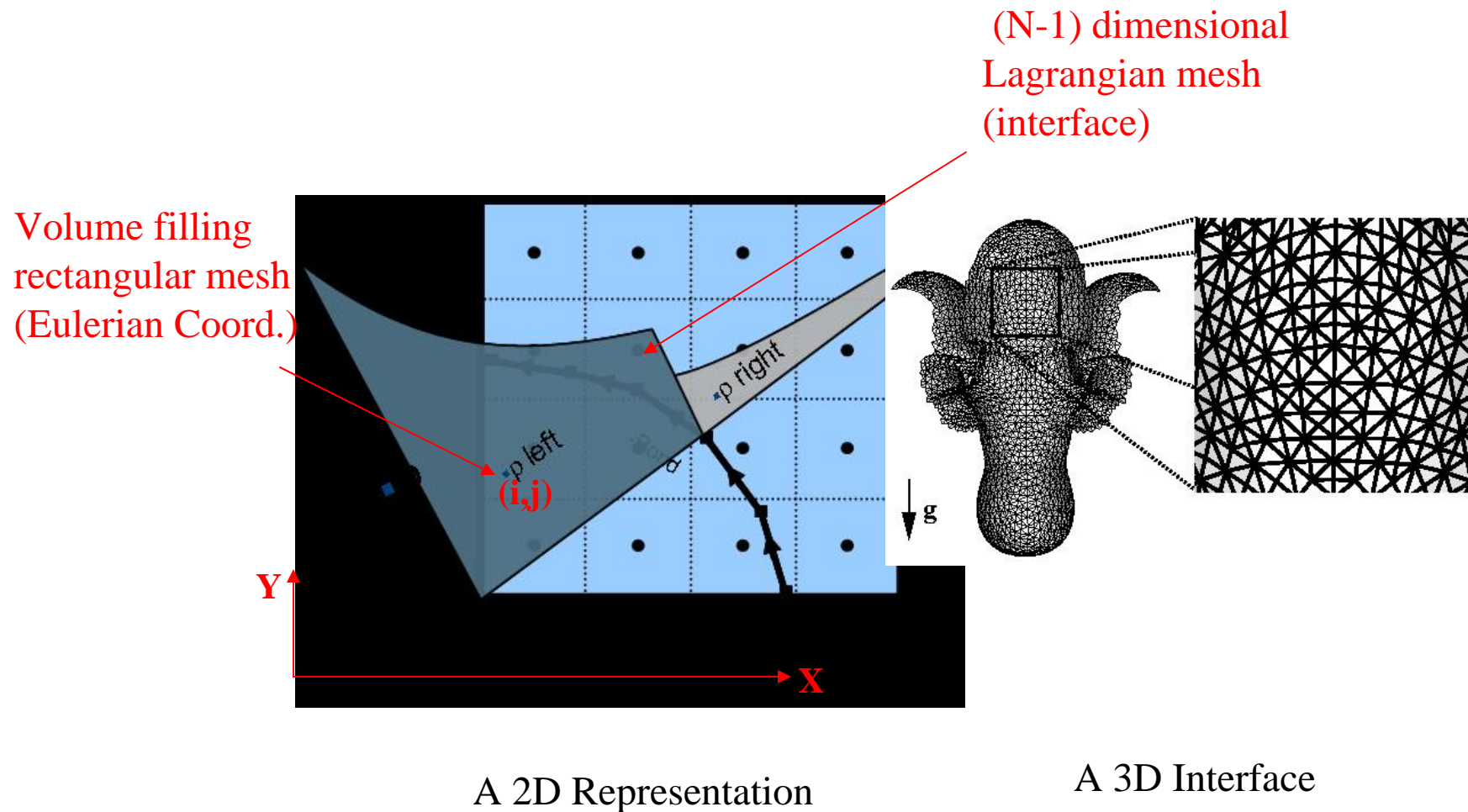# *FronTier* Challenges toward Petascale Computing

*Xiaolin Li and the FronTier team*
*(J. Glimm, X. Jiao, R. Samulyak, W. Bo, B. Fix,*
*R. Kaufman, et al)*
*Department of Applied Math and  Statistics*
*SUNY at Stony Brook*

# The Discrete Mesh Representation in Front Tracking



(N-1) dimensional Lagrangian mesh (interface)

Volume filling rectangular mesh (Eulerian Coord.)

(i,j)

p left

p right

Y

X

g

A 2D Representation

A 3D Interface

# Front Tracking: Scientific applications to interfacial physics, the methodology and software

Front tracking was first introduced
By Richtmyer in 1950's. It was
Used by Moretti for computation
In aerodynamics problems.

