The Center for Astrophysical Thermonuclear Flashes

Exploiting the Extensibility of the FLASH Code Architecture for Unsplit Time Integration

A. Dubey, D. Lee, K. Olson, K. Weide, K. Antypas

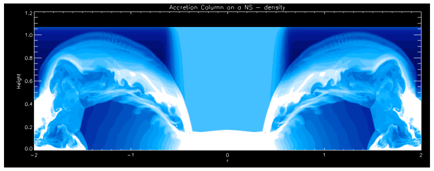
June 29, 2009

An Advanced Simulation & Computing (ASC)
Academic Strategic Alliances Program (ASAP) Center
at The University of Chicago

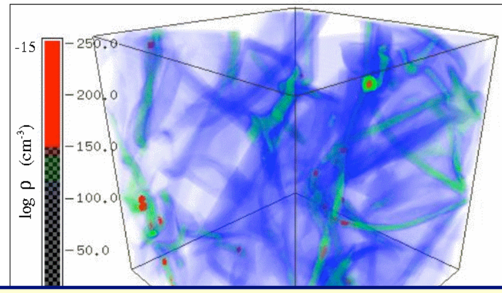
The FLASH Code Contributors

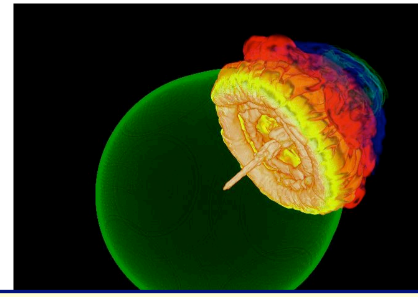
- Active Contributors
  - Dongwook Lee, Klaus Weide, Chris Daley, Anshu Dubey, Lynn Reid, Paul Rich, Paul Ricker, Dean Townsley, Cal Jordan, John Zuhone, Kevin Olson, Marcos Vanella
- Past Major Contributors:
  - Katie Antypas, Alan Calder, Jonathan Dursi, Robert Fisher, Timur Linde, Andrea Mignone,Tomek Plewa, Katherine Riley, Andrew Siegel, Dan Sheeler, Frank Timmes, Natalia Vladimirova, Greg Weirs, Mike Zingale

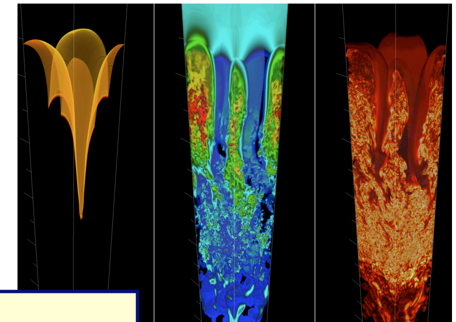
FLASH Capabilities Span a Broad Range…



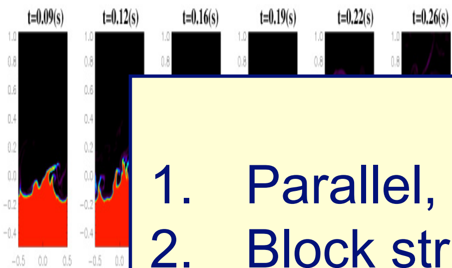
Shortly: Relativistic accretion onto NS







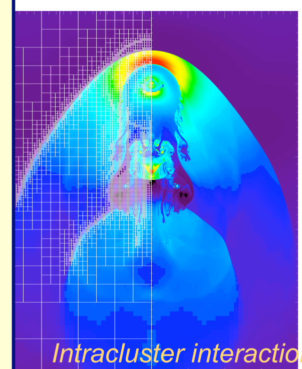
clear Burning



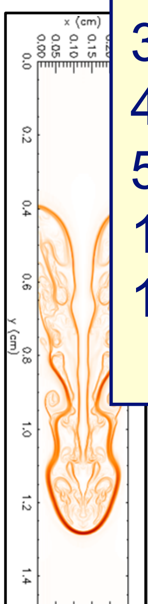
Wave break

The FLASH code

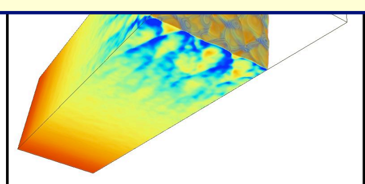
1. Parallel, adaptive-mesh refinement (AMR) code
2. Block structured AMR; a block is the unit of computation
3. Designed for compressible reactive flows
4. Can solve a broad range of (astro)physical problems
5. Portable: runs on many massively-parallel systems
11. Scales and performs well
12. Fully modular and extensible: components can be combined to create many different applications



