v_{i+1/2,j+1/2})) |\text{sign}(v_{i+1/2,j+1/2})|$$

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4. New Upwind-MEC (U-MEC)



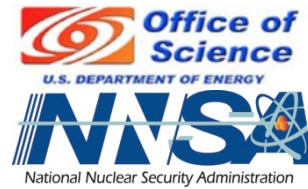
- ❑ New upwind biased modified electric field construction (upwind-MEC), Lee, JCP, submitted, 2012. **Considering $u > 0, v \rightarrow 0$:**

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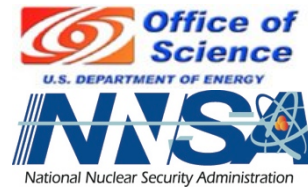


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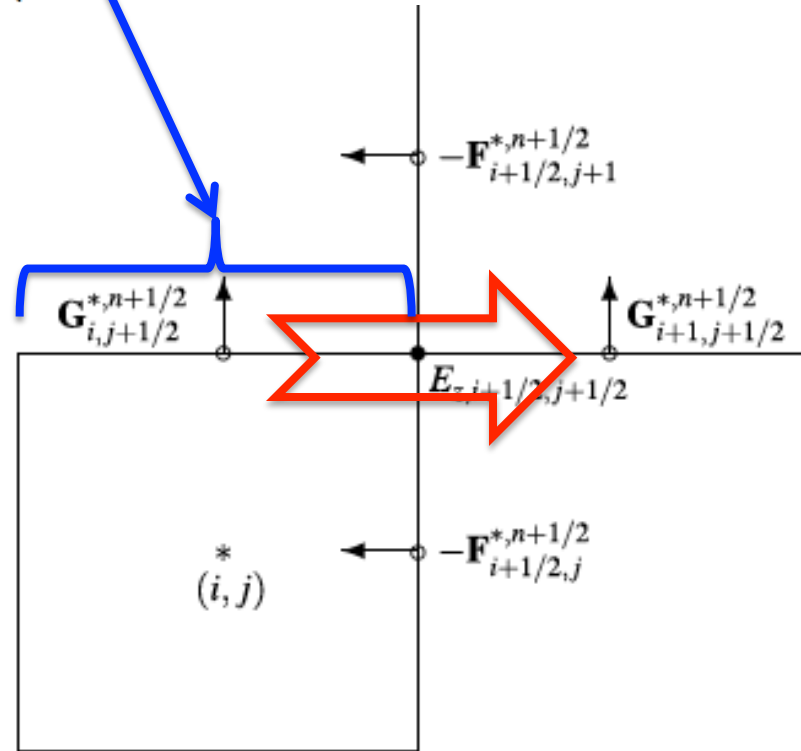


