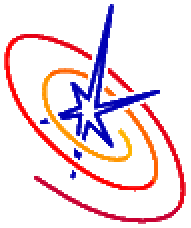

The Center for Astrophysical Thermonuclear Flashes

A Case Study of Verifying and Validating an Astrophysical Simulation Code

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October 23, 2002

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Academic Strategic Alliances Program (ASAP) Center
at The University of Chicago

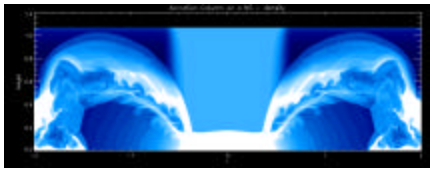
Outline

- Our V&V methodology
- Flash code
- Hydrodynamics method- context of tests
- Verification test: Isentropic vortex advection
- Validation tests
  - Laser-driven shock
  - Rayleigh-Taylor
- Summary, conclusions, and spear catching

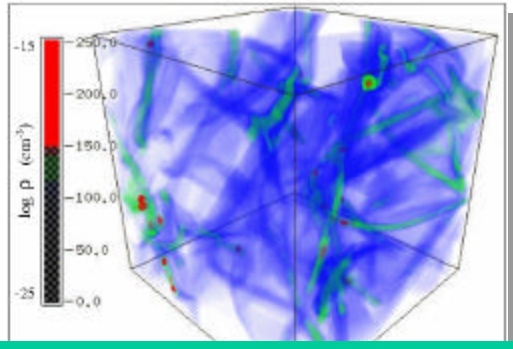
Our V&V Methodology

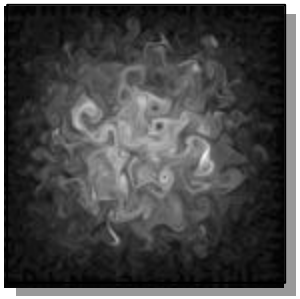
- Choose V&V tests/problems for particular code modules e.g. hydrodynamics.
- Verification test problems
  - Investigate convergence of error with resolution
  - Investigate error in secondary modules e.g. EOS
  - Regularly re-verify with nightly/weekly automated tests
- Validation problems
  - Quantify measurements in experiment and simulation
  - Quantify error and uncertainty in experiment and simulation
  - Resolution study