Extension to 2D and 3D started
By J. Glimm and O. McBryan
In 1980's at Courant Institute.
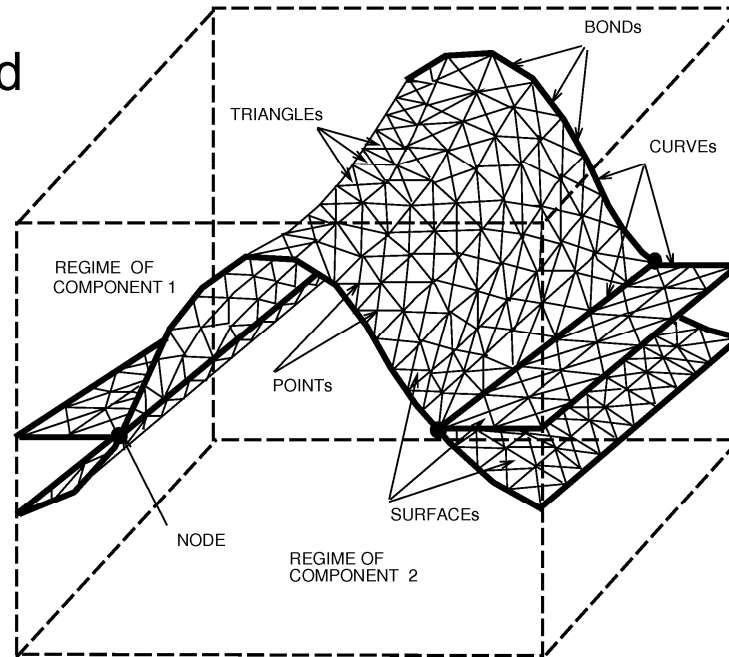


1. **2006-2008, over 26,000 new lines of code, removal of hundreds of run-time bugs, set up benchmarks.**
2. **Collaborations with ANL, BNL, LLNL, ORNL, PNNL, Oxford.**
3. **Over 20 publications and many conference presentations.**
4. **Implemented iMesh interface, support SciDAC applications.**
5. **Interoperability with Hypre and PETSc, coupling with parabolic and elliptic solvers, implicit and Crank-Nicolson and incompressible solver.**

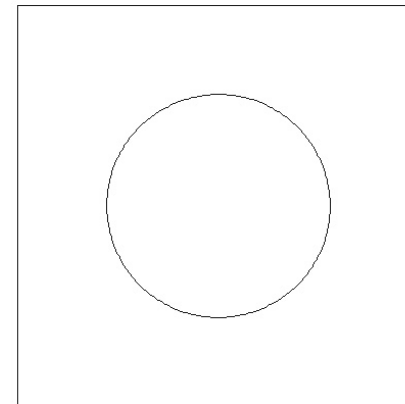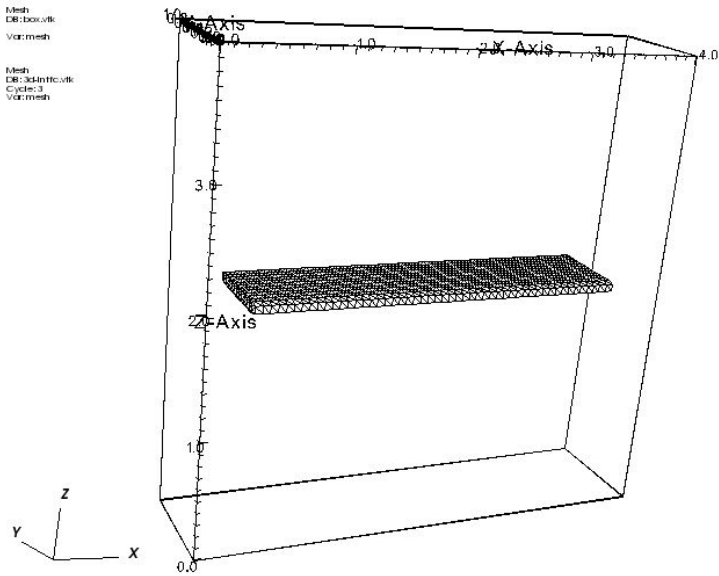# Geometry preservation, accuracy and high (subgrid) resolution