4. New Upwind-MEC (U-MEC)



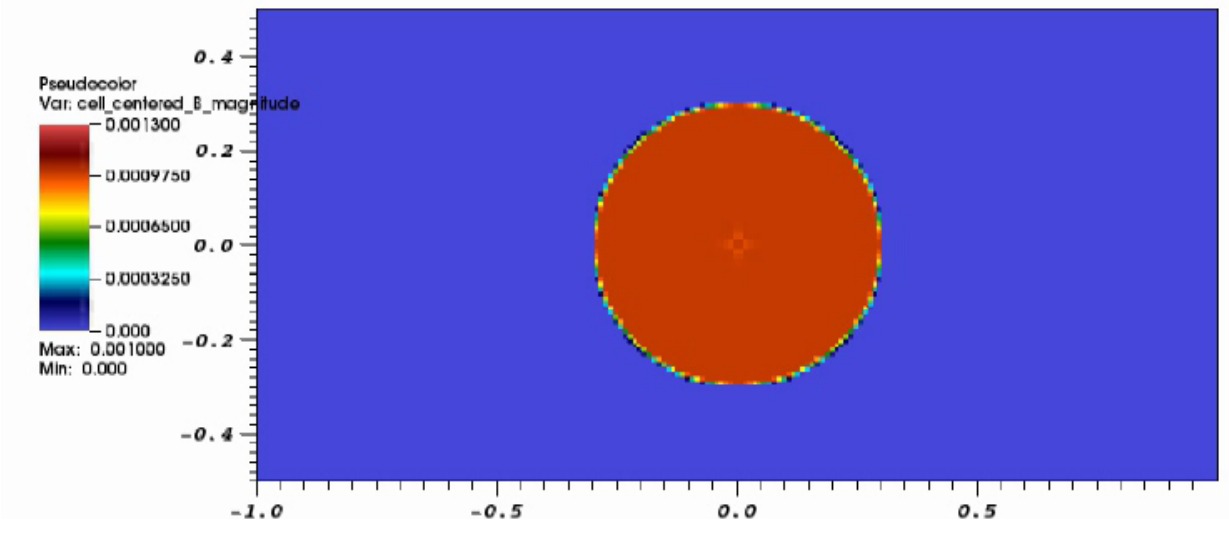
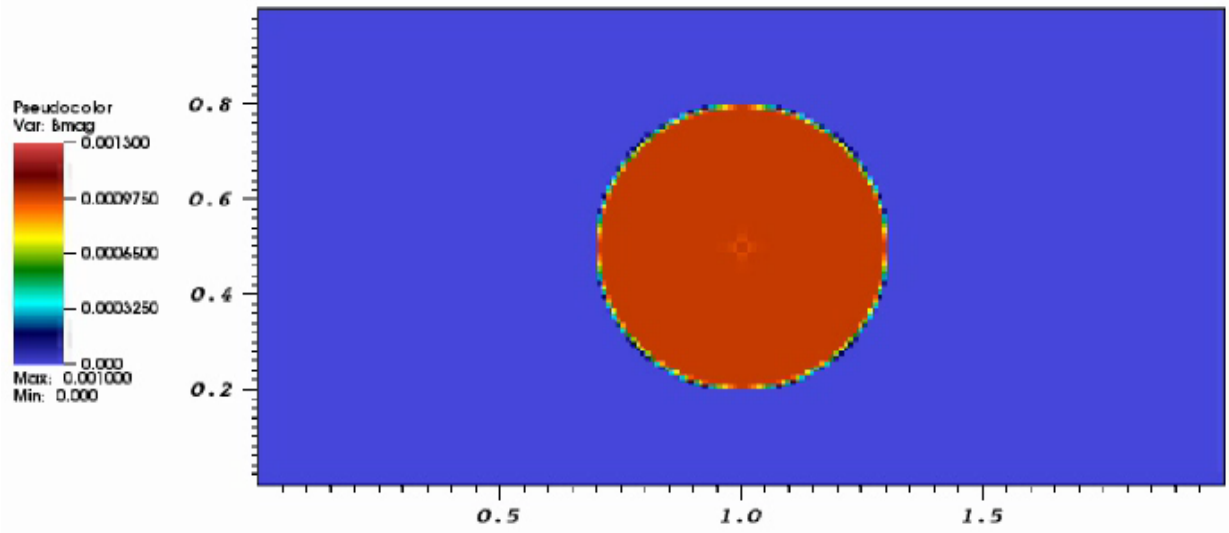