The Flash Code

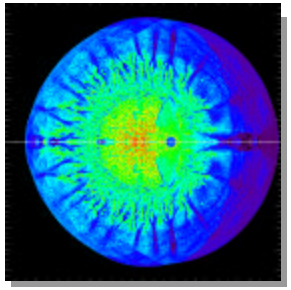


Shortly: Relativistic accretion onto NS

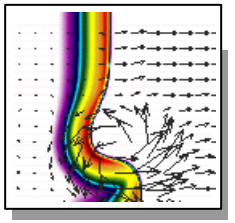




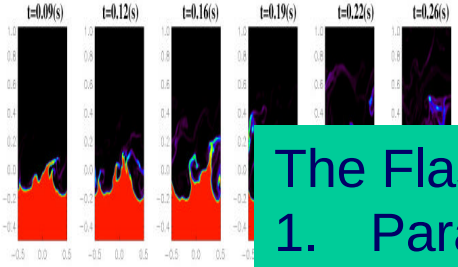
Compressed turbulence



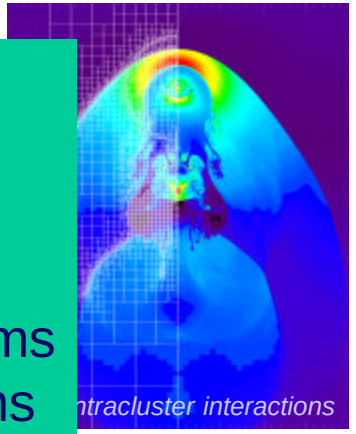
Type Ia Supernova



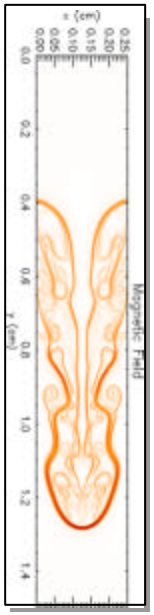
Flame-vortex interactions



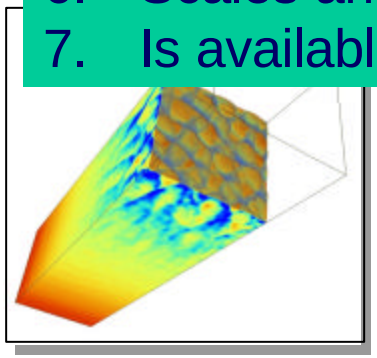
Wave breaking on w



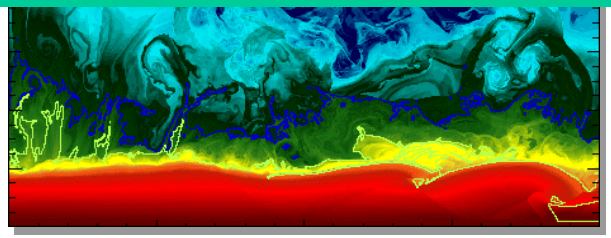
ntracluster interactions



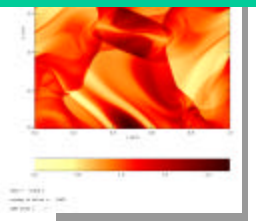
Magnetic Rayleigh-Taylor



Cellular detonation



Helium burning on neutron stars



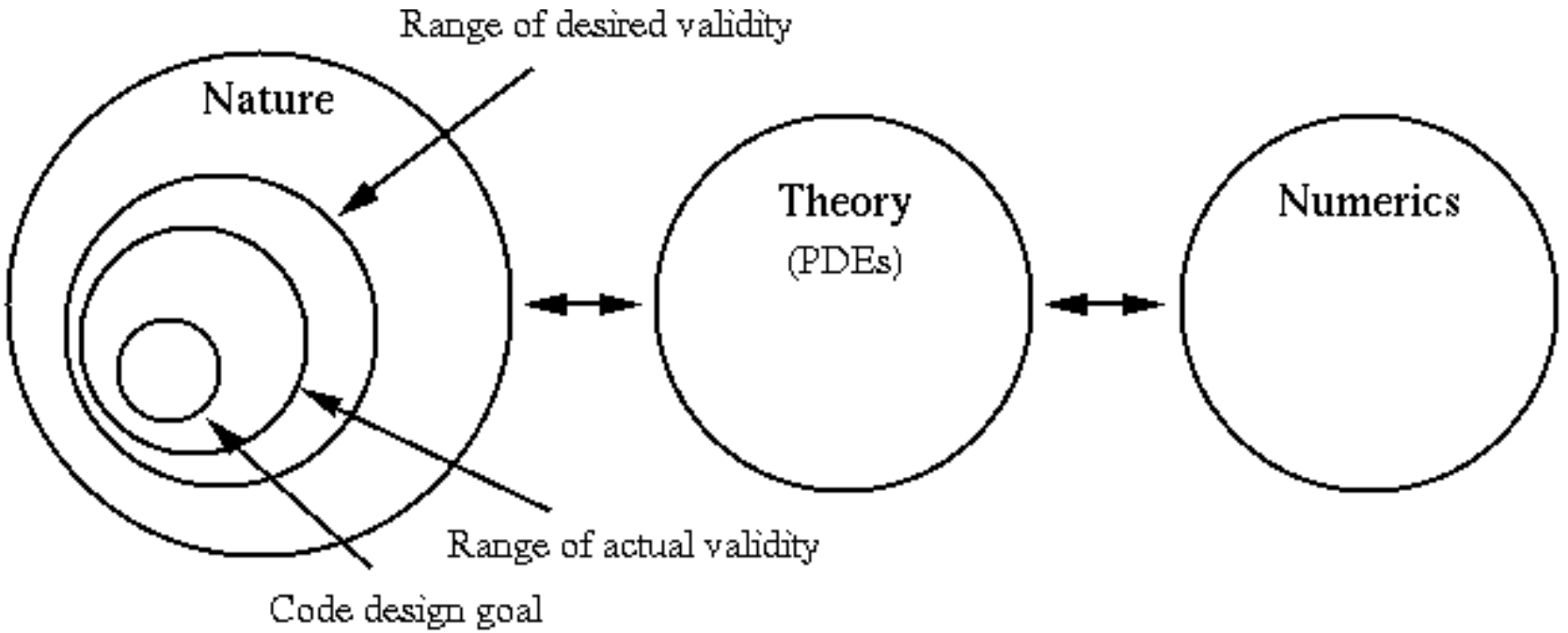
Orzag/Tang MHD vortex

Richtmyer-Meshkov instability

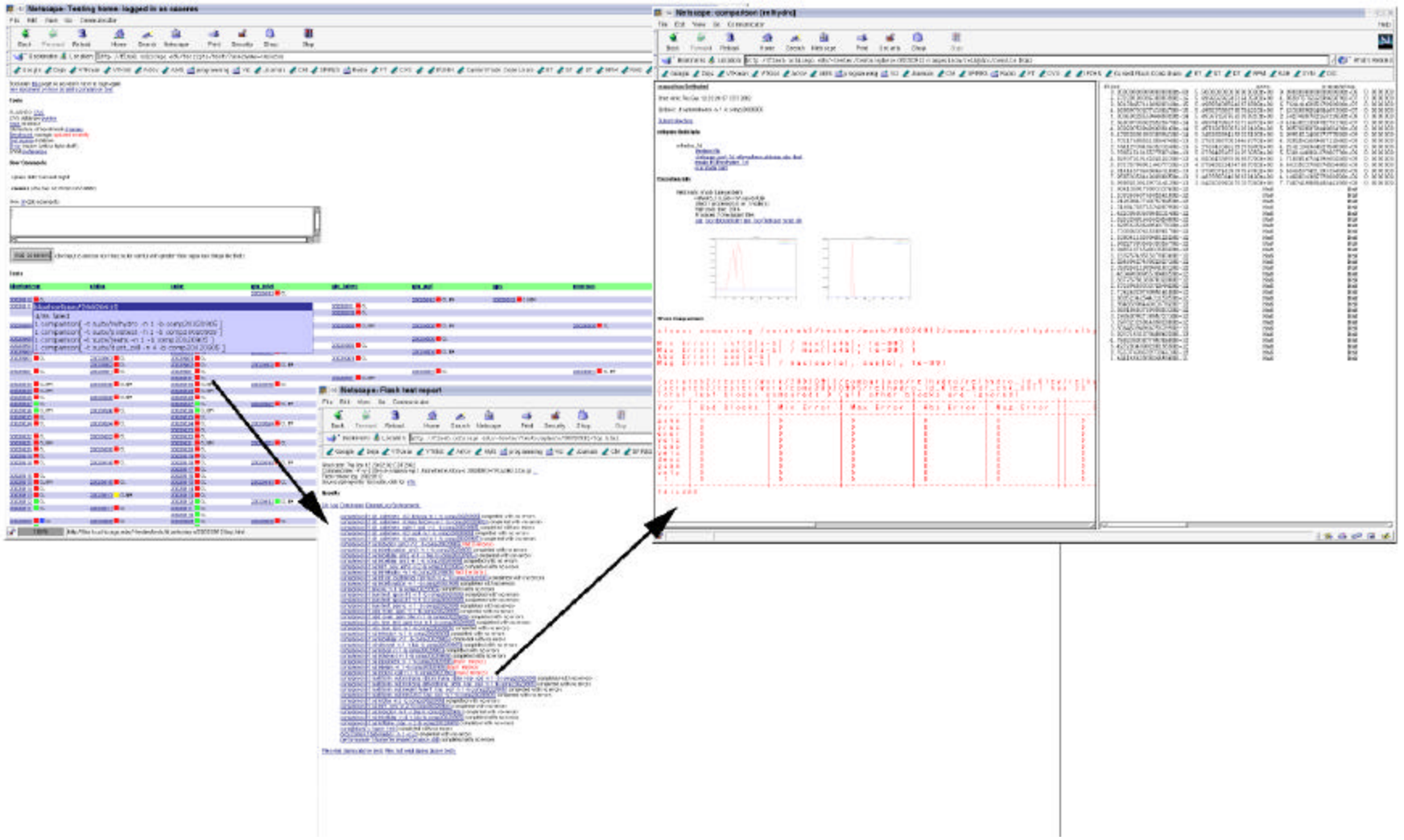
The Flash code

1. Parallel, adaptive-mesh simulation code
2. Designed for compressible reactive flows
3. Has a modern CS-influenced architecture
4. Can solve a broad range of (astro)physics problems
5. Portable- runs on many massively-parallel systems
6. Scales and performs well
7. Is available on the web: http://flash.uchicago.edu

