

Cartesian Grid Embedded Boundary Methods for Solving Applied PDEs

Terry J. Ligocki, Phil Colella, Dan Graves
Peter Schwartz, Brian Van Straalen

Applied Numerical Algorithm Group
Lawrence Berkeley National Laboratory
Berkeley, CA

ICIAM 2003 Minisymposium
Cartesian Grid Methods for Embedded Boundaries
Sydney, Australia
July 8, 2003

Overview

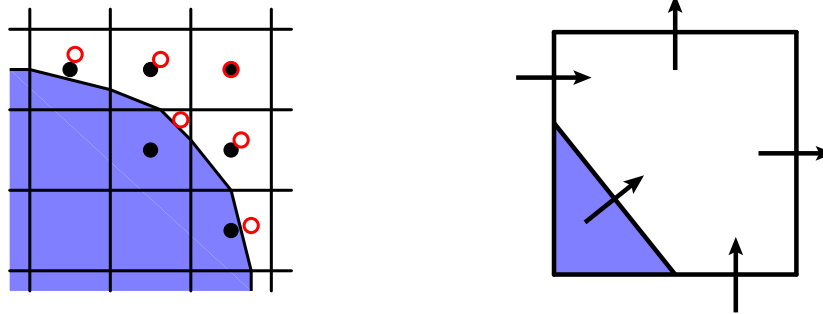
- Algorithms
 - Fundamental Concepts
 - Recent Developments
- Software
 - Design Overview
 - Grid Generation
- Results
 - AMR Hyperbolic Solver
 - Diffusion with a Moving Boundary
 - Wind over Mountains
- Future & Related Work
- Acknowledgments

Algorithms - Fundamental Concepts

- Consider PDEs written in conservation form:

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

- Primary dependent variables approximate values at centers of Cartesian cells



- Divergence theorem over each control volume leads to “finite volume” approximation for $\nabla \cdot \vec{F}$ (fluxes are at centroids):

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

Algorithms - Fundamental Concepts (cont.)

- Away from the boundaries, method reduces to standard conservative finite difference method
- $D \cdot \vec{F}^h$ is consistent and accurate enough on cut cells to obtain 2nd order solution accuracy
- $D \cdot \vec{F}^h$ seems to be singular from both the standpoint of stability and accuracy - the elliptic and hyperbolic cases are handled differently

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

Algorithms - Recent Developments

- **Hyperbolic PDEs:**

- Consistent, conservative discretization with small control volume stability using weighted flux computation and redistribution

- **Elliptic PDEs:**

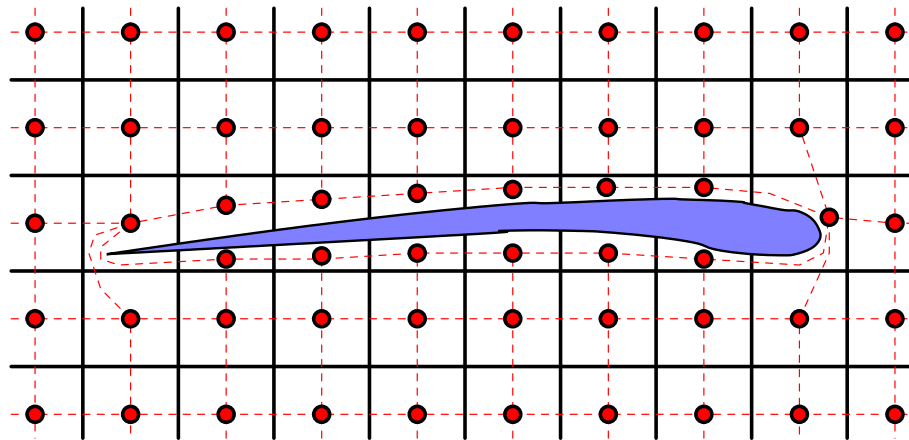
- Consistent, stable flux calculation in 2D using linear interpolation and in 3D using bilinear interpolation

- **Parabolic PDEs:**

- 2^{nd} order accurate, L_0 -stable implicit Runge-Kutta (Twizell, Gumel, and Arigu - 1996)
- Moving boundaries represented as a sequence of equivalent fixed boundary problems (McCorquodale, Colella, Johansen - 2001)