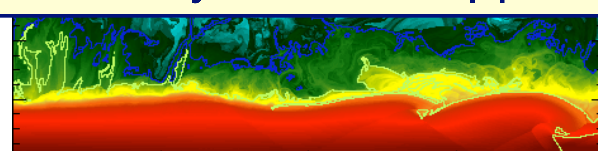
Intracluster interactions



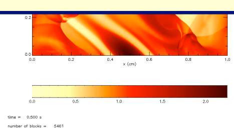
Magnetic Rayleigh-Taylor



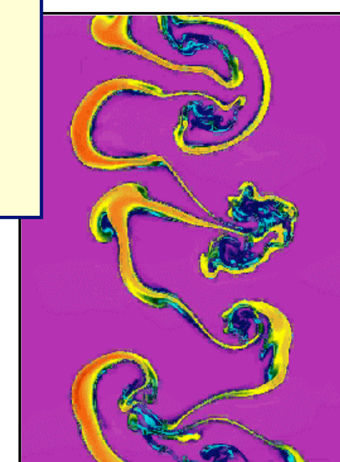
Cellular detonation



Helium burning on neutron stars

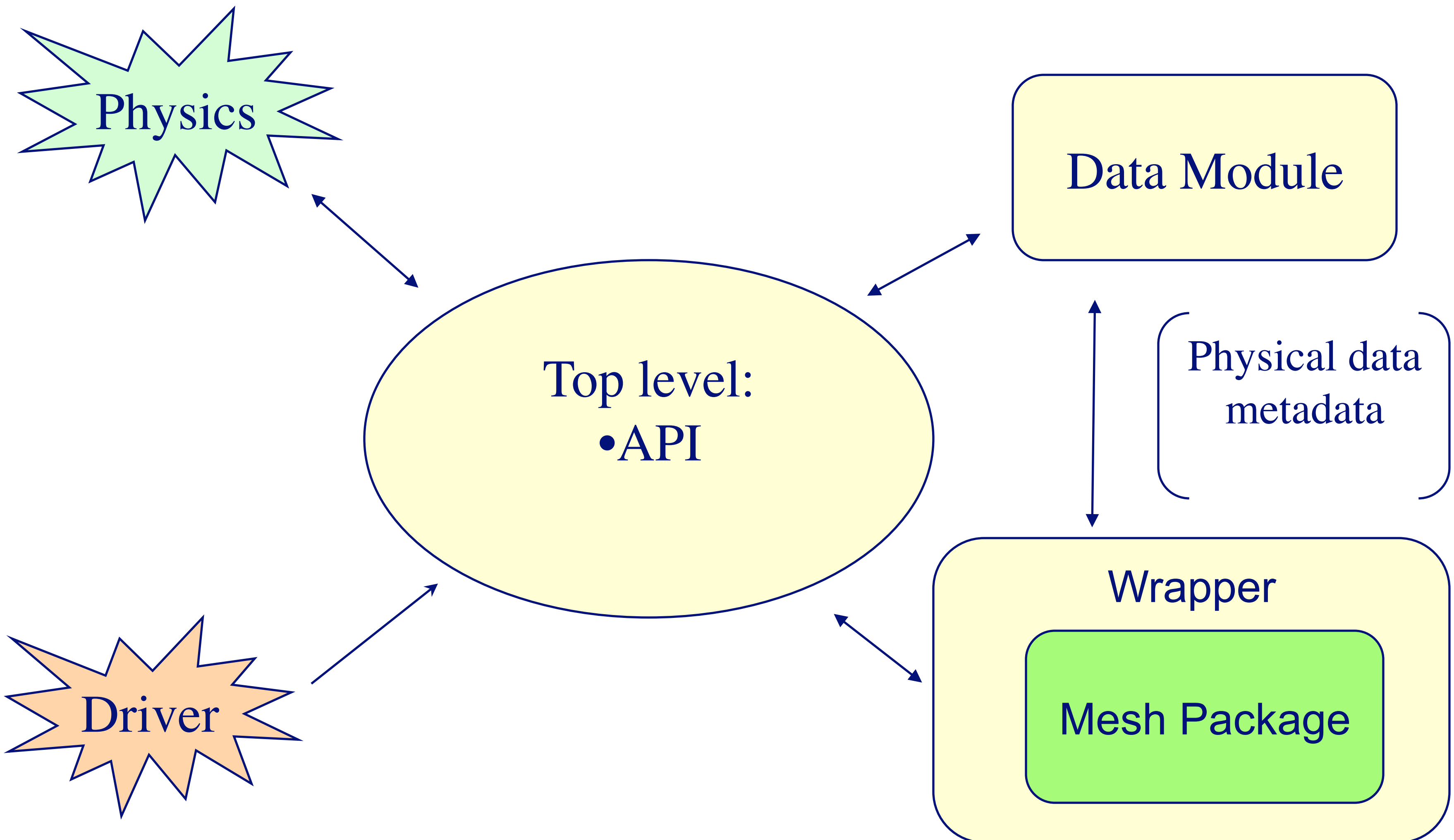


Orzag/Tang MHD vortex



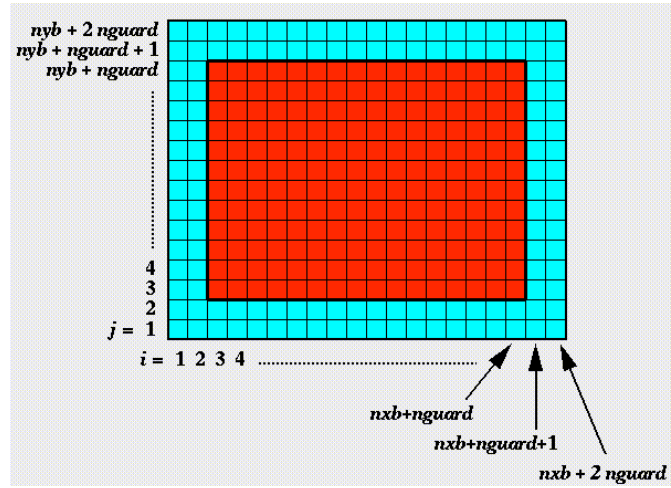
Richtmyer-Meshkov instability