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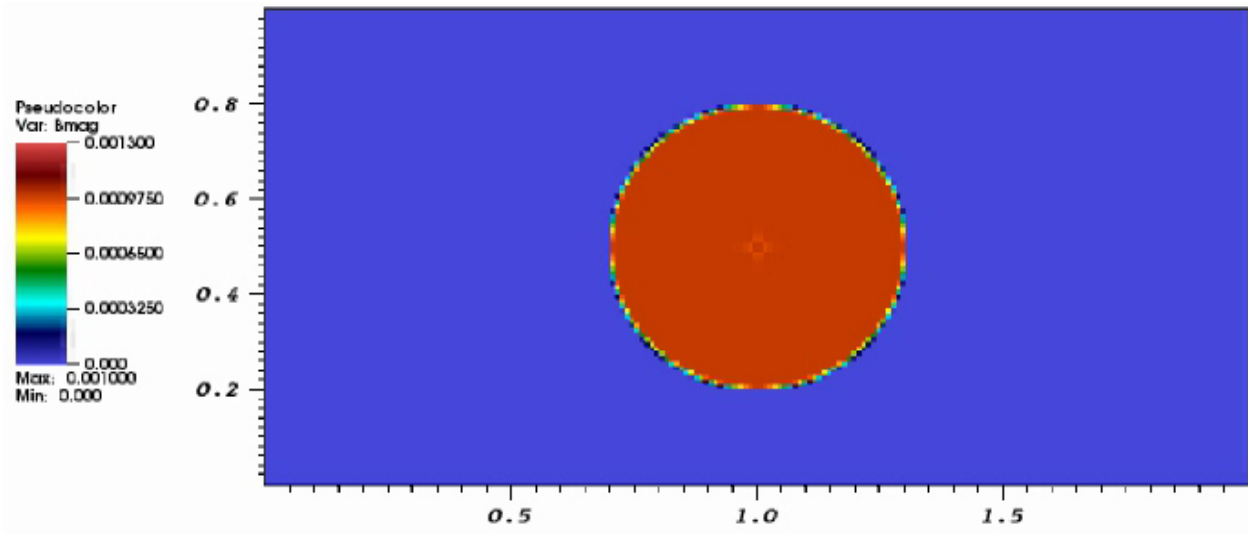
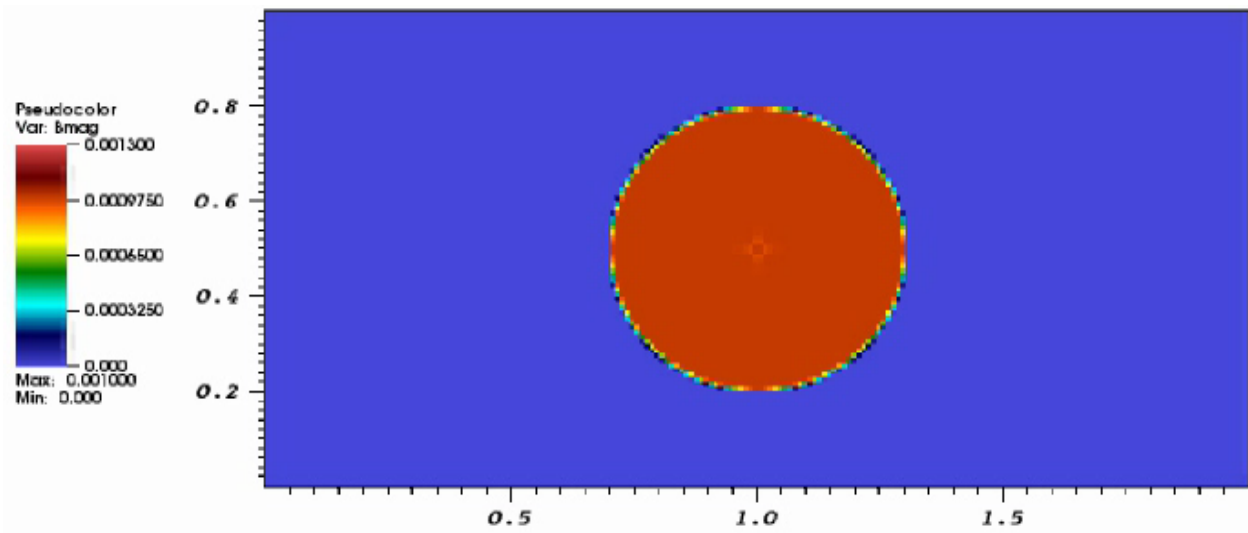