Software - Design Overview

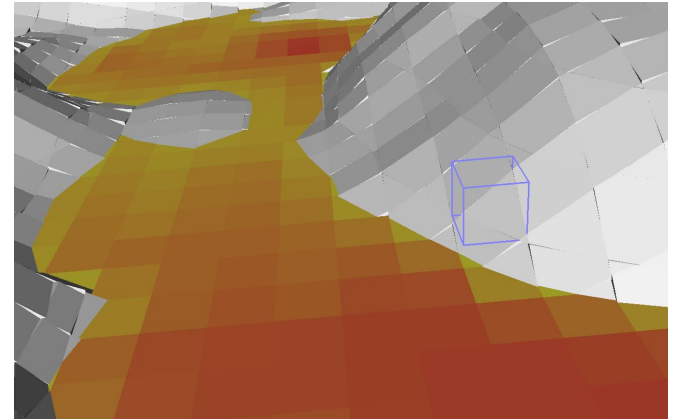
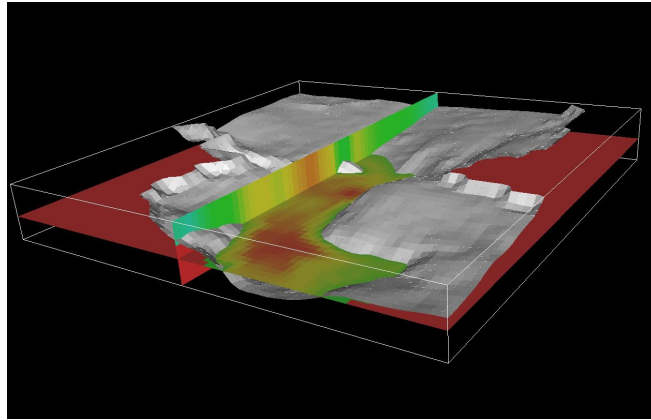
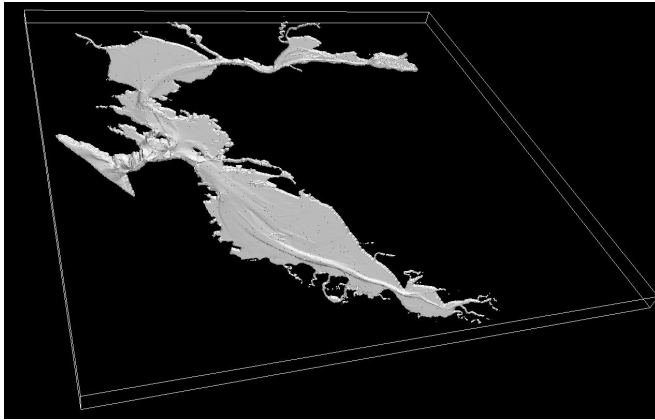
We generalize rectangular array abstractions to represent more general graphs that map into the rectangular lattice \mathbb{Z}^D . The nodes of the graph are the control volumes, while the arcs of the graph are the faces across which fluxes are defined.



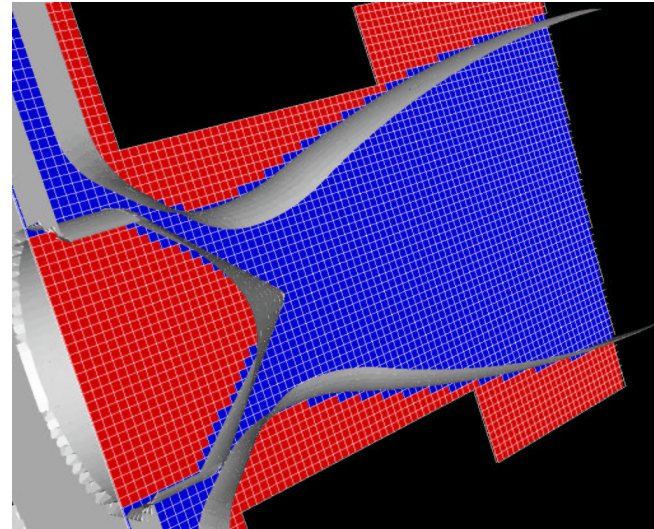
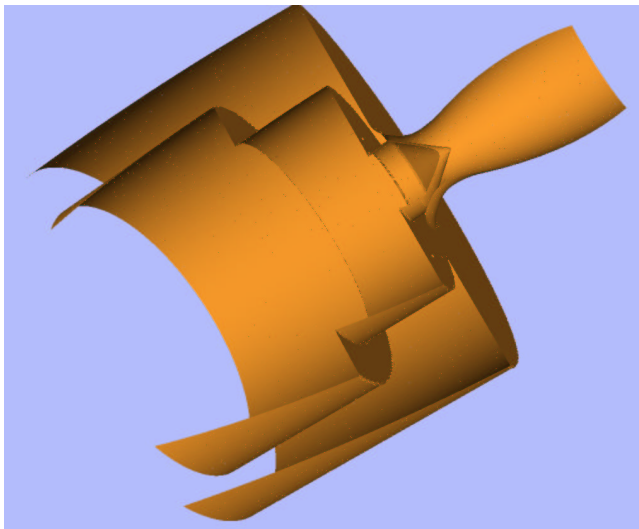
	EB Chombo
Index space = \mathbb{Z}^D	EBIndexSpace
Index (point) $\in \mathbb{Z}^D$	VolIndex, FaceIndex
Rectangular set of indices	EBISBox
Rectangular array	BaseEBCellFAB, BaseEBFaceFAB

