The Chombo Framework for Block-Structured Adaptive Mesh Refinement Algorithms

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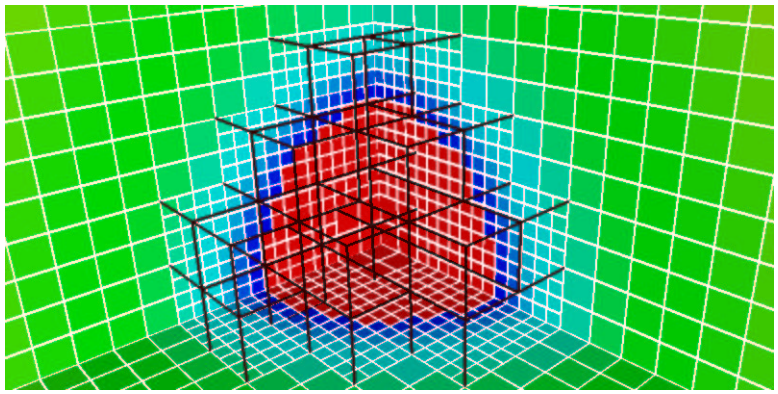
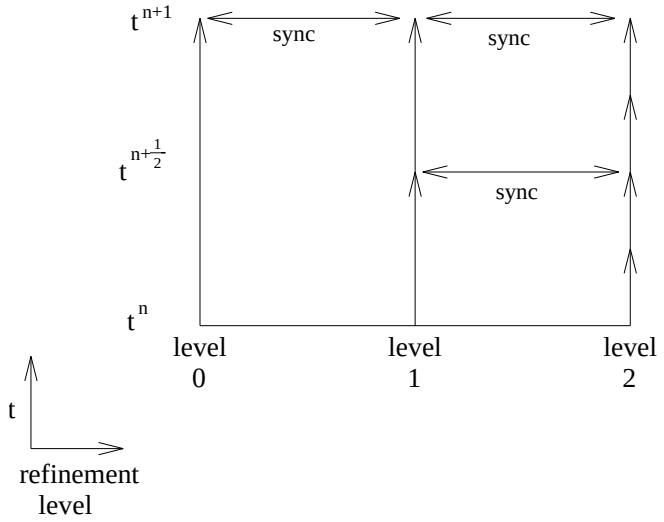
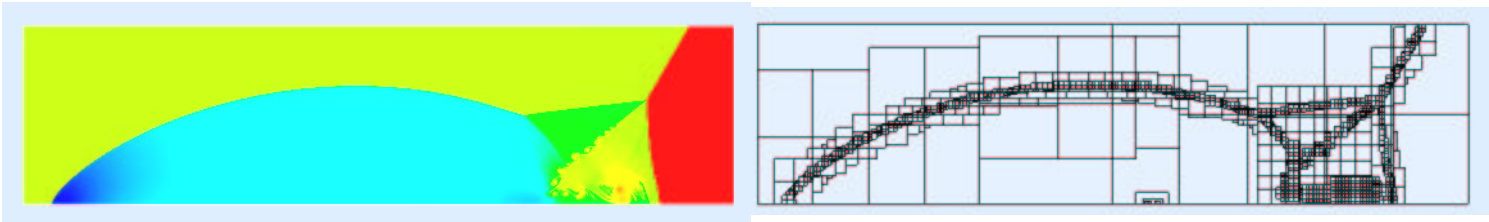
Block-Structured Local Refinement (Berger and Oliger, 1984)





Refined regions are organized into logically rectangular patches

Refinement performed in time as well as in space.



Chombo: a Software Framework for Block-Structured AMR

Requirement: to support a wide variety of applications that use block-structured AMR using a common software framework.

• Mixed-language model: C++ for higher-level data structures, Fortran for regular single-grid calculations.

• Reuseable components. Component design based on mapping of mathematical abstractions to classes.

• Build on public-domain standards: MPI, HDF5, VTK.

• Interoperability with other SciDAC ISIC tools: grid generation (TSTT), solvers (TOPS), performance analysis tools (PERC).

Previous work: BoxLib (LBNL/CCSE), KeLP (Baden, et. al., UCSD), FIDIL (Hilfinger and Colella).

Layered Design

• **Layer 1.** Data and operations on unions of boxes – set calculus, rectangular array library (with interface to Fortran), data on unions of rectangles, with SPMD parallelism implemented by distributing boxes over processors.

• **Layer 2.** Tools for managing interactions between different levels of refinement in an AMR calculation – interpolation, averaging operators, coarse-fine boundary conditions.

• **Layer 3.** Solver libraries – AMR-multigrid solvers, Berger-Oliger time-stepping.

• **Layer 4.** Complete parallel applications.

• **Utility layer.** Support, interoperability libraries – API for HDF5 I/O, visualization package implemented on top of VTK, C API's.

AMR Applications (Layer 4)

• A general driver for an unsplit second-order Godunov method for hyperbolic conservation laws. User provides physics-dependent components (characteristic analysis, Riemann solver).

• Level solvers, AMR multigrid solvers for Poisson, Helmholtz equations.

• Incompressible Navier-Stokes solver using projection method. Includes projection operators for single level, AMR hierarchy. Advection-diffusion solvers.

• Wave equation solver.

• Time-dependent Ginzburg-Landau equation solver.

• Volume-of-fluid algorithm fluid-solid interactions.

AMR Utility Layer

• API for HDF5 I/O.

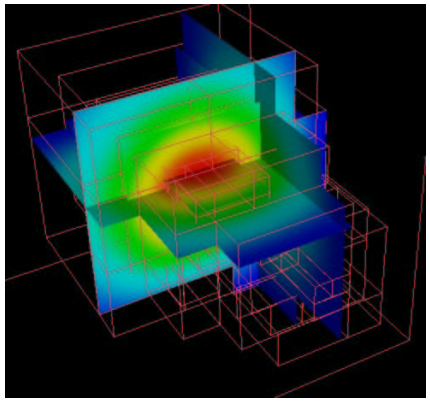
• Interoperability tools. We are developing a framework-neutral representation for pointers to AMR data, using opaque handles. This will allow us to wrap Chombo classes with a C interface and call them from other AMR applications.