BSCT & GSCT





LD-MEC & BSCT with Upwind





4. New Upwind-MEC (U-MEC)

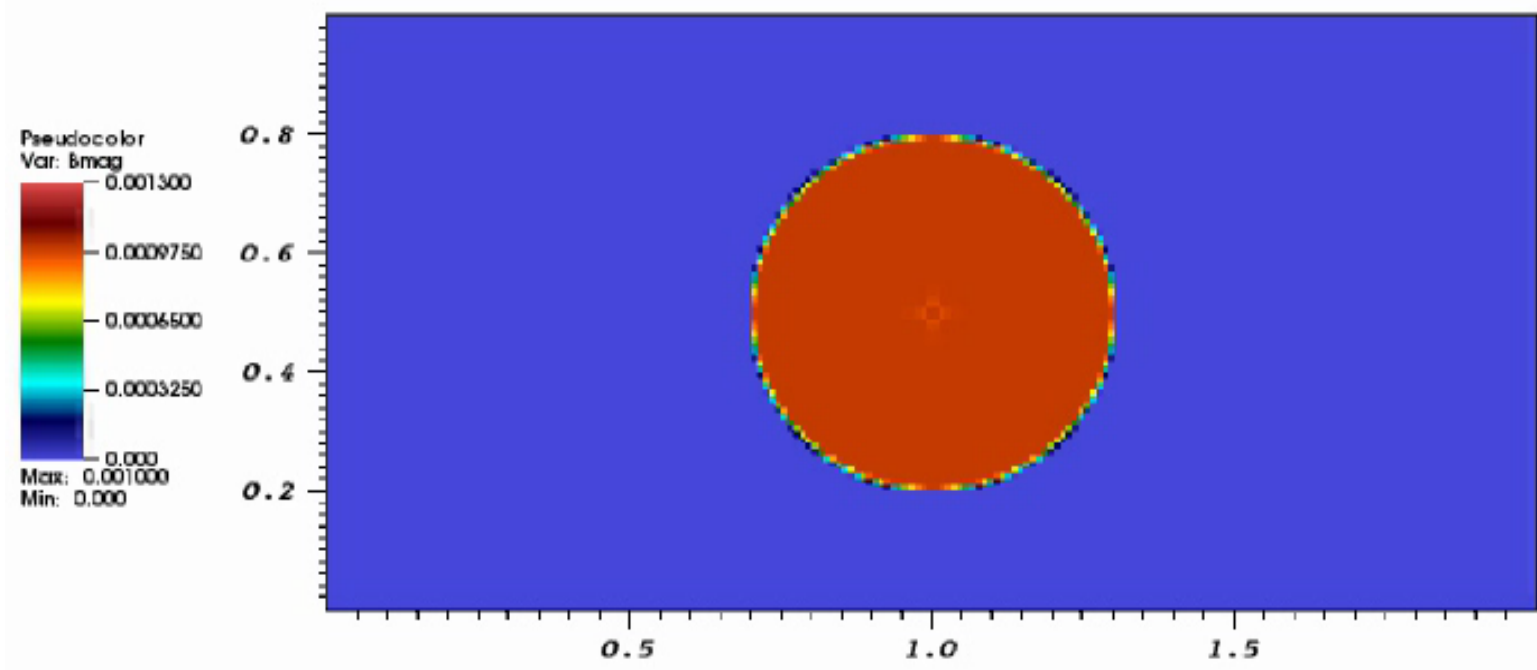
- New upwind biased modified electric field construction (upwind-MEC), Lee 2012:

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High Order Terms!