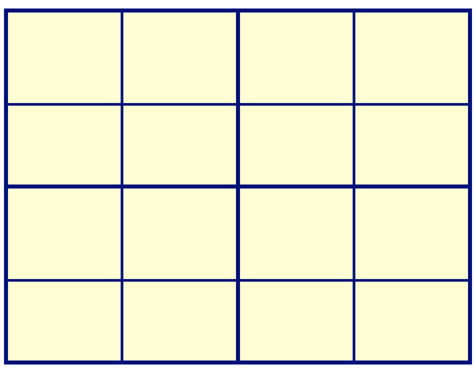
Grid Abstraction Through Unit Architecture



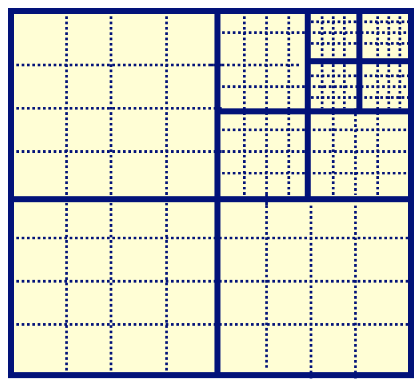
Blocks and Mesh Packages

- Mesh package can be selected at configuration time
- The basic abstraction is a block of interior cells surrounded by guard cells
- Grid unit makes sure that blocks are self contained before being given to the solvers