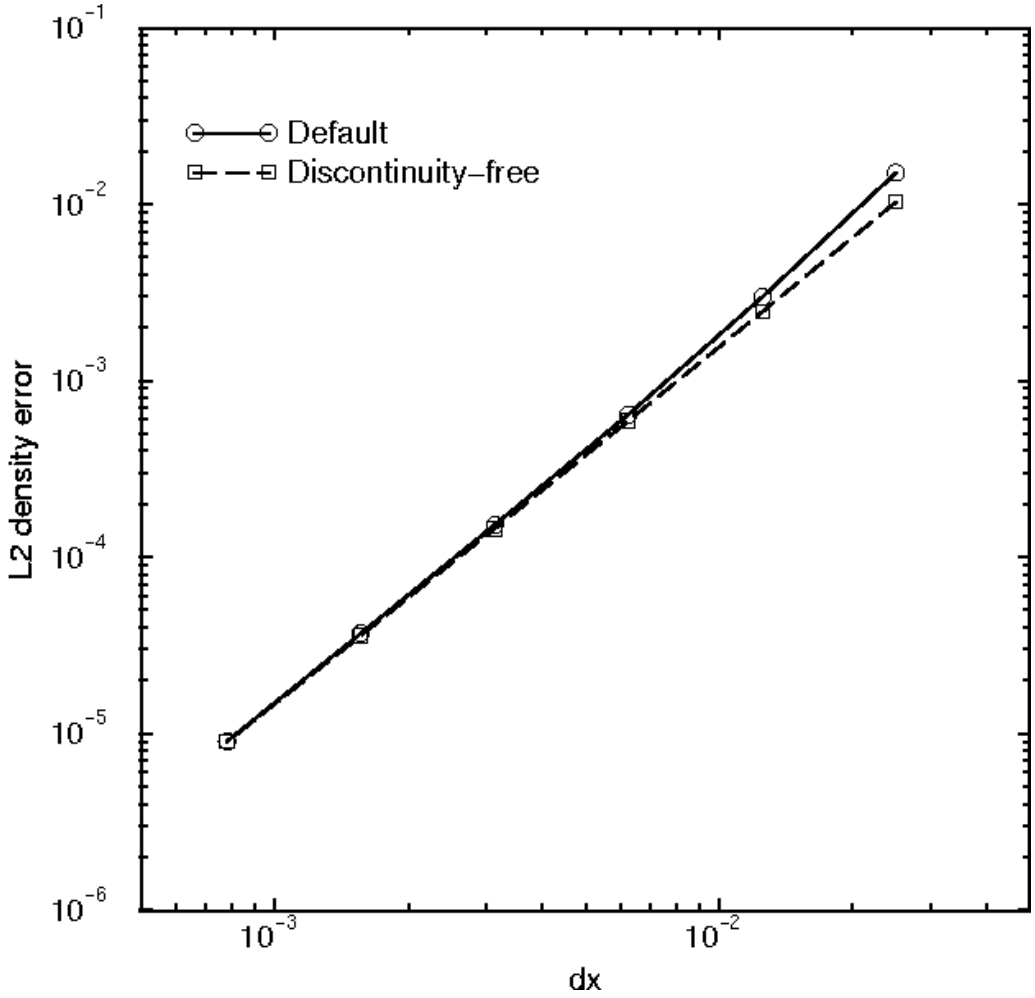
Verification and Validation



Software Verification: Nightly Test Suite



Verification Test: Isentropic Vortex



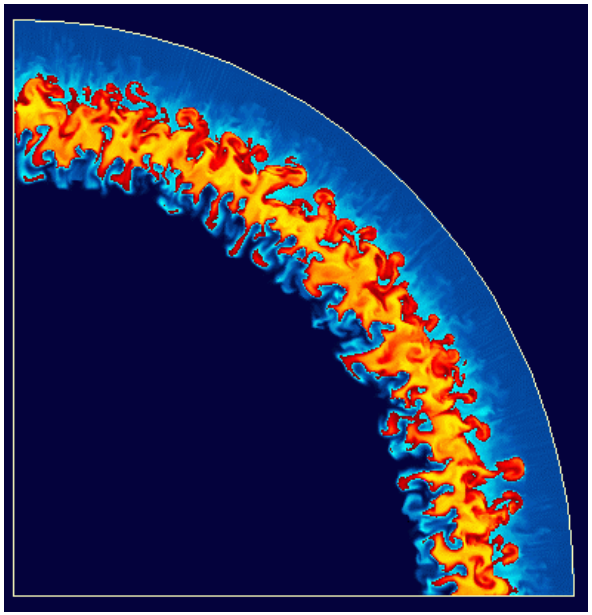
Demonstrates expected 2nd order convergence of error

Motivation For Choice of Validation Problems

- Problem must test non-trivial, nonlinear behavior
  - Validation, not Verification
  - Problem should relate to the astrophysics of interest
- Problem must have a well-documented laboratory counterpart
  - Collaboration with National Labs (LANL, LLNL, Sandia)
  - Collaborations with other groups
- Problem must be intrinsically interesting
  - Non-trivial problems are hard
  - Fundamental aspect of research
- Likely candidates involve fluid instabilities