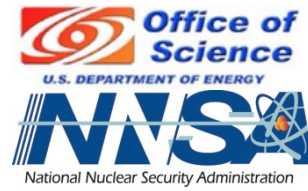


U-MEC

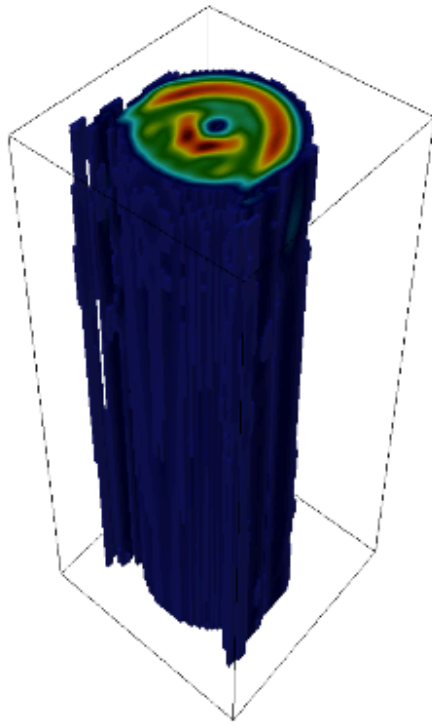




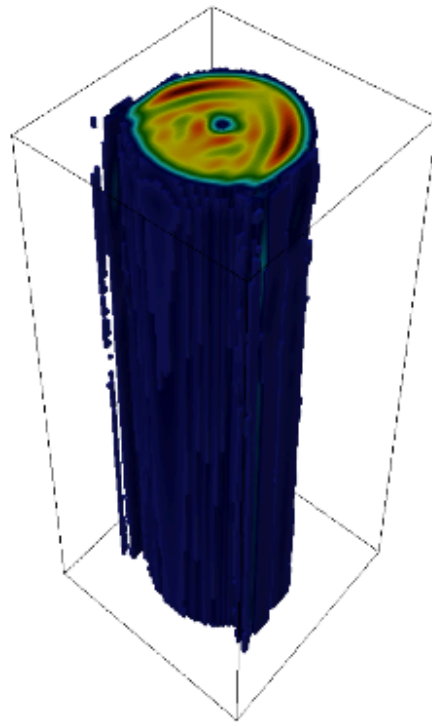
BSCT, LD-MEC & U-MEC



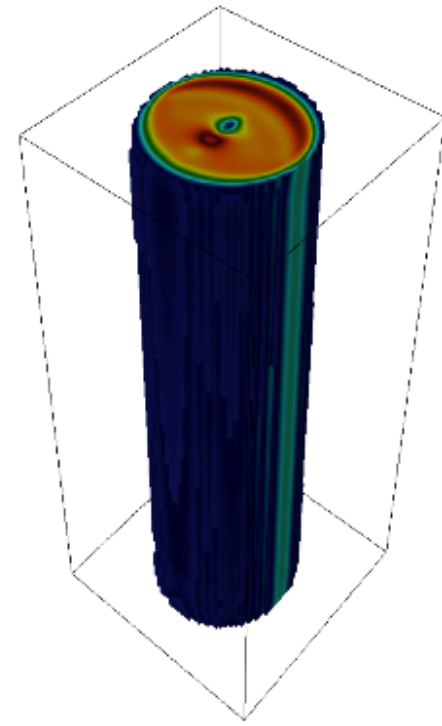
Small angle advection of the 3D field loop: $\theta = \tan^{-1}(0.01) = 0.573^\circ$



(a) B_p using the standard CT at $t = 2$.



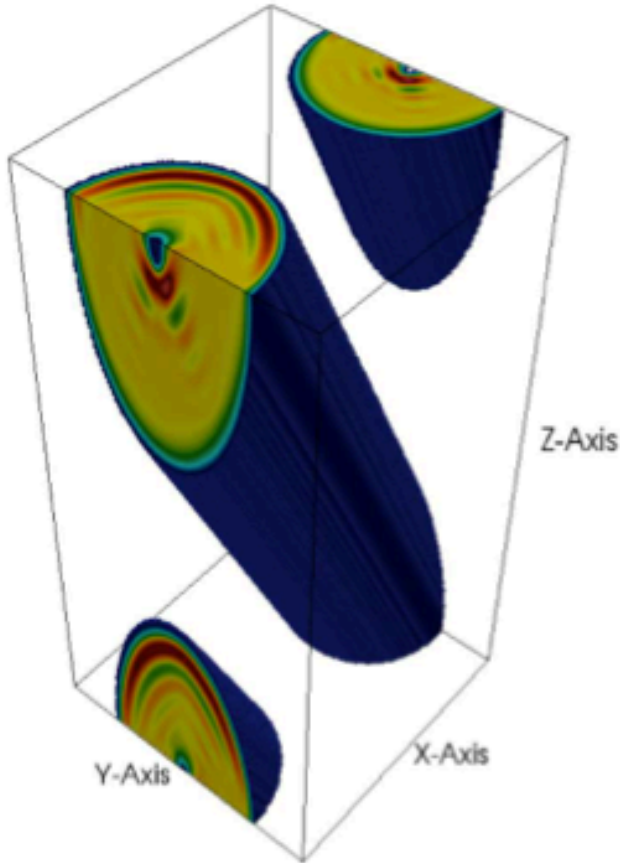
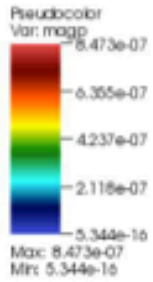
(b) B_p using the standard MEC at $t = 2$.