**2D**
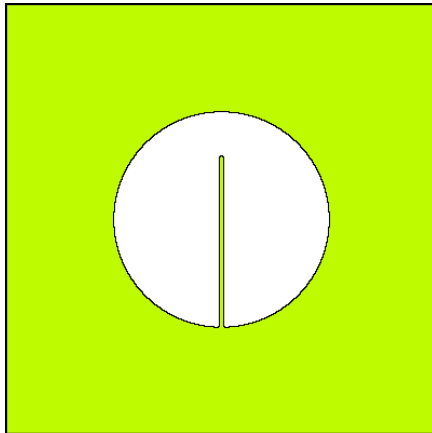
**3D**
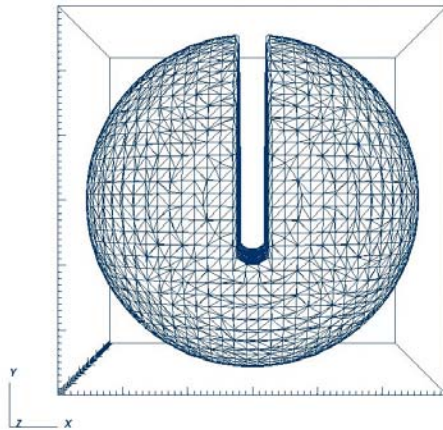
**Accuracy**

**Geometry preservation**

**Subgrid resolution**

# Robust geometry and topology functions



**Robust topological bifurcation**

**Efficient mesh deformation**
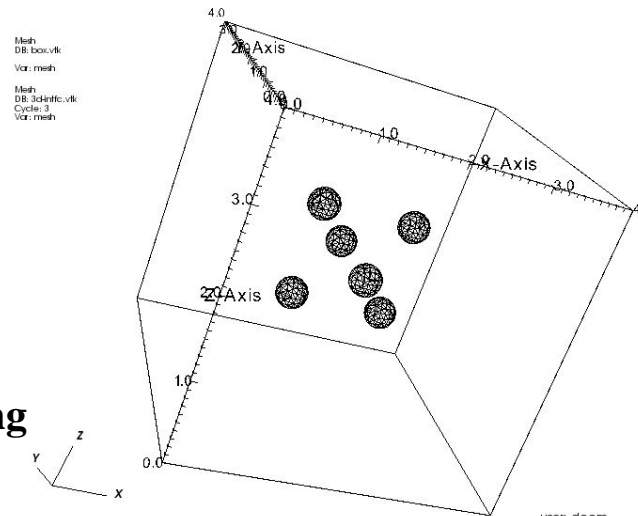
**Robust mesh merging**

# FronTier application: chaotic mixing
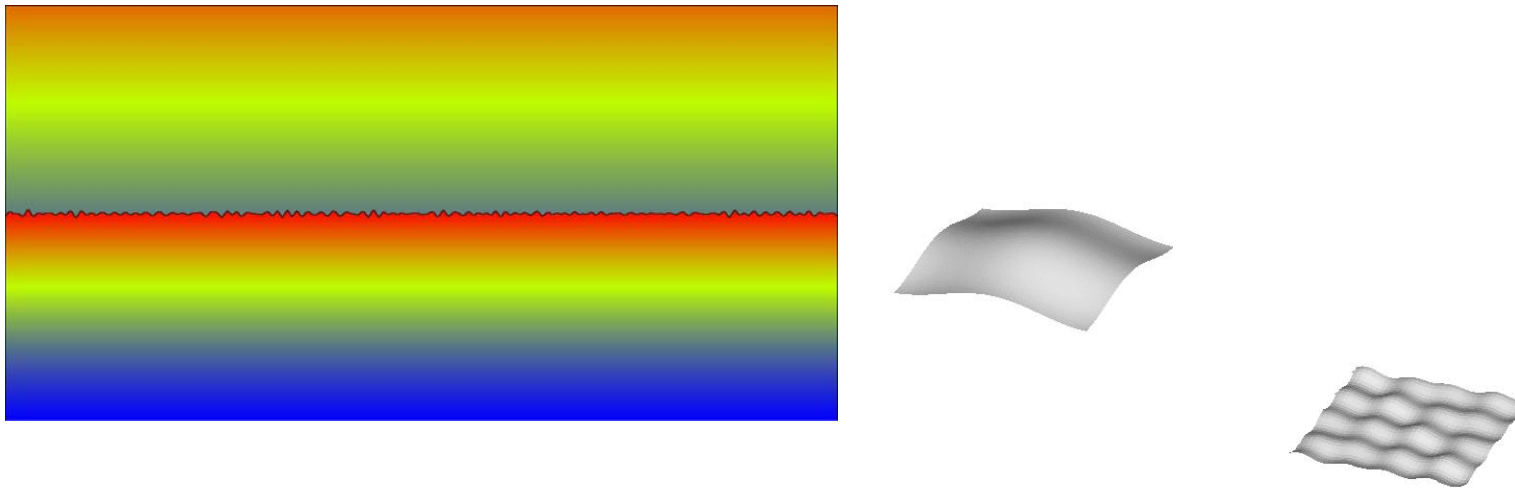


Chaotic mixing is not only important to ICF, but also a test of large scale FronTier application to petascale computing. We have implemented a load balanced parallel algorithm and ran up to 1024 processors on New York Blue. Collaboration with B. Cheng, John Grove, and D. Sharp at LANL.

6

# FronTier application: solute precipitation (growth of crystal) and subsurface flow.
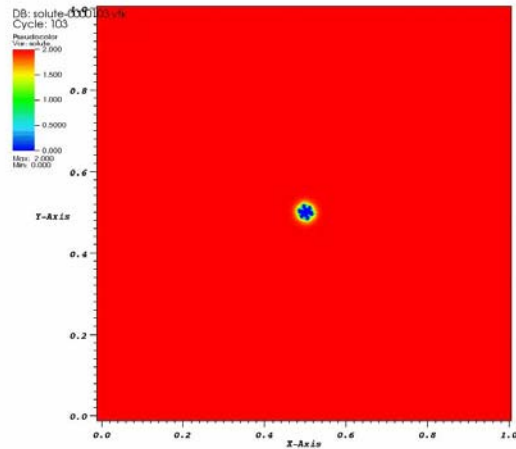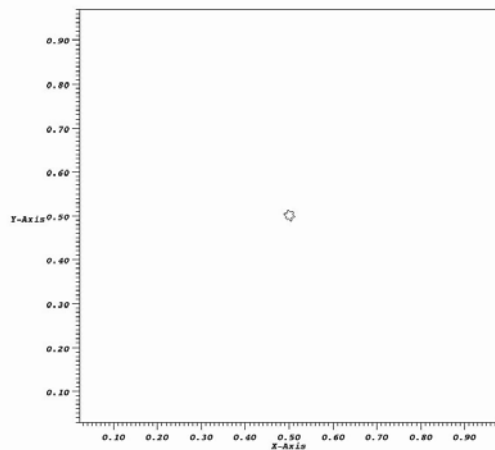