Software - Grid Generation

- Cut cell generation via local function values:



- Cut cell generation via CAD description and Cart3D:



Results - AMR Hyperbolic Solver

Dan Graves

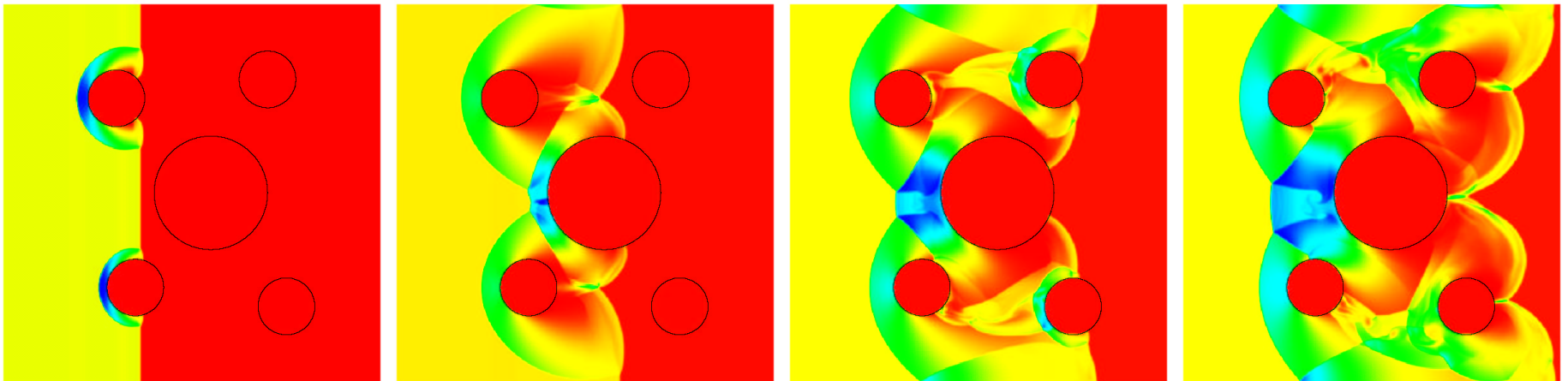
Goal: EB AMR Hyperbolic Solver using unsplit Godunov scheme

Status:

- 2D, 2^{nd} order accurate, x-y/r-z solver
- 3D, 2^{nd} order accurate solver underway

Issues:

- 2^{nd} order accurate, robust discretization of irregular control volume
- Performance - time and space
- Parallel load balancing



Results - Diffusion with a Moving Boundary

Peter Schwartz

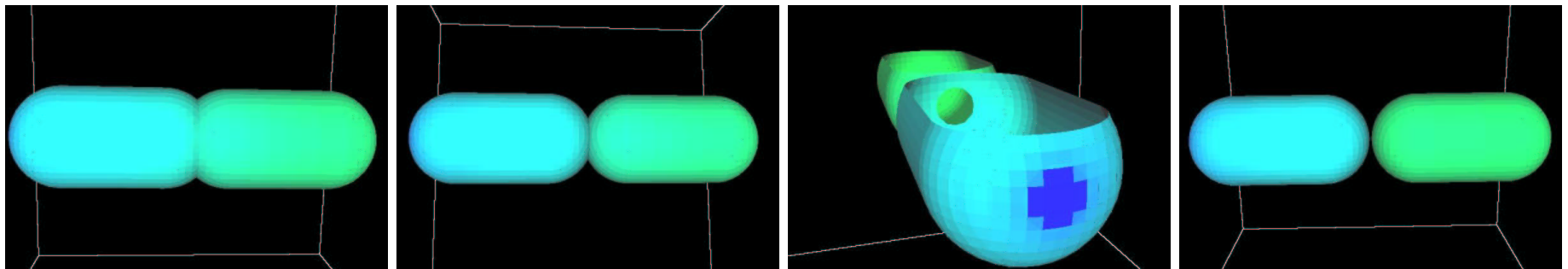
Goal: Moving boundary with diffusion on interior and boundary with chemical coupling between boundary and interior

Status:

- 2^{nd} order accurate interior diffusion with a stationary boundary
- 2^{nd} order accurate interior diffusion with a moving boundary underway
- 1^{st} order accurate coupling of chemistry using operator splitting