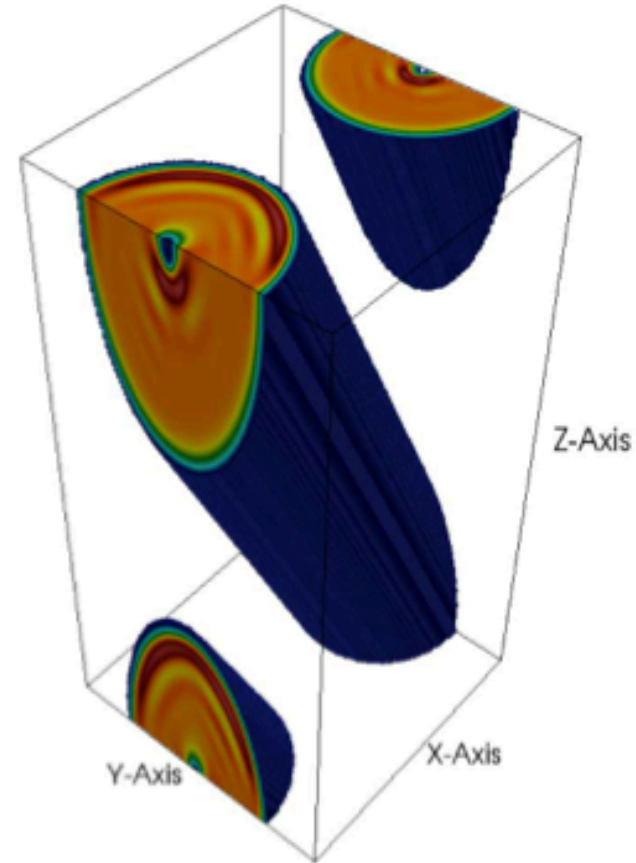
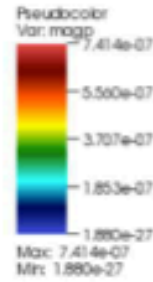
(c) B_p using the upwind MEC at $t = 2$.



LD-MEC & U-MEC



(a) B_p using the standard-MEC CT at $t = 1$.

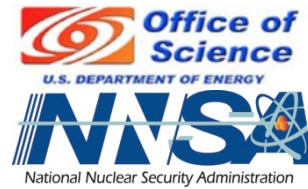


(b) B_p using the upwind-MEC at $t = 1$.

Fig. 6. The standard field loop advection problem at time $t = 1$ using PPM and the Roe Riemann solver. The minmod slope limiter is used for taking slope gradients of characteristic variable in the PPM reconstruction step. All results are resolved on $128 \times 128 \times 256$ grid cells.