• Chombo Fortran - a macro package for writing dimension-independent Fortran and managing the Fortran / C interface.

• `ParmParse` class from BoxLib for handling input files.

• Visualization and analysis tools (ChomboVis).

ChomboVis Interactive Visualization and Analysis Tools



• "AMR-aware"

– Block-structured representation of the data leads to efficiency.

– Useful as a debugging tool (callable from debuggers (gdb))

• Visualization tools based on VTK, a open-source visualization library.

• Implementation in C++ and Python

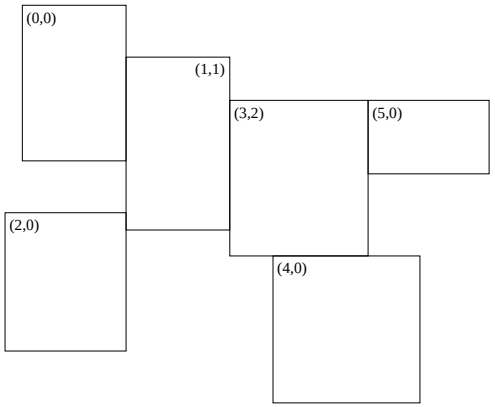
– GUI interface for interactive visualization

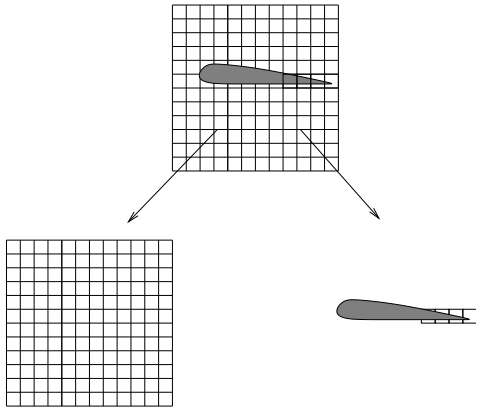
– Command-line python interface to visualization and analysis tools, batch processing capability – goal is a full analysis tool.

• Interface to HDF5 I/O along with C API provides access to broad range of AMR users. ("Framework-neutral")

Mechanisms for Re-use

- **Algorithmic reuse:** Identify mathematical components which cut across applications. Easy example: solvers. Less easy example: Layer 2.
- **Reuse by templating data holders:** Easy example: rectangular array libary – array values are the template type. Less easy example: data on unions of rectangles – "rectangular array" is a template type.





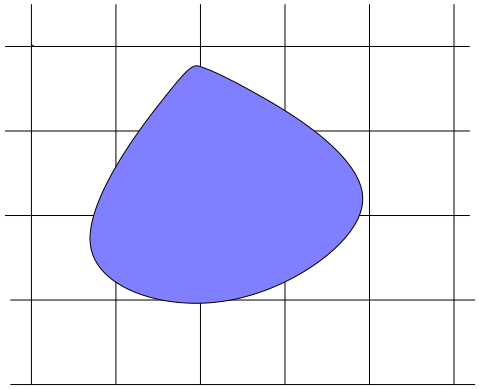
- **Reuse by inheritance:** Control structures (multigrid, CG, Berger-Oliger AMR timestepping) are independent of the data, operations on that data. Use inheritance to isolate the control structure from the details of what is being controlled (interface classes).

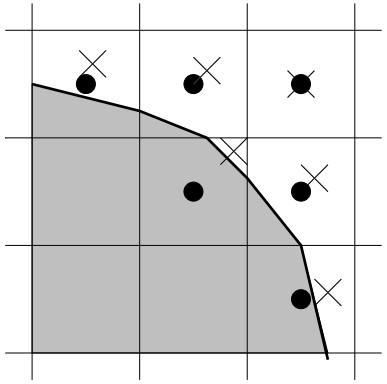
AMR Software Development Milestones

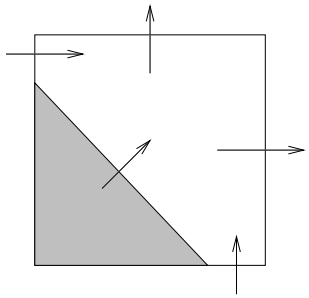
- **Solvers**
  - Constant- and variable-coefficient elliptic solvers for unions of rectangles, AMR hierarchies
  - Hyperbolic PDE packages – user supplies physics-dependent components.
  - Parabolic solvers for AMR with refinement in time
  - AMR-PIC method for RF accelerator modeling.
  - Shortly-Weller solver for nodal-point discretization of Poisson's equation in complex geometries.
- **Interoperability**
  - Interface to PAPI performance monitoring tools
  - Chombo interface to Hypre multigrid solver package.
  - Design and implementation of framework-neutral AMR data alias, based on AMR CCA proposal.
  - Preliminary interface to UW CLawPack hyperbolic package.

Cartesian Grid Representation of Irregular Boundaries (`EBChombo`)

Based on nodal-point representation (Shortley and Weller, 1938) or finite-volume representation (Noh, 1964).





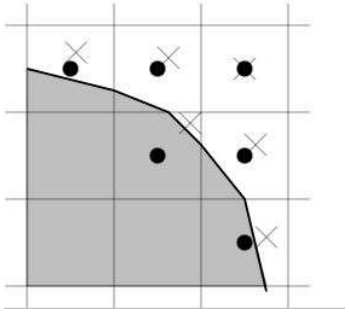


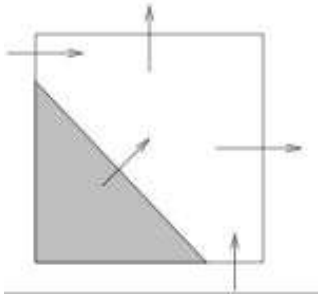
Advantages:

- Grid Generation is tractable
- Good discretization technology (e.g. finite differences on rectangular grids, geometric multigrid)
- Straightforward coupling to AMR

Embedded Boundary Discretization of Conservation Laws

$$\nabla \cdot \vec{F} = \rho \ , \ \vec{F} = \nabla \phi \qquad \frac{\partial U}{\partial t} + \nabla \cdot \vec{F}(U) = 0$$





- Primary dependent variables approximate values at cell centers.