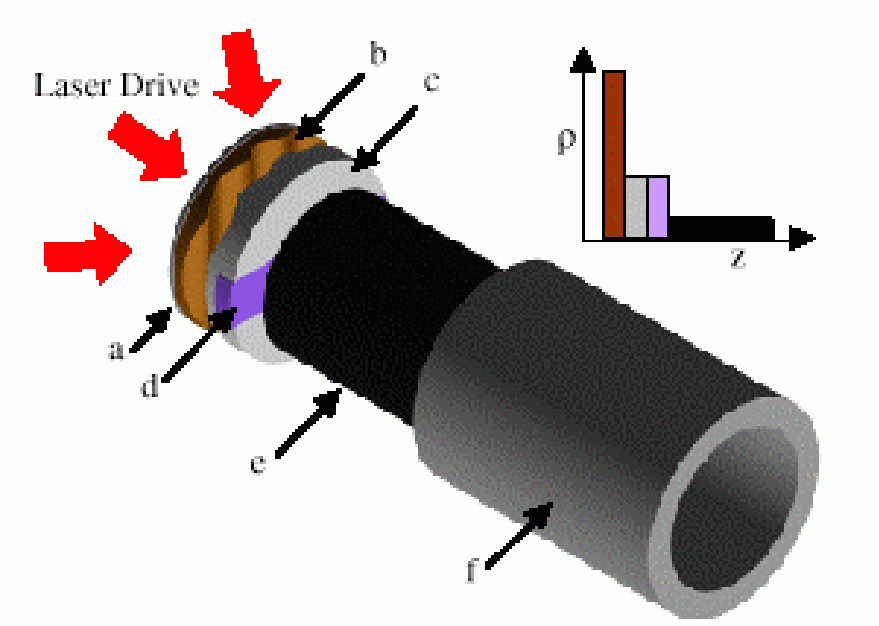
Fluid Instabilities in Astrophysics

STScI



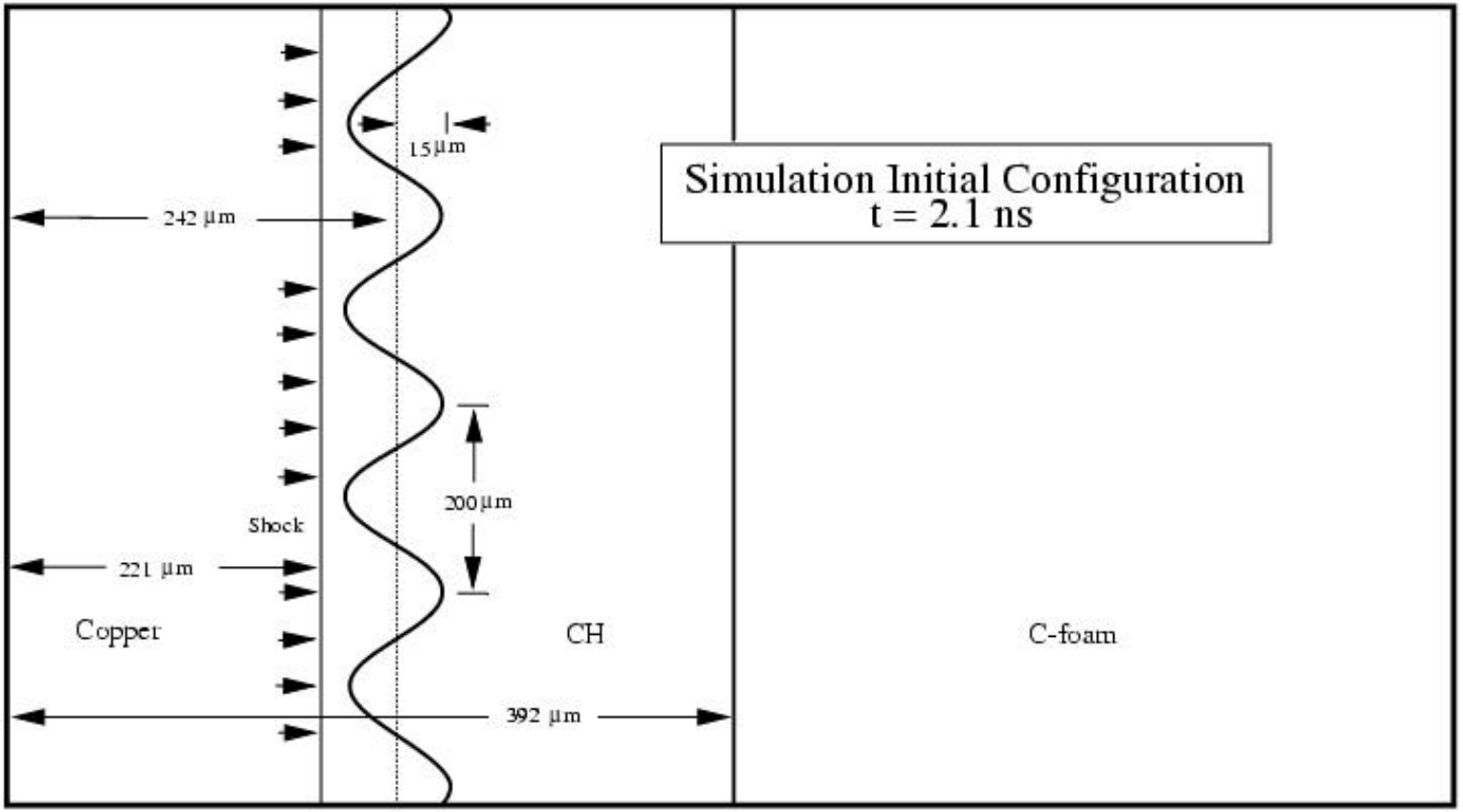
- Observations of astrophysical phenomena, *e.g.* ^{56}Co in SN 1987A, indicate that fluid instabilities can play an important role
- Astrophysical observations often are indirect, but laboratory experiments offer direct observation