Conclusions



□ *Part 1: Applications*

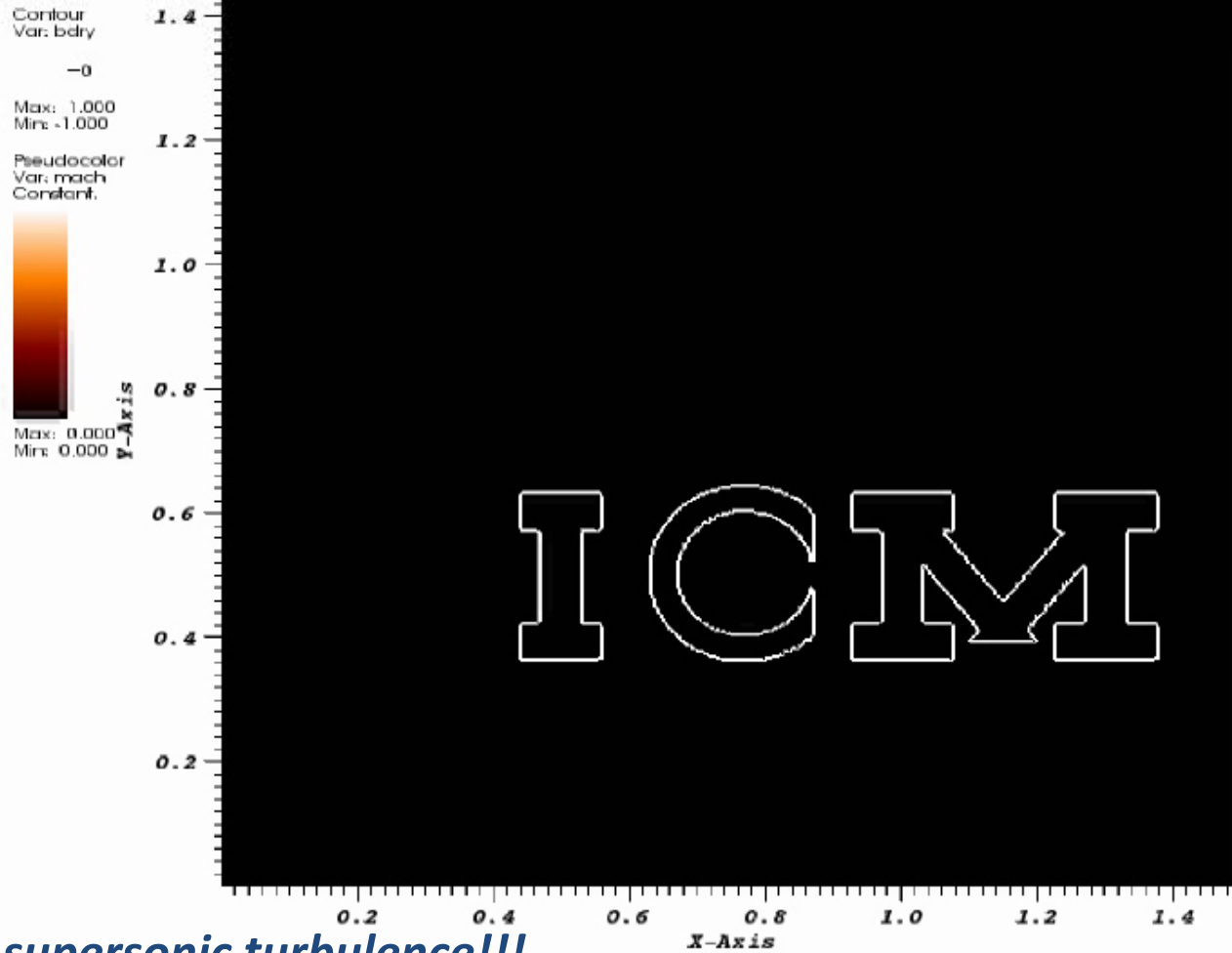
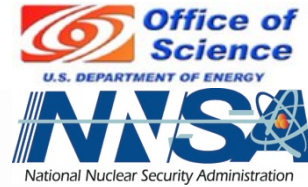
- FLASH has been extended to simulating HEDP lab experiments
- Validating lab experiments using simulations is doable but hard
- If successful, simulations can provide strong support in experimental design, data analysis through extensive diagnostics, and serve as a powerful tool for predictive science!

□ *Part 2: Algorithms*

- A small angle field loop advection test reveals a special care for CT in conventional Godunov schemes based on 1D Riemann solves
- An upwinding scheme can improve handling numerical dissipations in preserving circular symmetry for the small angle advection
- Alternatively, a genuinely multidimensional Riemann solves (Balsara, 2010) can be used



Thanks!



- ❑ **ICM supersonic turbulence!!!**
- ❑ Rigid body structures, PPM, MC limiter on characteristic variables with HLLC on 400x400