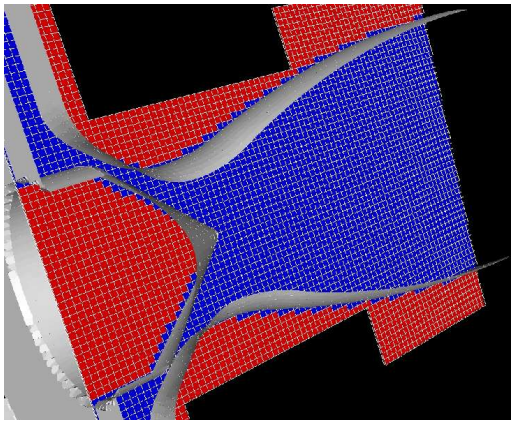
- Divergence theorem over each control volume leads to "finite volume" approximation.

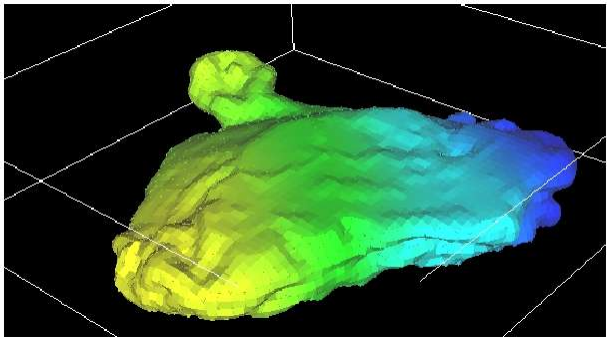
$$\nabla \cdot \vec{F} \approx \frac{1}{\kappa h^d} \int \nabla \cdot \vec{F} dx = \frac{1}{\kappa h} \sum \alpha_s \vec{F}_s \cdot \vec{n}_s + \alpha_B \vec{F} \cdot \vec{n}_B \equiv D \cdot \vec{F}$$

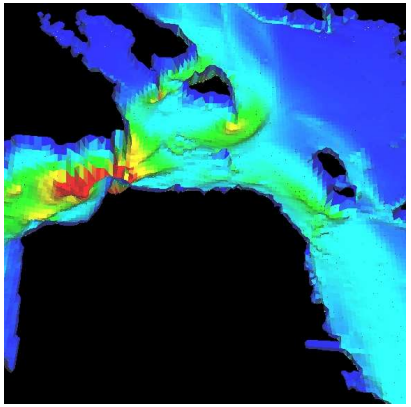
- Away from boundaries, methods reduce to standard conservative finite difference discretizations.

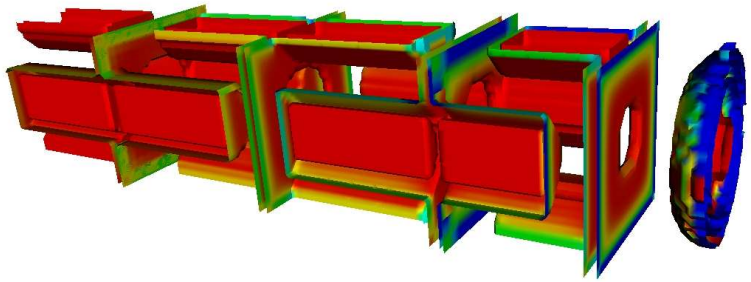
Embedded Boundary Methods for PDEs

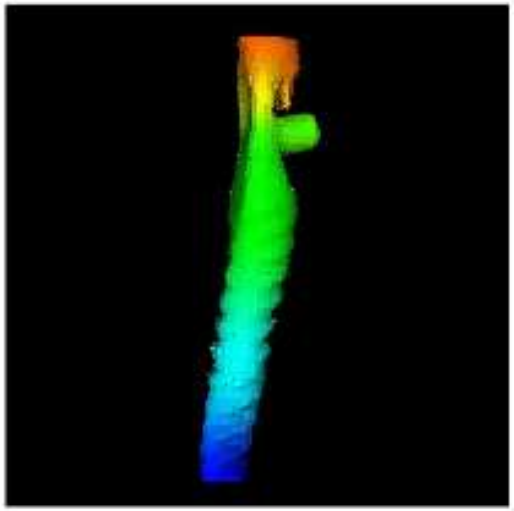
Easy grid generation, starting from CAD, image, or geophysical data.