Three-layer Shock Imprint Experiment



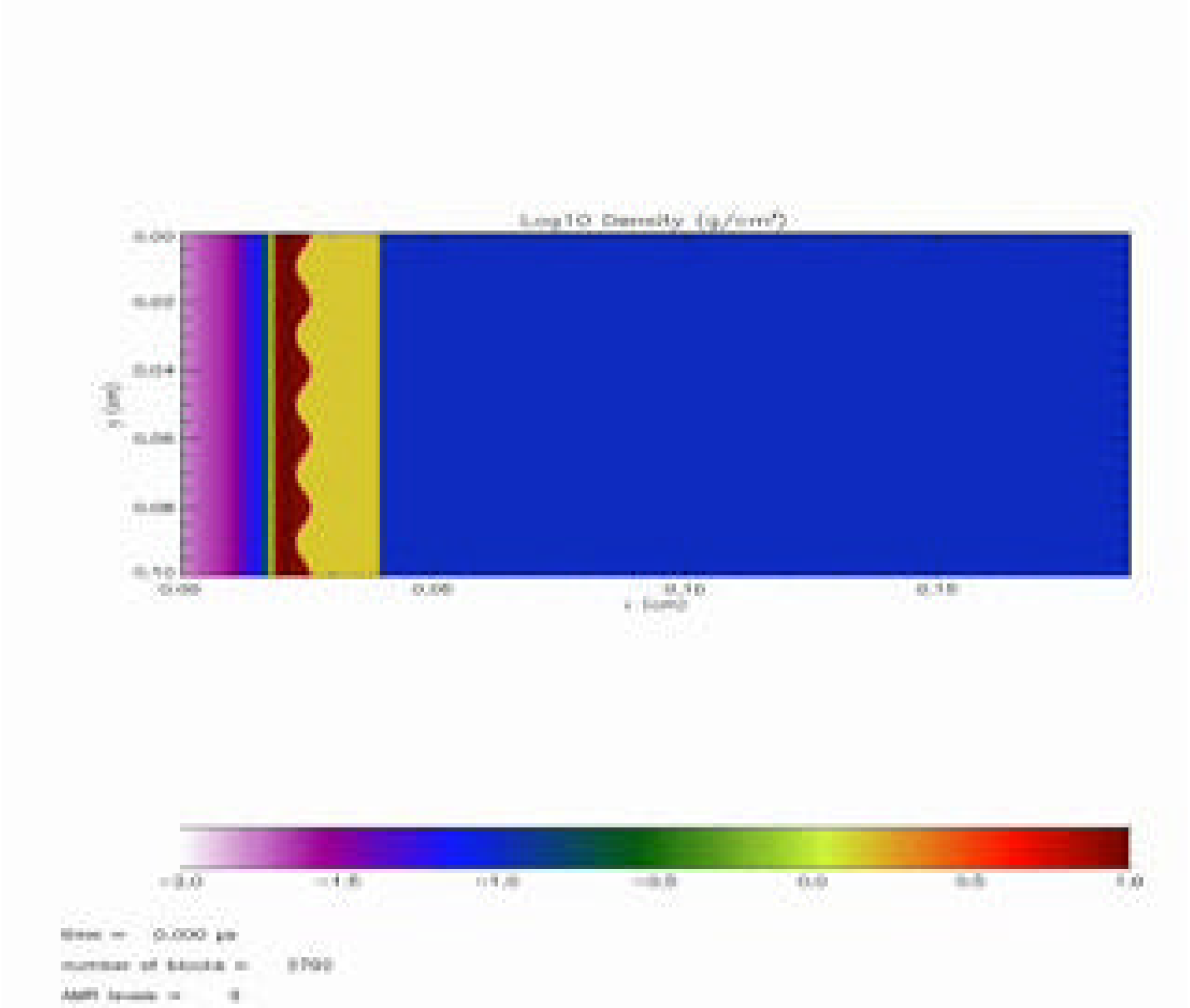
- Performed at the Rochester Omega laser facility
- Strong shock driven through a planar, copper-plastic-foam three-layer target
- Rayleigh-Taylor and Richtmyer-Meshkov instabilities
- Full details in Kane et al. 2001, Robey et al. 2001