Solute deposition is a component in the study of reactive transport and precipitation. It will be coupled with the Navier-Stokes Equation for the study of reactive subsurface flow in ground water simulation. Collaboration with H. Trease and A. Tartakovsky at PNNL (work in progress)

7

# Convection diffusion model
# Ground water precipitation

# Multiphase Hydro / MHD Flows for Energy Applications

## R. Samulyak, in collaboration with P. Parks at GA

**ITER fueling by injection of cryogenic pellets (in collaboration with General Atomics)**

• Developed algorithms for multiphase MHD and the pellet ablation model

• Simulations revealed new features of ablation flow

**Global Nuclear Energy Partnership**

• Deployment of high performance codes for Generation IV nuclear reactors

• SB task: simulation of failures in fuel rods

• Consortium of RPI, Stony Brook University, Columbia University, and Brookhaven Lab.

**Simulation of Plasma Jet Driven Magnetized Target Fusion**

• Computational evaluation of new promising ideas in fusion science

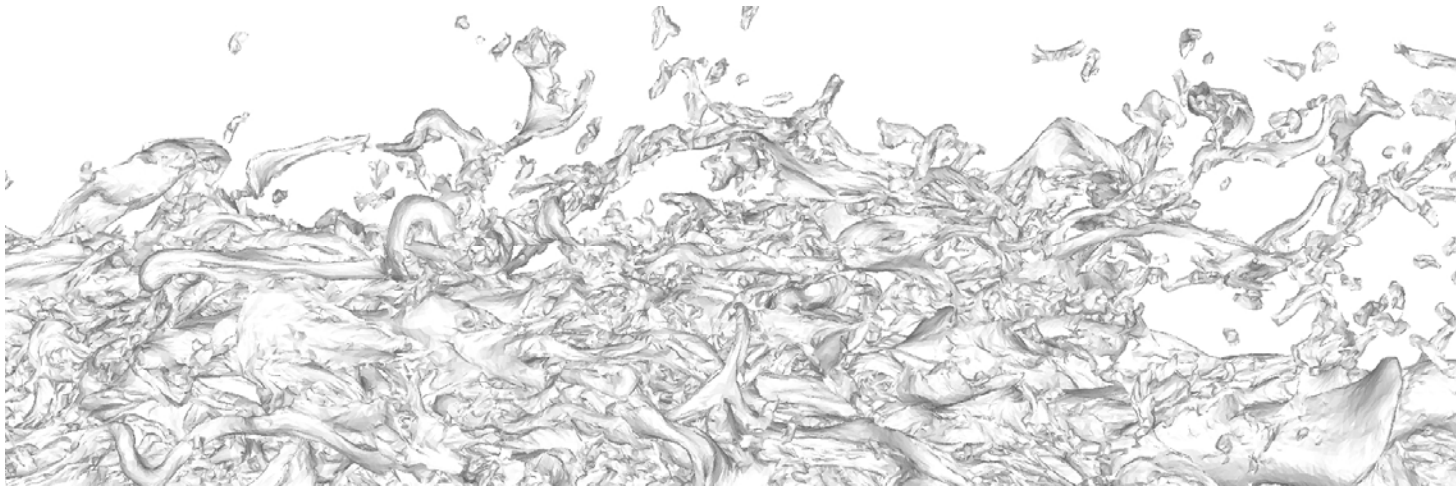• Preliminary work targeting future funding
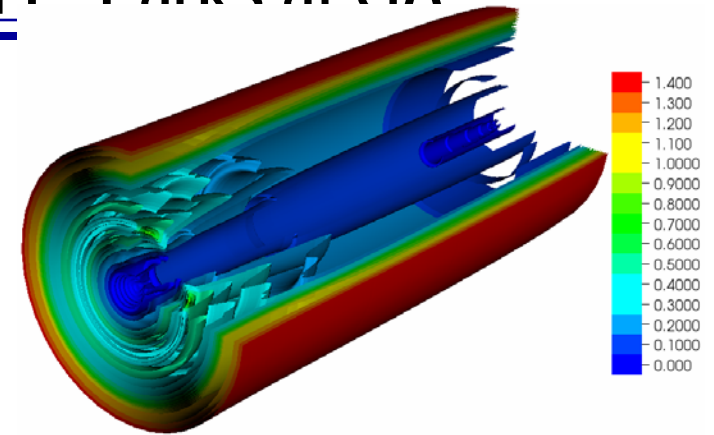