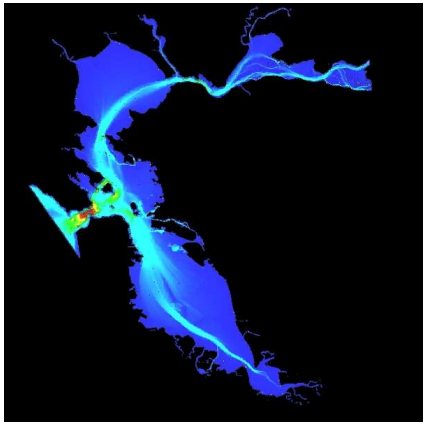












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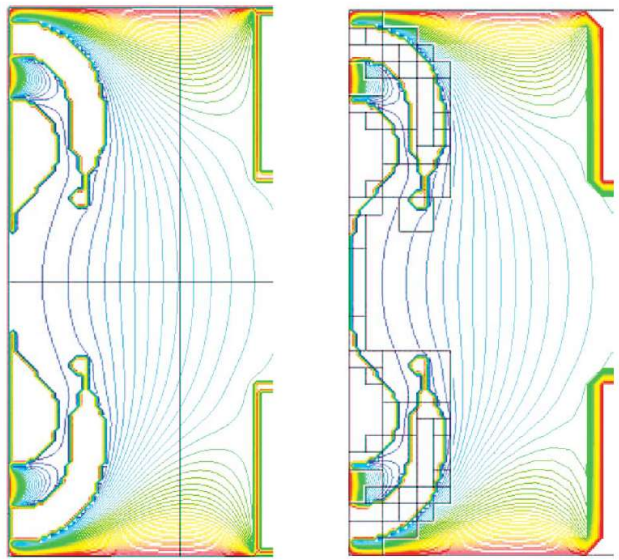
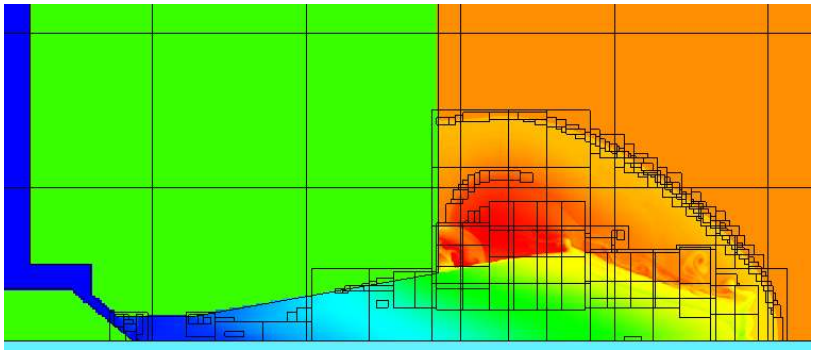
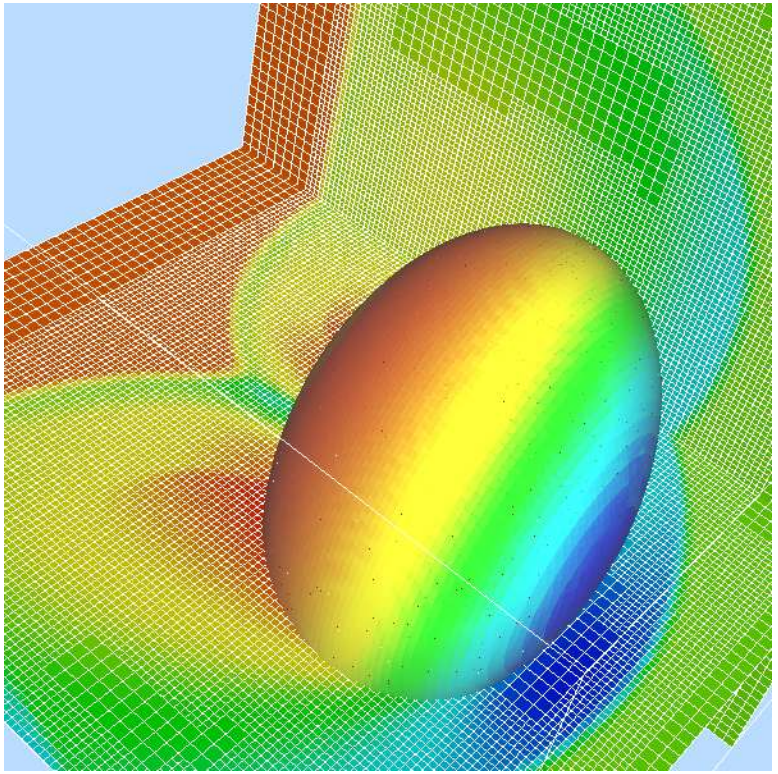
Embedded Boundary Methods for PDEs

Natural coupling to adaptive mesh methods.