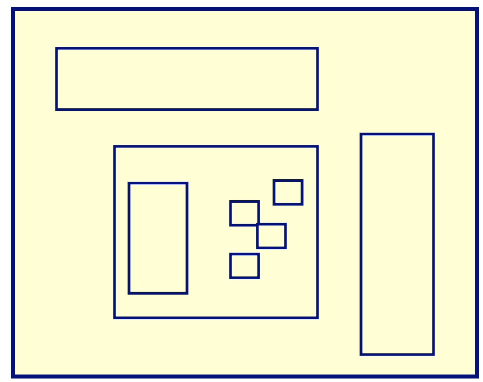




Uniform Grid



Oct tree based AMR

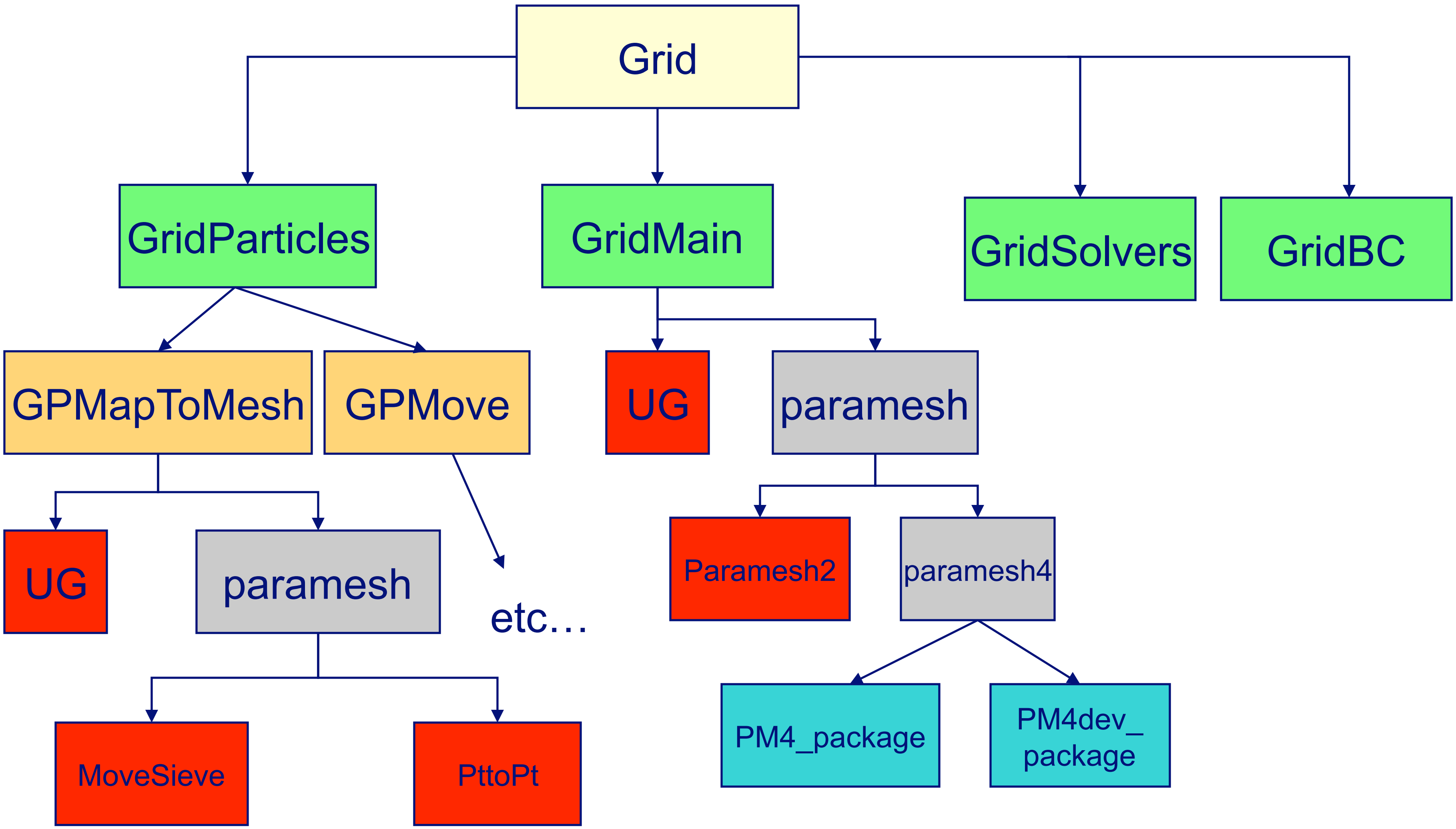


AMR with variable patch size

at concept

testing stage

The Grid Unit Organization



Hierarchical EOS interface Design

- Hierarchy in complexity of interfaces
  - For single point calculation scalar input and output
  - For sections of a block or full block vectorized input and output
    - wrappers to vectorize and configure the data
    - returning derivative quantities if desired
- Different levels in the hierarchy give different degrees of control to the client routines
  - Most of the complexity is completely hidden from casual users
  - More sophisticated users can bypass the wrappers for greater control
- Done with elaborate machinery of masks and defined constants