Issues:

- Geometry approximation consistent with the divergence theorem
- Stability of operator stencil in 3D
- Interactions between the interior and the surface
- Operator splitting to include chemistry and moving boundaries



Results - Wind over Mountains

Caroline Gatti-Bono

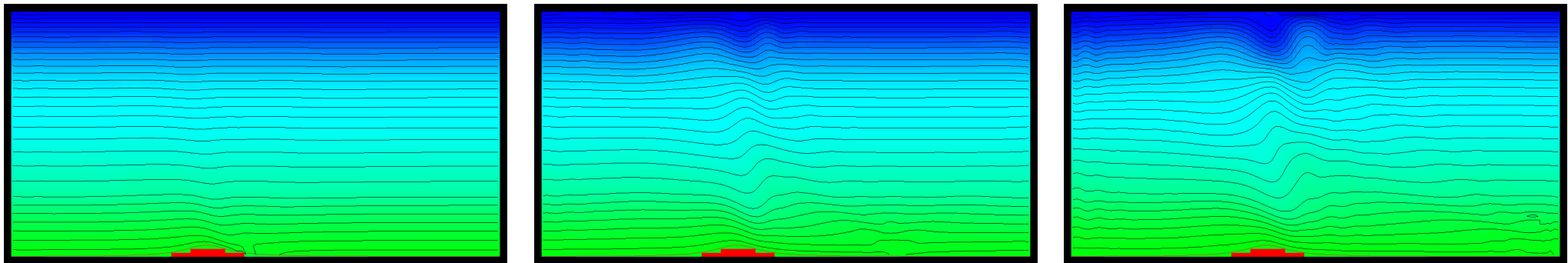
Goal: 3D flow over mountains for climate prediction

Status:

- 2D anisotropic, non-hydrostatic, allspeed formulation (Colella and Pao - 1999) with gravity
- Testing and validation underway

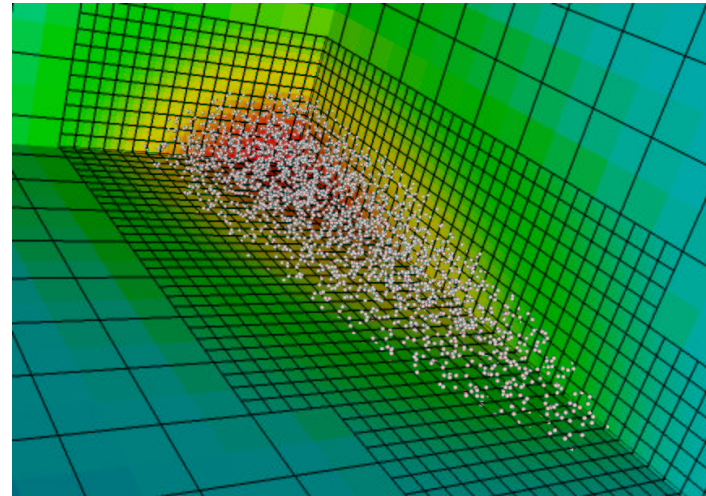
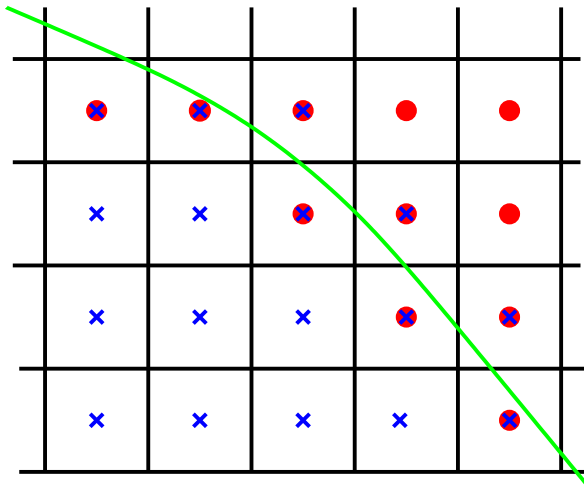
Issues:

- Anisotropic multigrid with line relaxation
- Higher order intersection points between geometry and cell boundaries for scalar advection
- 2^{nd} order accurate, robust discretization of irregular control volume



Future & Related Work

- Future:
 - BIOMEMS
 - Environmental Simulations
 - Magnetohydrodynamics (MHD)
- Related:
 - Multifluid AMR
 - Particle AMR



Acknowledgments

Work at the Lawrence Berkeley National Laboratory is sponsored by the US Department of Energy Office of Science SciDAC program under contract DE-AC03-76SF00098.