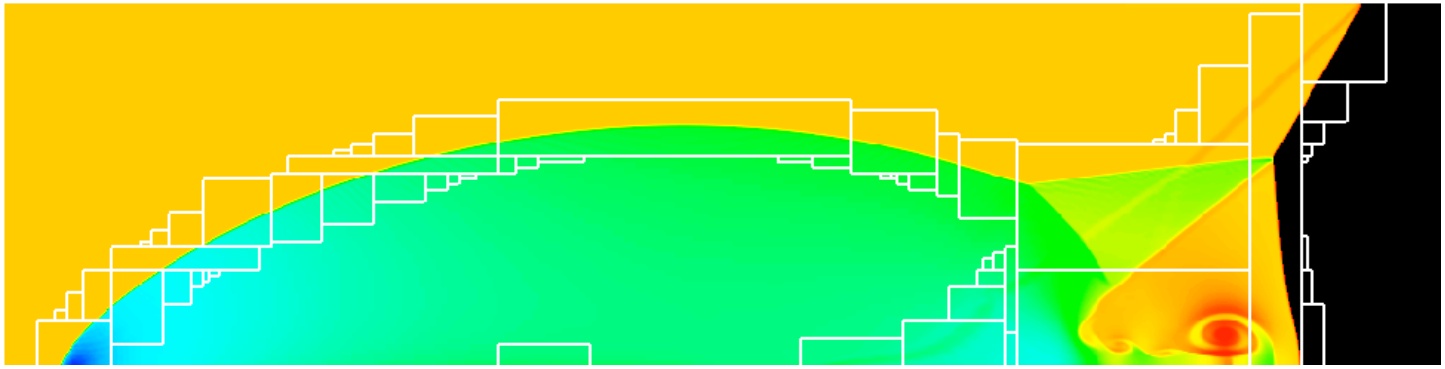


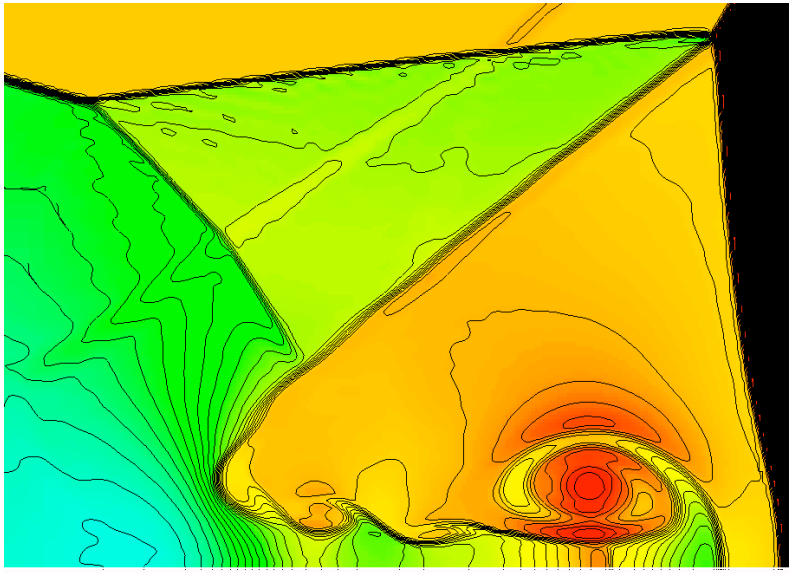


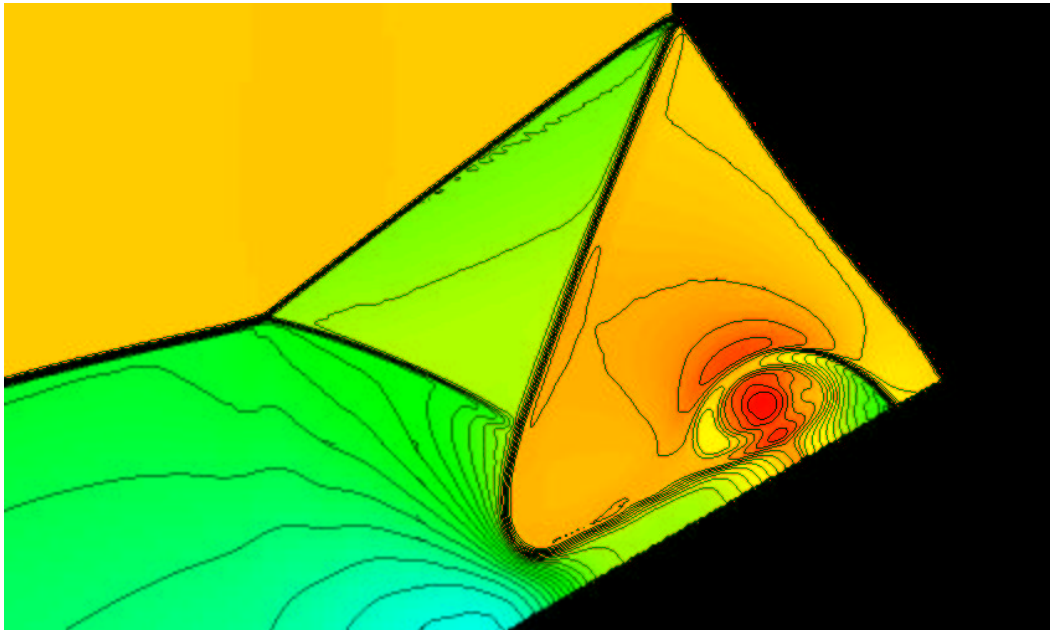
Gas Dynamics

Unsplit higher-order Godunov scheme with AMR for hyperbolic systems of equations (AMRGodunov).

Includes flux correction at coarse-fine interfaces for conservation.







Elliptic Equations

AMR elliptic solver – used as standalone code (AMRPoisson) or as solver library (AMRElliptic: AMRSolver class)

- Implements a multigrid solver for an AMR hierarchy of refined grids.
- Uses multilevel discretizations of the elliptic operators to maintain accuracy in the presence of coarse-fine interfaces.

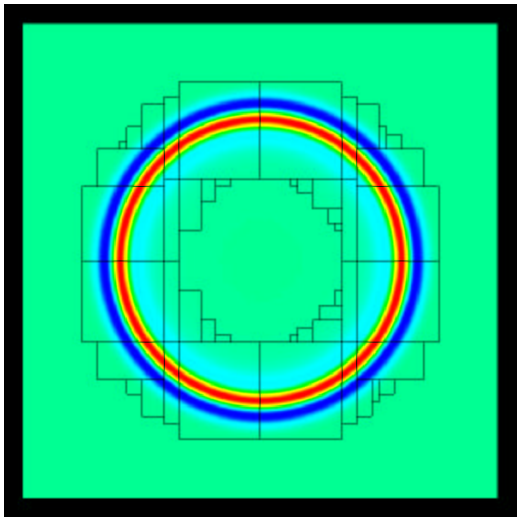
Wave Equation Solver

• Write second-order wave equation as first-order system in time.

$$\frac{\partial \varphi}{\partial t} = \pi$$
$$\frac{\partial \pi}{\partial t} = \Delta \varphi$$