Rotational Mach number in pellet ablation flow. The observed supersonic rotation is the most likely cause of striation instabilities, presently now well understood.
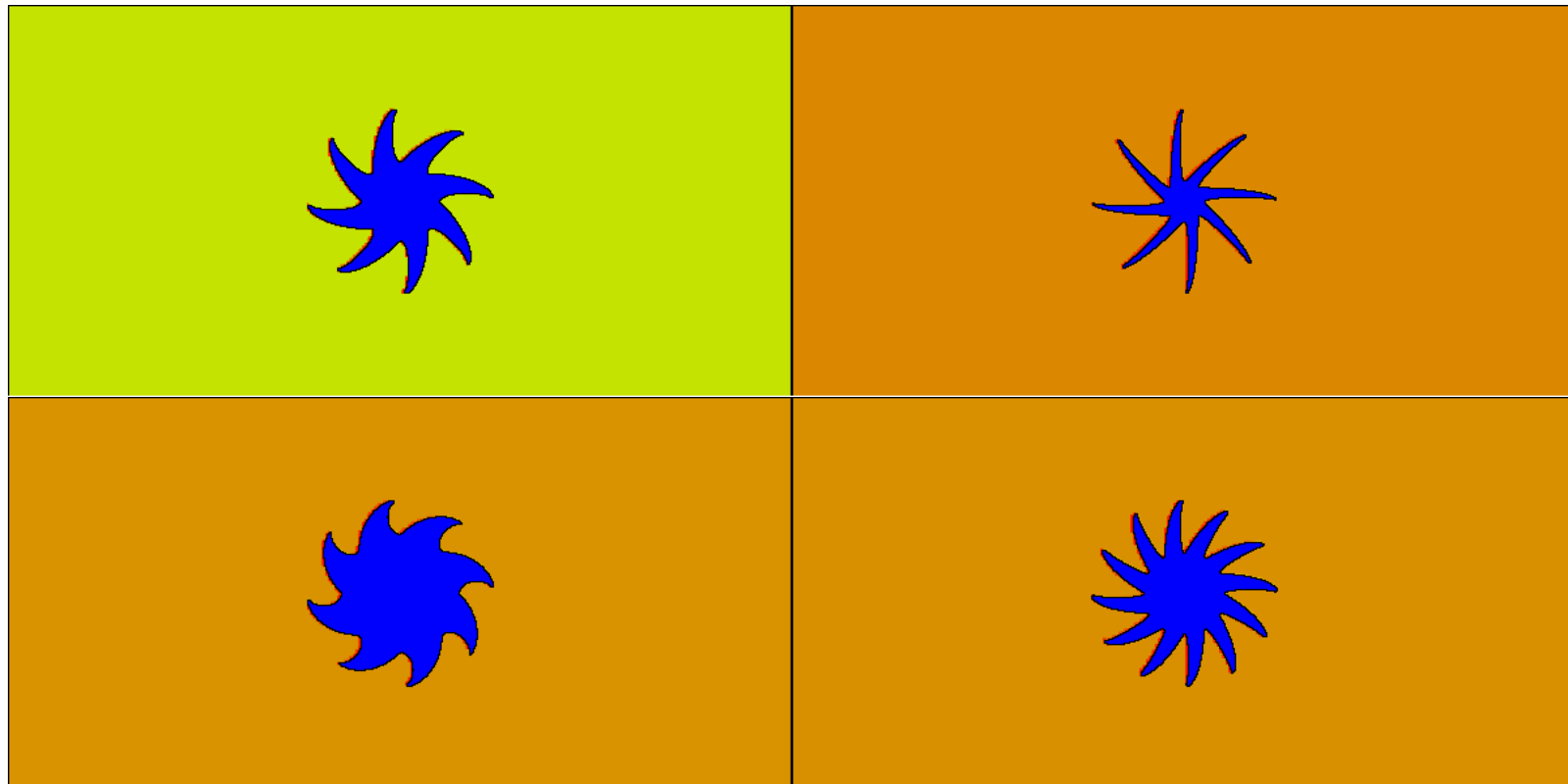