How FLASH Architecture Helped Unsplit Solver

- To implement un-split time integration
  - Alternative implementation of the Driver unit
  - No impact on other units in the code because of encapsulation
- Use of face centered variables and scratch variables
  - Generalized interfaces for handing guardcells can handle all datatypes
  - Hierarchical design of the Eos unit doesn’t distinguish between grid data structures
- Availability of UG also made it easier to develop the solver
  - Isolate the complexity
  - Easier to create testing framework and diagnostic tools

Unsplit MHD and Hydro Solvers in FLASH3

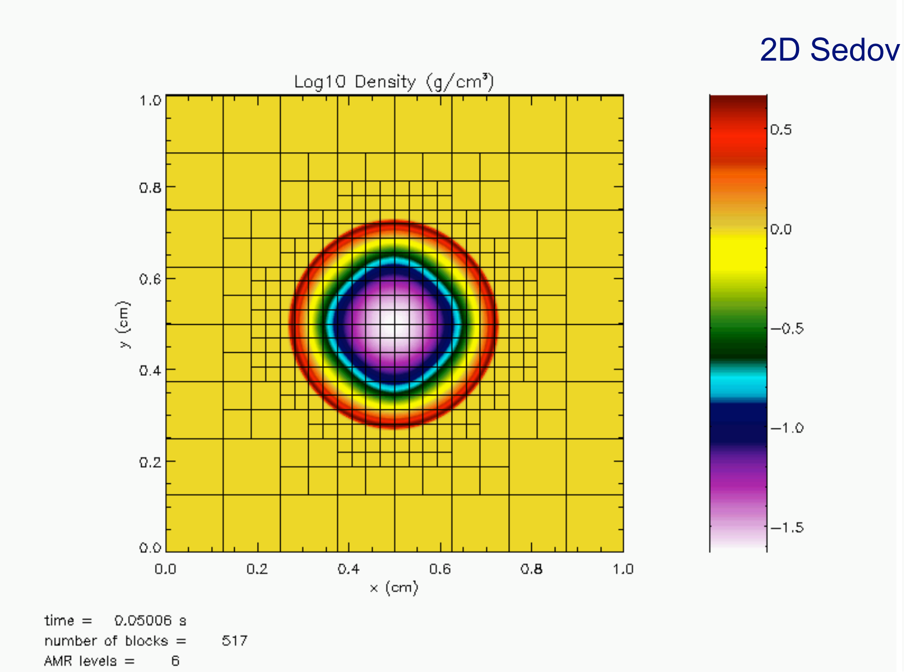
- Physics
  - Ideal and non-ideal flows
    - Magnetic resistivity (MHD), themal conductivity, and viscosity
  - EOS
    - Ideal gamma, multiple gamma, Helmholtz (degenerate EOS)
  - Gravity
  - Multiple species, particles
  - Well tested for wide ranges of plasma flows for MHD: $10^{-6} \le \beta(\equiv p/B_p) \le 10^{6}$