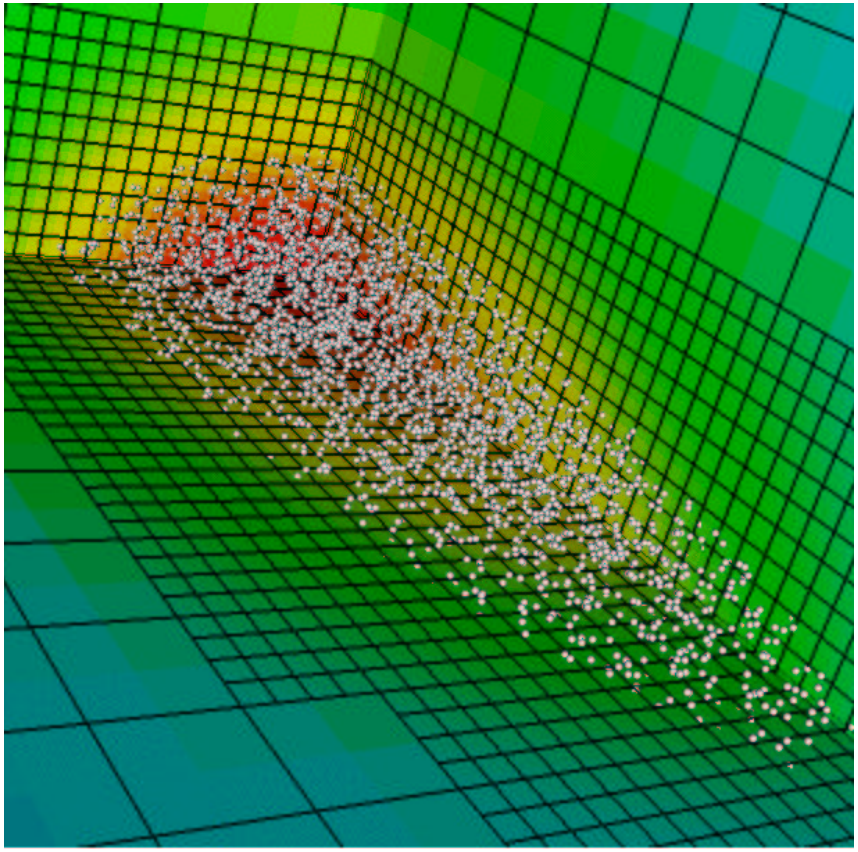
• Discretize Laplacian on AMR grid using RK4 in time, quadratic interpolation in space for coarse-fine boundary conditions.

• Refinement in time: linear interpolation in time for coarse-fine boundary conditions, treat π as a conserved quantity for the purpose of refluxing.



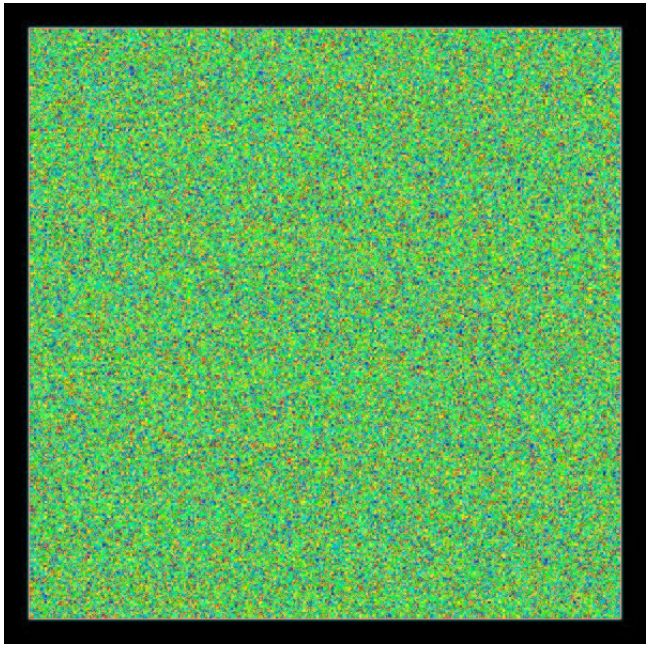
Particles

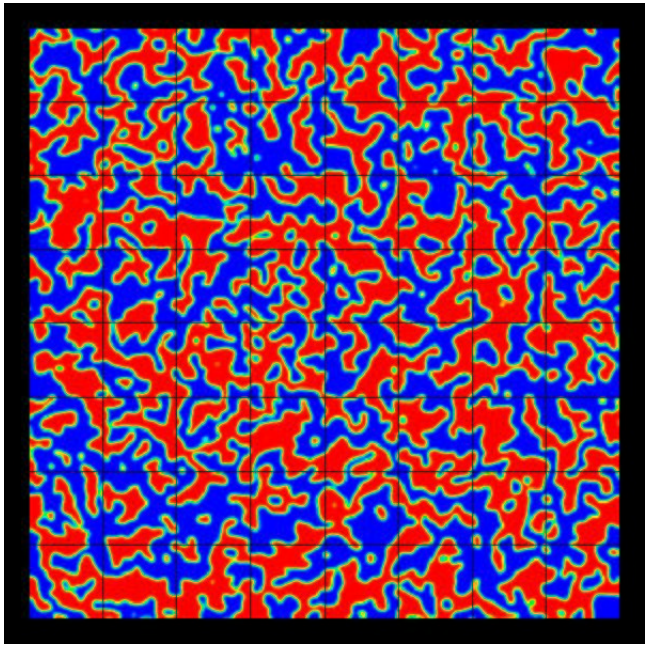
AMR-PIC code used in accelerator modelling

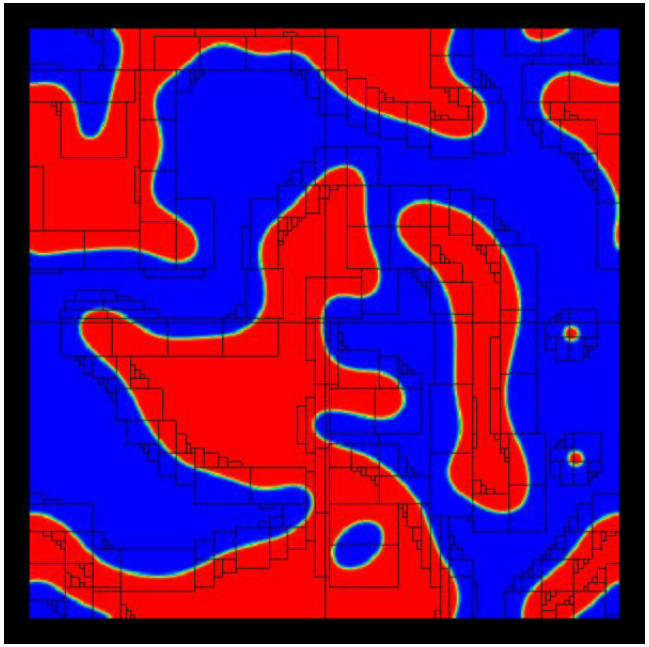


Time-dependent Ginzberg-Landau Equations

Diffusion equation with a nonlinear source term – used to model phase-field dynamics (crystal growth, etc) (with F. Alexander, LANL)