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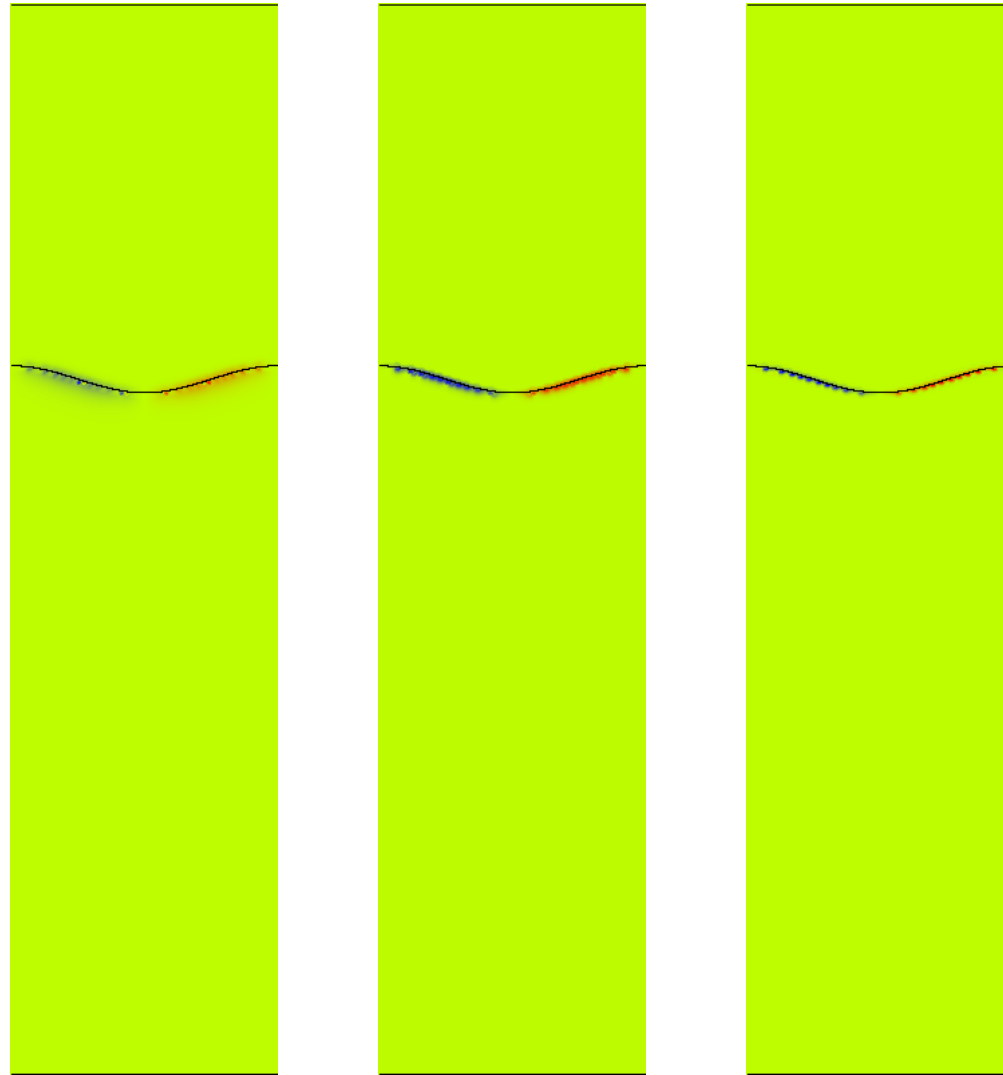
# Simulation of Spherical RM
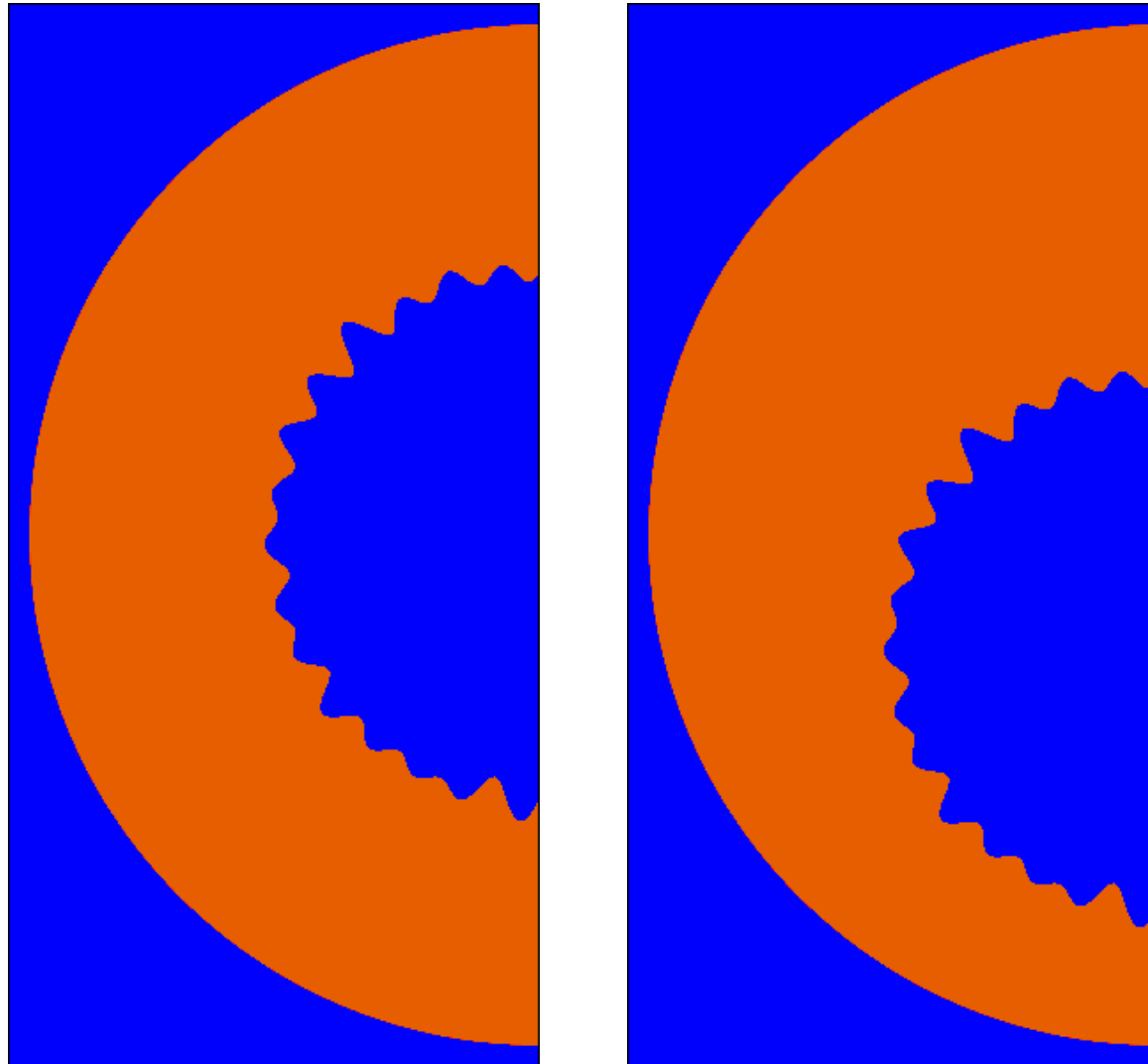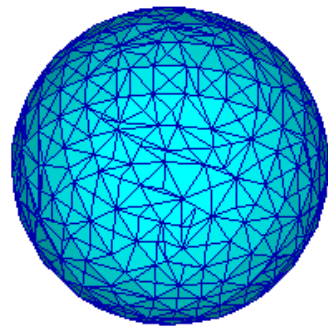
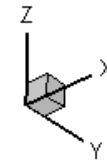# 3D Jet Atomization Simulation