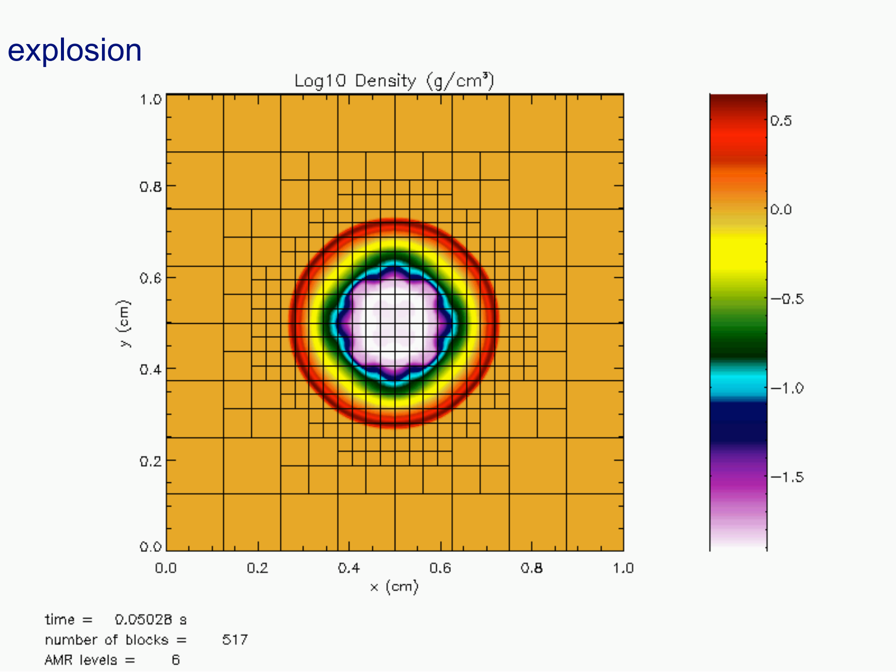
- Implementations and algorithms
  - 2nd order MUSCL-Hancock in space and time (PPM interpolation will be available in future release)
  - Riemann solvers
    - Roe (default), Lax-Friedrichs, HLLE, HLLC for both, and HLLD for MHD
    - Carbuncle, even-odd instability fix for Roe solver
  - Strong shock-rarefaction detection algorithm (Balsara, 1998)
  - Various slope limiters (Minmod, MC, Van Leer, hybrid)
  - Two prolongation methods (Balsara's & direct injection) of divergence-free B fields on AMR for MHD
  - Use of face-centered variables, and edge-centered variable for MHD
  - Wide ranges of CFL limit: CFL < 1 for 1D, 2D and 3D for both solvers

Unsplit Gas Dynamics Hydro Solver

- **Unsplit pure-Hydro solver (New in FLASH3; Lee, 2009)**
  - Reduced version of USM-MHD solver without magnetic and electric fields
  - 2nd order MUSCL-Hancock in space and time
  - Preserves better flow symmetries (Roe solver with Carbuncle instability fix)