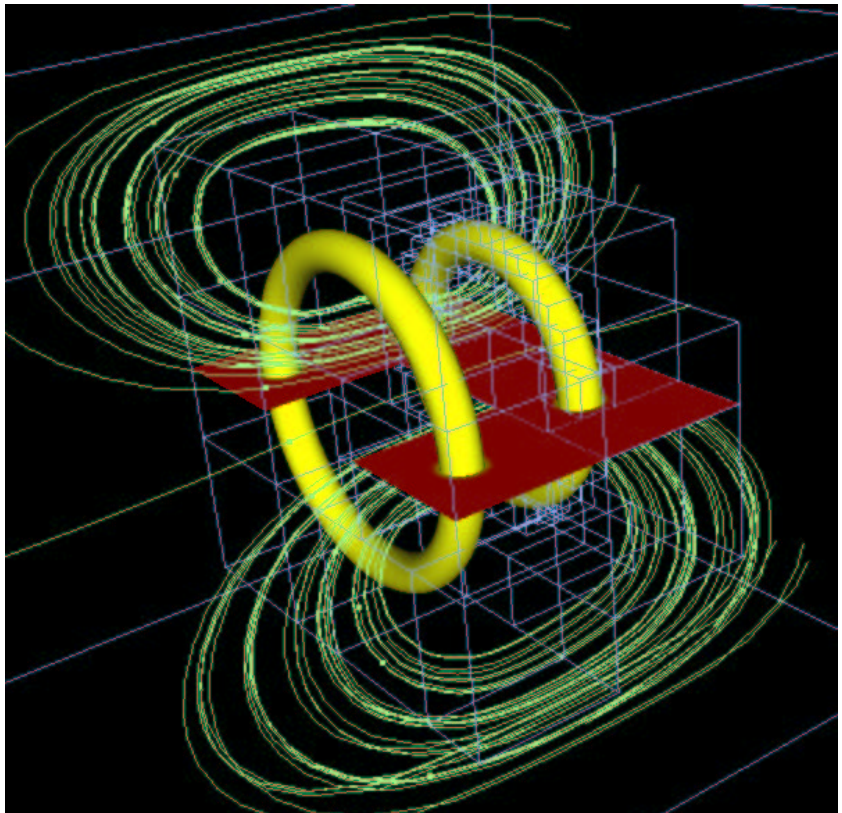




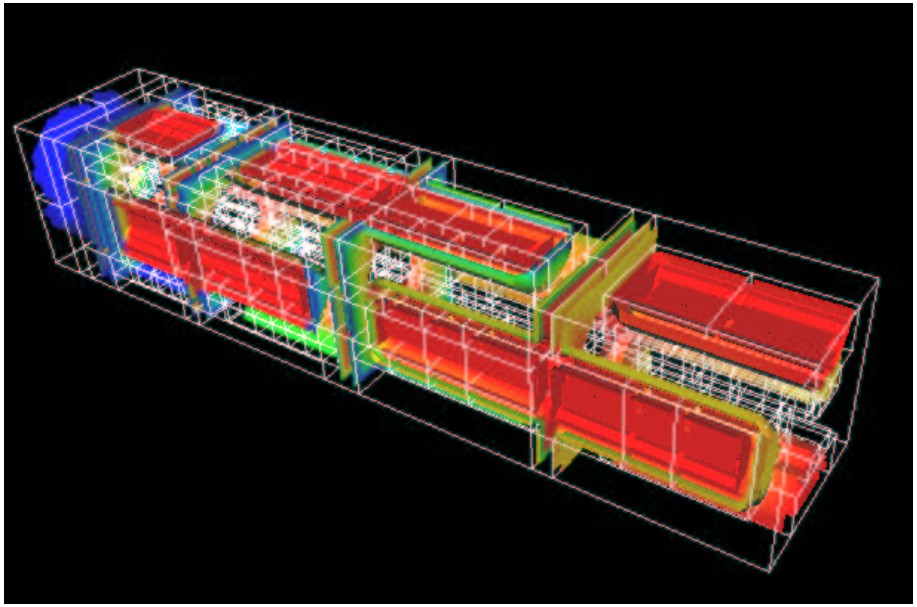
Incompressible AMR Navier-Stokes

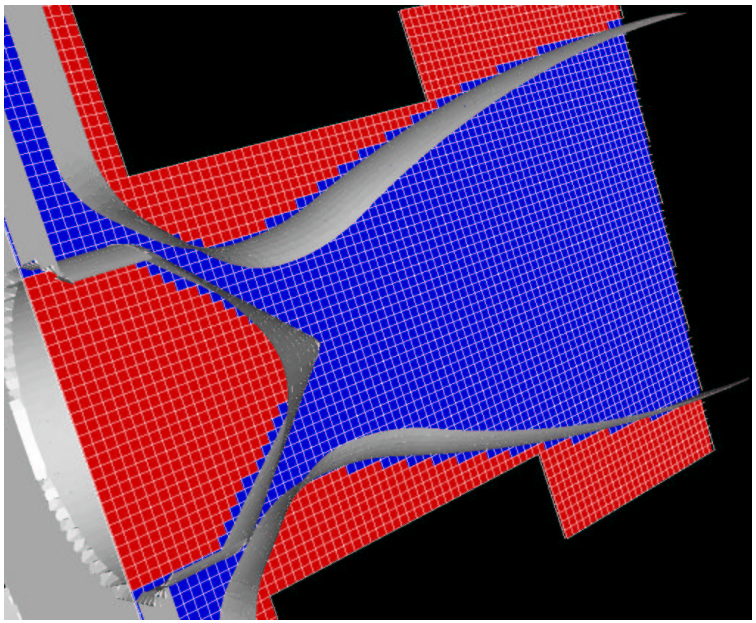
AMRINS code

- Implements a projection method for incompressible viscous flow.
- Freestream preservation maintained approximately in the presence of coarse-fine interfaces using an advection velocity correction computed using an auxiliary advected scalar.
- Viscous updates performed using L_0-stable semi-implicit Runga-Kutta scheme