Three-layer Target Simulation

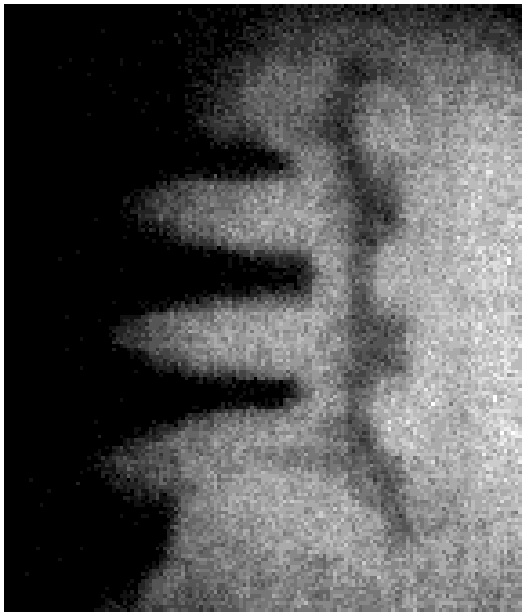


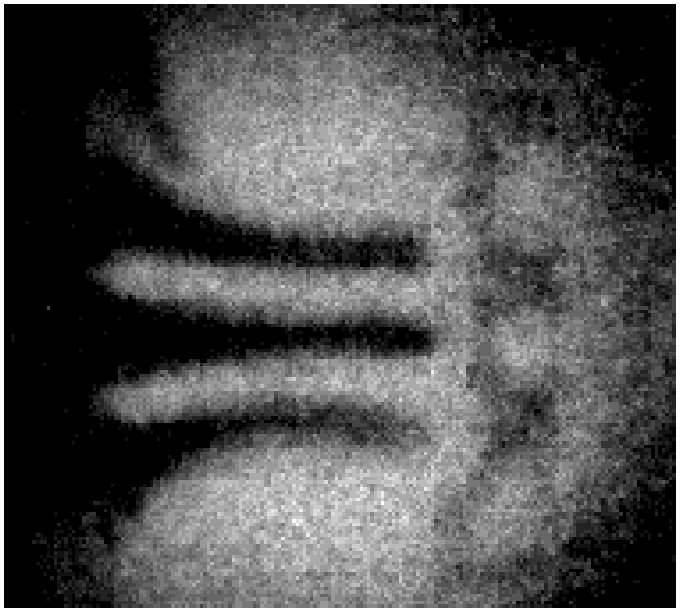
Initial Conditions

Three-layer Target Simulation



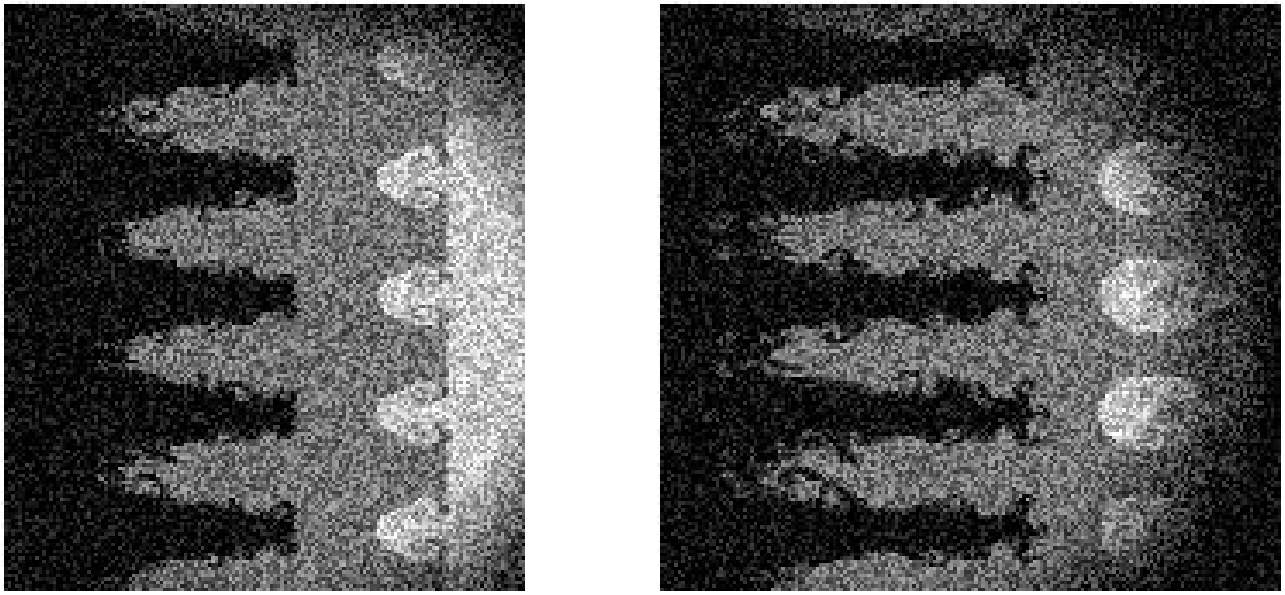
Three-layer Target Simulation





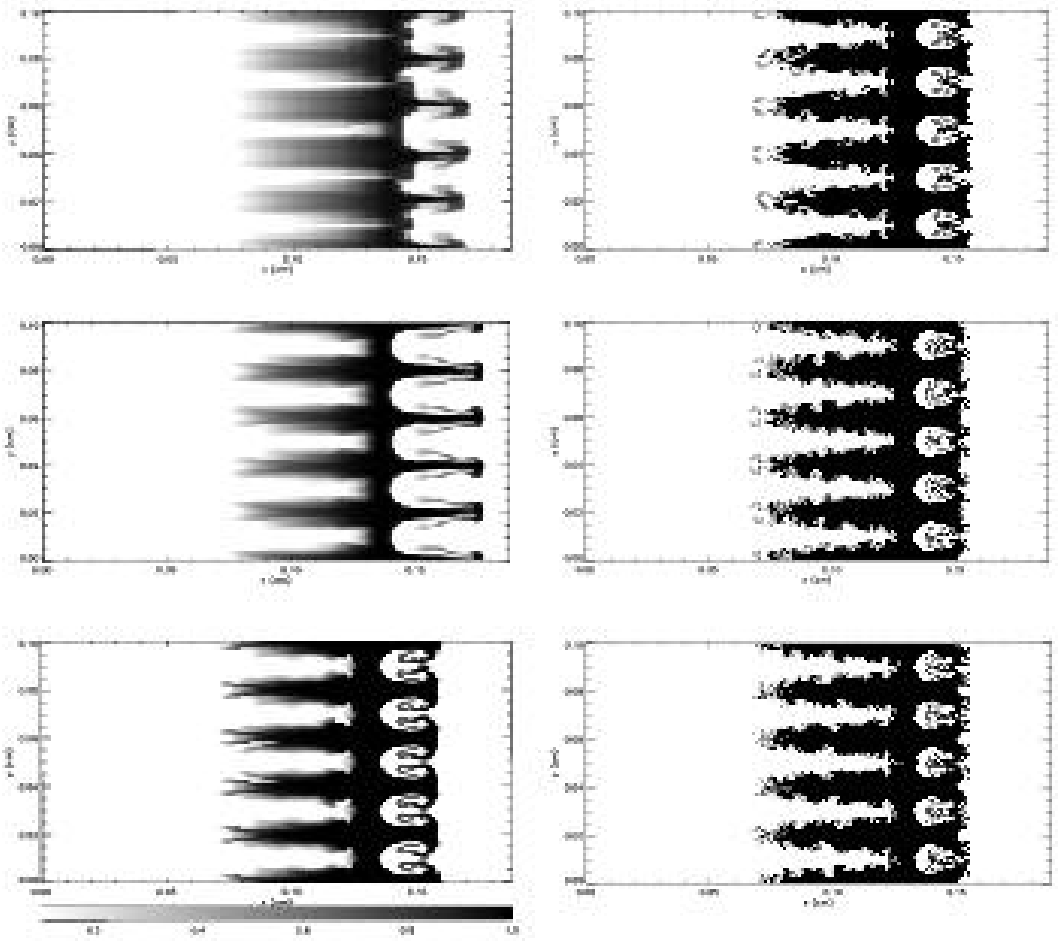
Images from the experiment