2D Sedov explosion



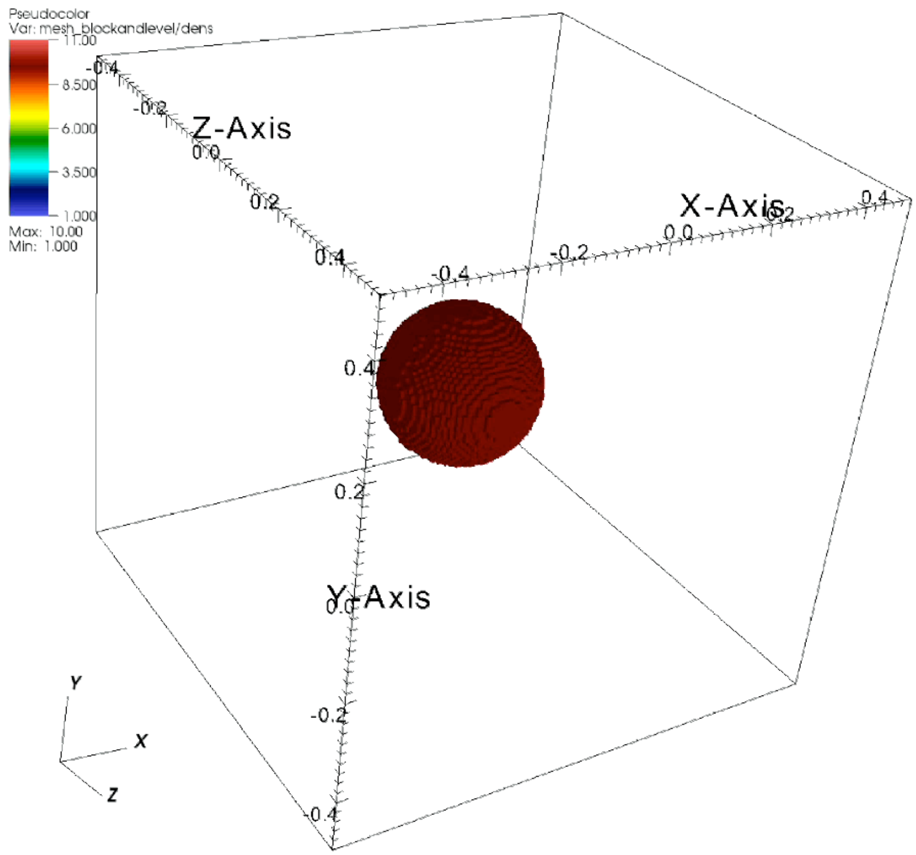


Unsplit MUSCL-Hancock

Split PPM

CFL Stability Test

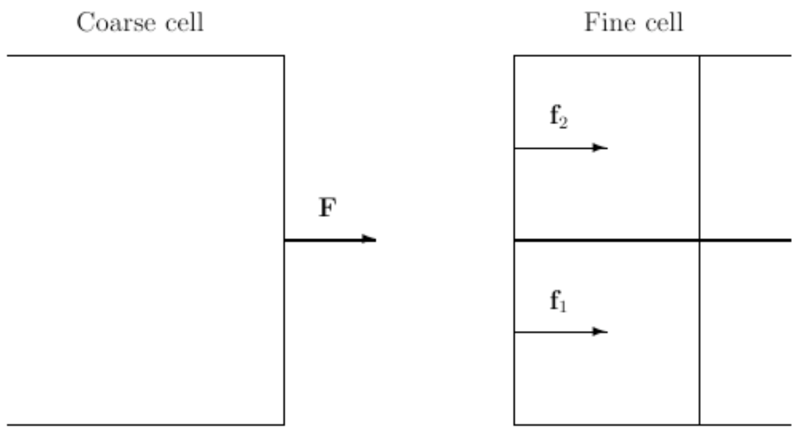
Advecting a 3D density ball in a periodic domain



CFL = 0.8 using the unsplit hydro solver

Unsplit Staggered Mesh MHD Solver on AMR

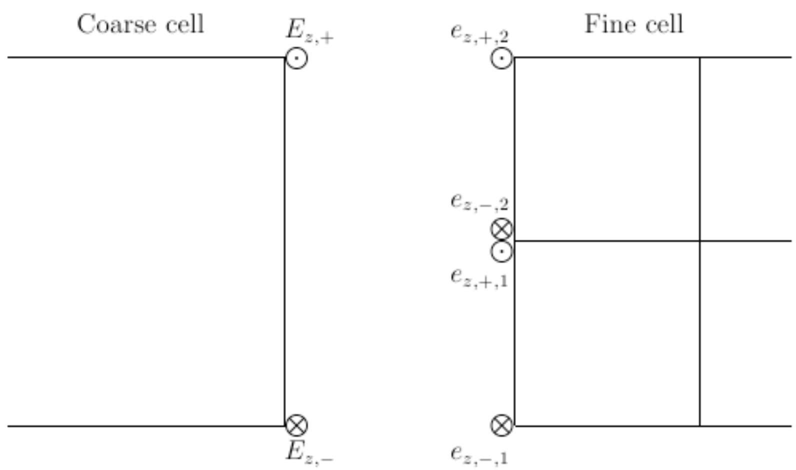
- **Unsplit Staggered Mesh (USM) MHD solver (Lee, 2006; Lee and Deane 2009)**



Flux conservations on fine-coarse boundary

- Conservation of high-order Godunov fluxes on AMR grid
- Grid_conserveFlux.F90 to get consistent flux values:

$$\mathbf{F} = \mathbf{f}_1 + \mathbf{f}_2$$

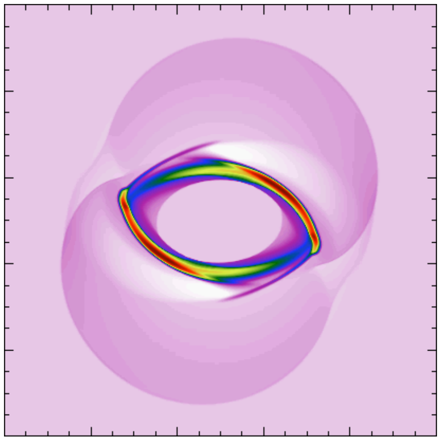


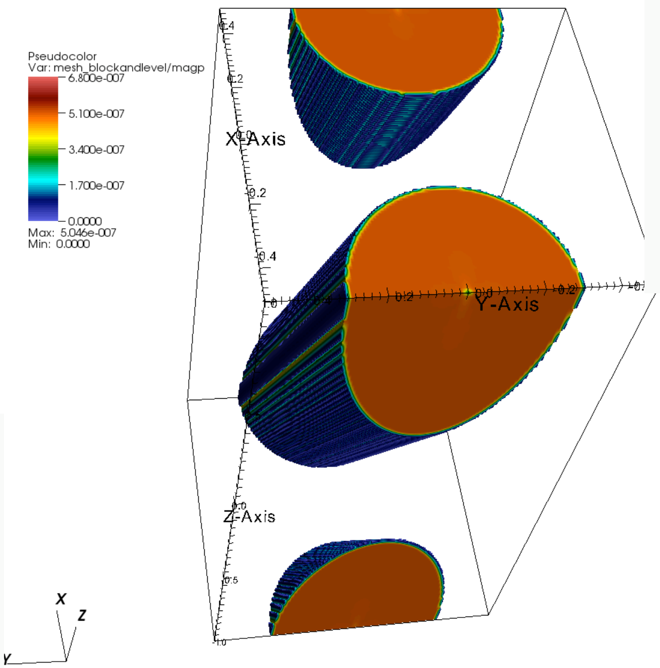
Electric field correction on fine-coarse boundary

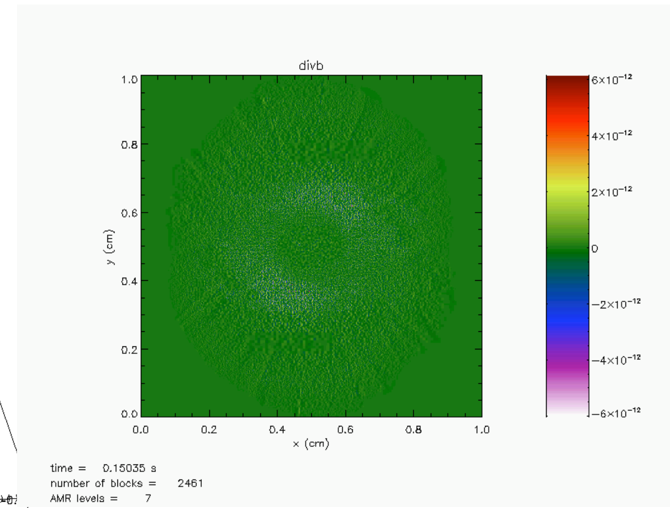
- Use of “edge” structures in PARAMESH
- Grid_conserveField.F90 to get consistent field values:

$$E_{z,+} = e_{z,+,2},\, E_{z,-} = e_{z,-,1}$$

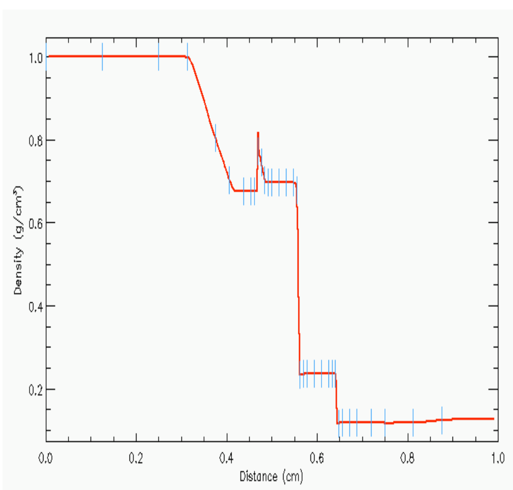
Applications





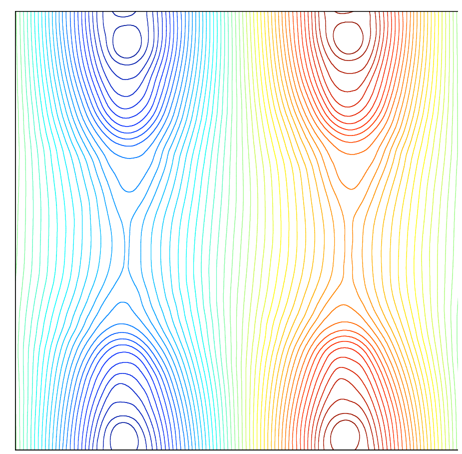


Rotor



Brio-Wu MHD shock-tube

3D Field Loop advection



Magnetic Reconnection

Performance on IBM BG/L