# Fluid-Rigid body interaction

# Incompressible Rayleigh-Taylor instability on Reynold number
# (from left: 14,140,1400)

# Simulation of Cell Migration

# 4. Tracking Front Parallely

# FronTier Parallel Implementation

1. Partition is based on rectangular subdomain division.
2. Mesh is cut at the subdomain boundary.
3. Ghost entities are patched to the "buffer zone" of subdomain.
4. Mesh entities are divided into domestic and foreign parts.
5. Operations are on both domestic and foreign entities.
6. Only owned and boundary entities will remain.
7. Buffer update mainly via floating point match.
8. Global indexing serves as supplement for matching.
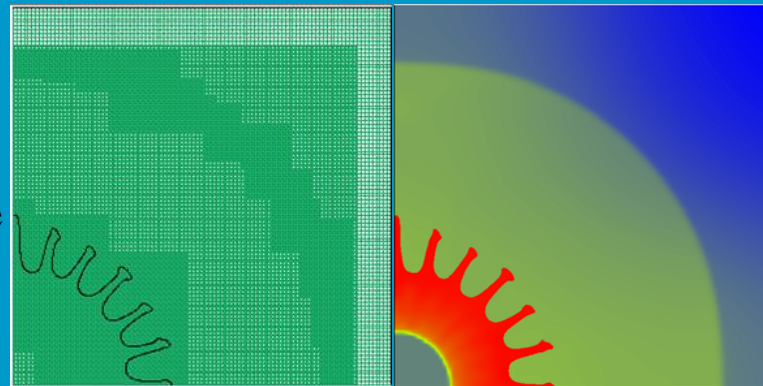
# Parallelization of Front Tracking
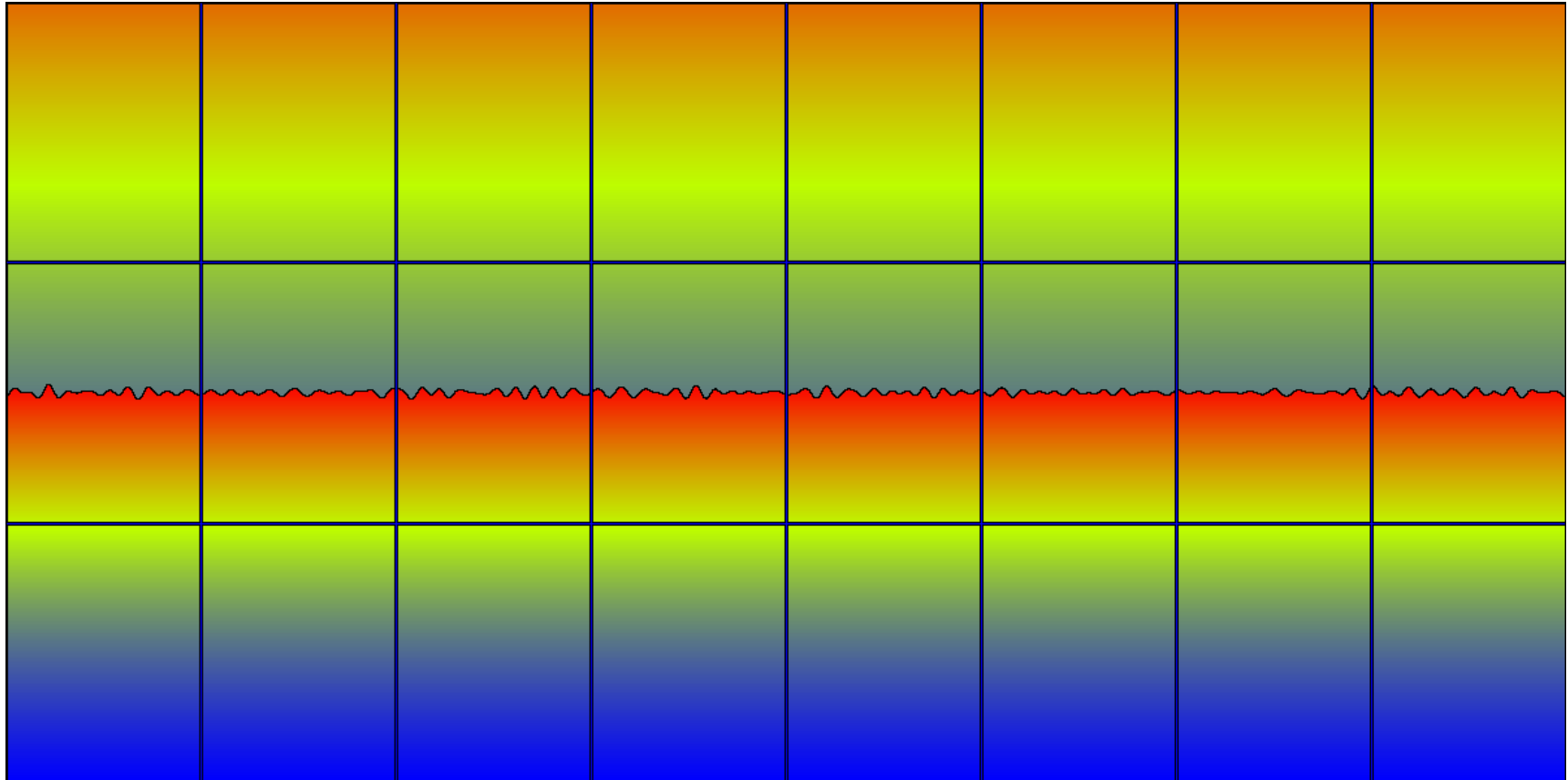
# Parallel load balancing
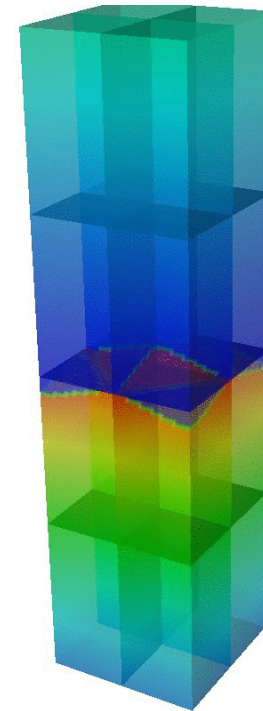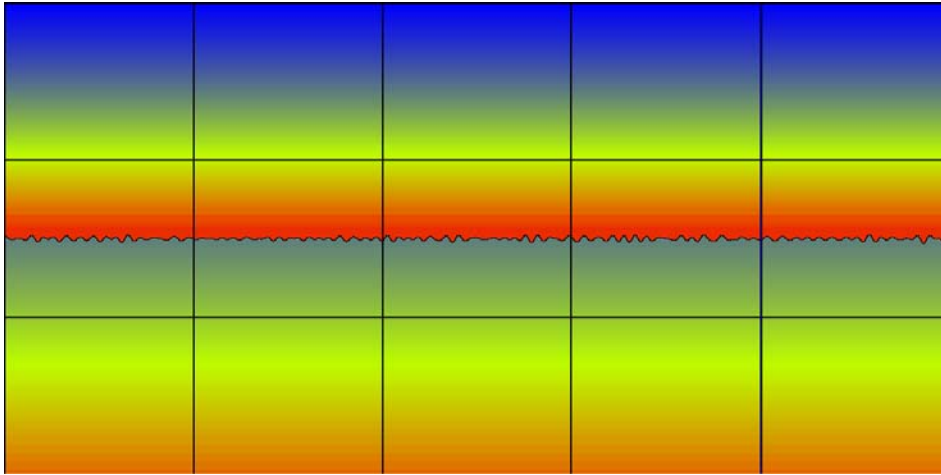


Like AMR, FronTier has encountered great
Obstacle in load balancing and parallel
scaling. One important development is
adaptive partition load balancing.Up to
8196 processors have been tested. No
better for number larger than that.

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# AMR FronTier

1. Interoperability of FronTier with AMR packages including Overture, Chombo and Samrai are underway
2. FronTier has developed a interface for elliptic PDE solvers using the embedded boundary method, this service will be used in MHD study of fusion pallet injection, subsurface flow simulation and many other applications.

3. FronTier has implemented interoperability with linear PDE solvers such as PETSc and Hypre
4. Our collaborators include J. Grove at LANL, H. Trease at PNNL, Helen Yee at LLNL, etc.



FronTier and AMR interoperation

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