Accelerator Design

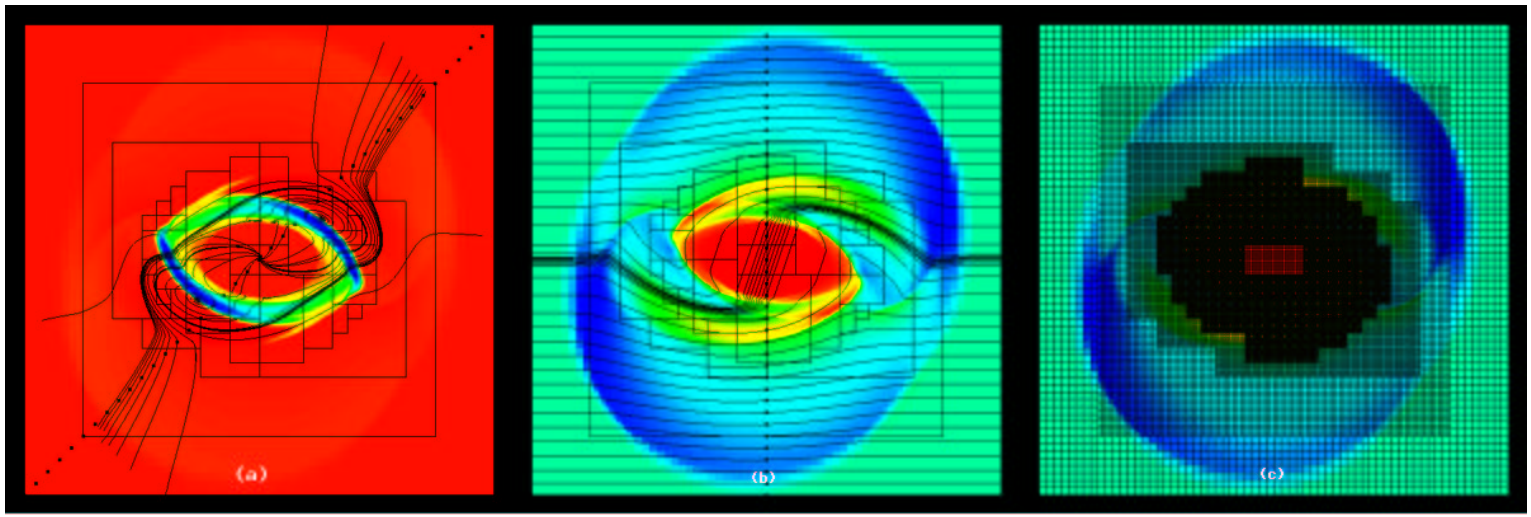




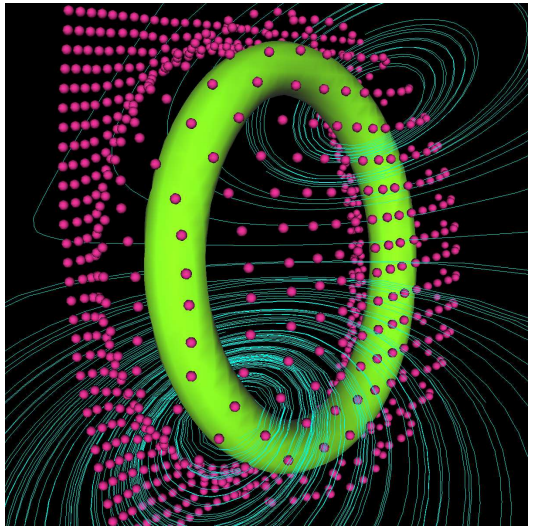
Magnetohydrodynamics (Samtaney, et. al., 2003)

Fluid representation: AMR for magnetohydrodynamics, based on semi-implicit methods.

- Explicit upwind discretizations for hyperbolic terms.
- Implicit discretizations for parabolic operators.
- Projection to enforce $\nabla \cdot \vec{B} = 0$ constraint.



Other Current Applications (partial list)

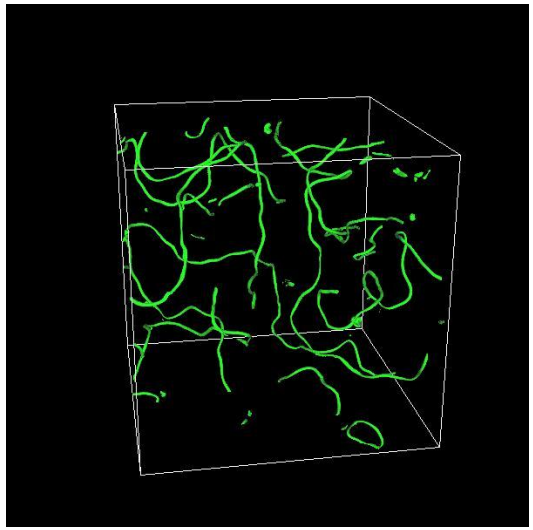


• Star formation; multiphase microgravity flows (NASA CT Program).

• Solid mechanics (G. Miller, UC Davis and LBNL).

• Cosmology (F. Miniati, MPI-Garching).

• Low-Mach number geophysical, astrophysical flows (UC Davis, Univ. of Chicago ASCI Center).



• Semi-local strings (J. Borrill, LBNL).

Chombo, ChomboVis available from the ANAG website:

- http://seesar.lbl.gov/ANAG/software.html
- Chombo version 1.4.6 released April 28, 2004
- ChomboVis version 4.4.1 released October 1, 2004.

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