Three-layer Target Simulation



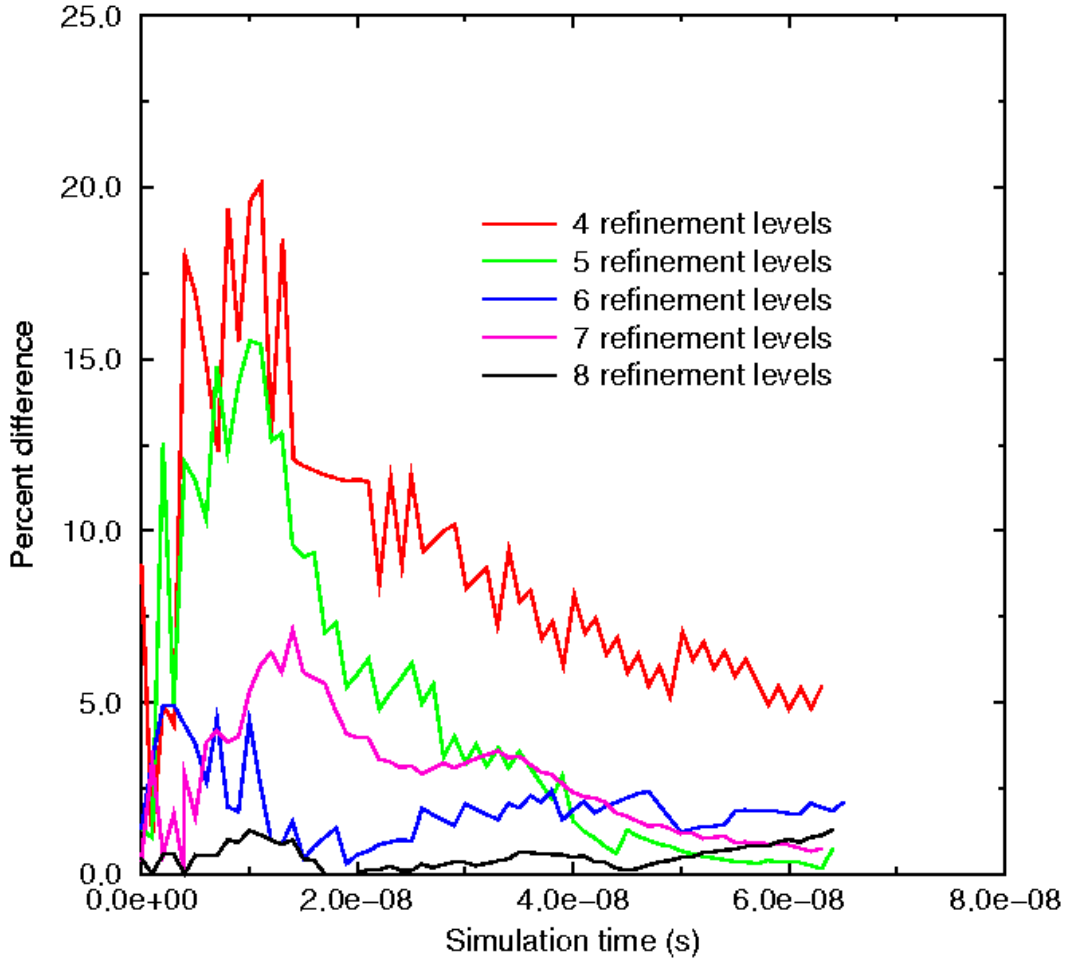
Simulated radiographs

Three-layer Target Simulation



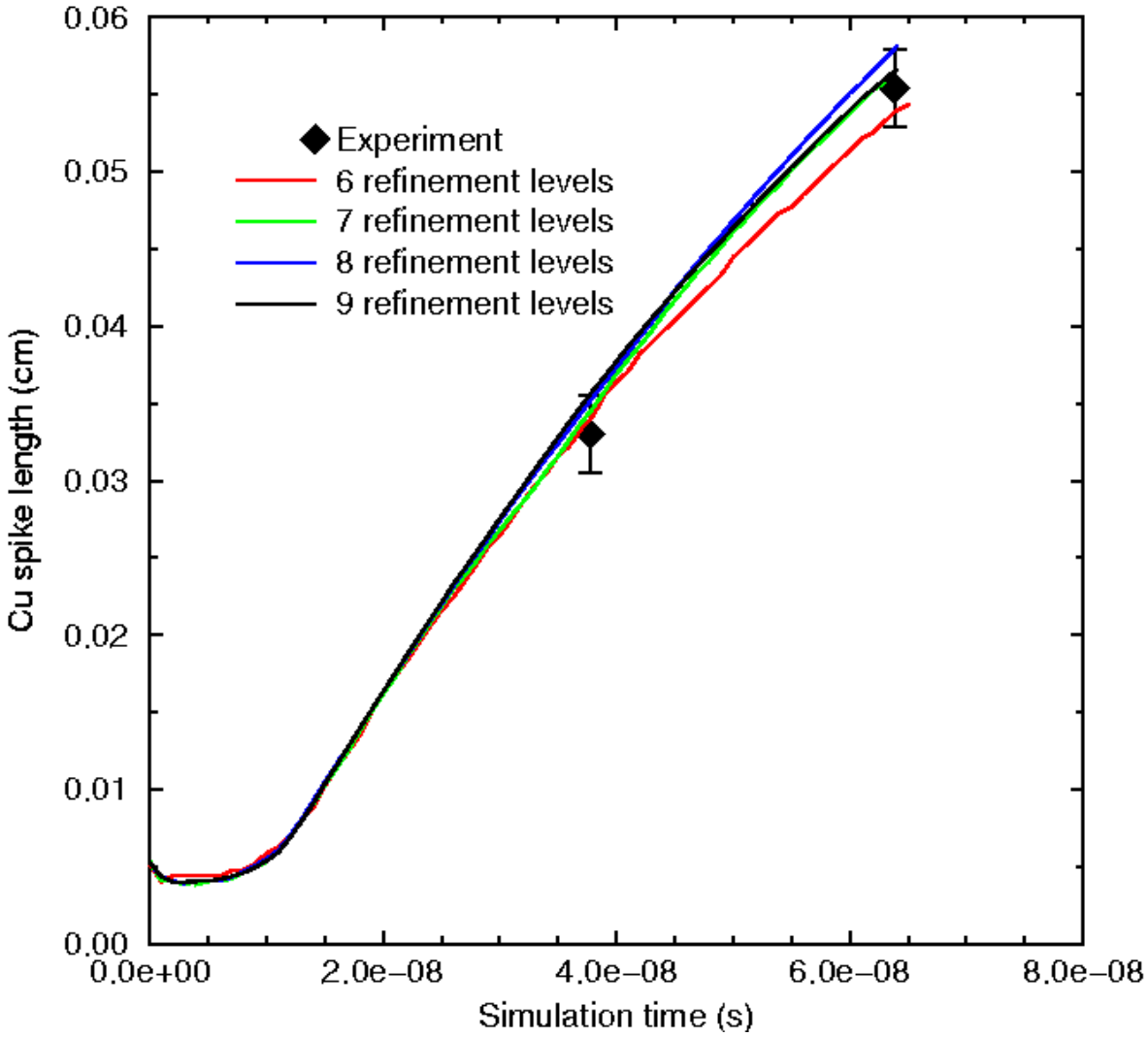
Resolution Study

Three-layer Target Simulation

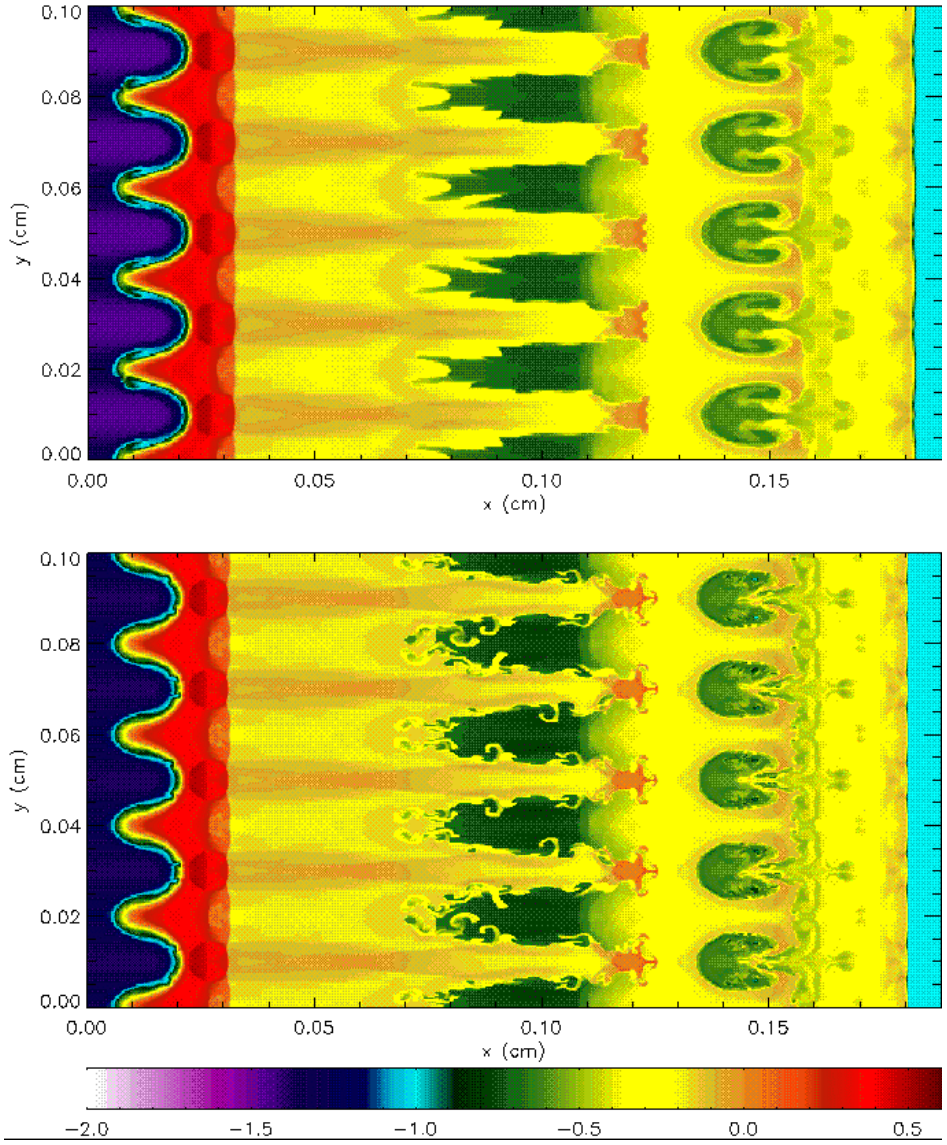


Convergence results: percent difference

Three-layer Target Simulation



Three-layer Target Simulation

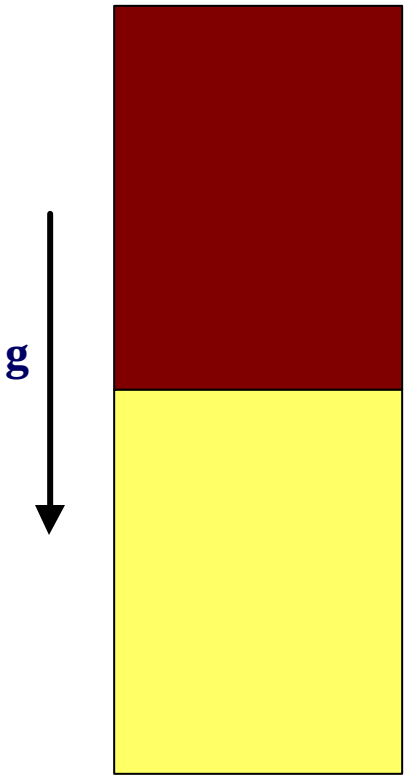


Shortcomings: Incomplete Physics

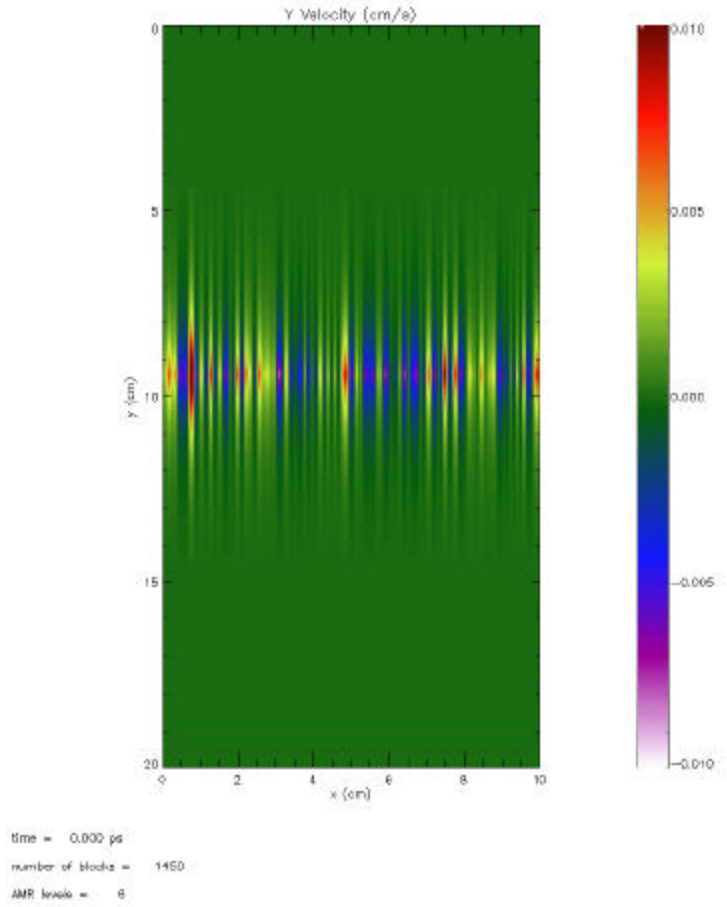
- Simulations used a gamma-law EOS, $P = (\gamma - 1)\rho\varepsilon$, with choice of gamma to match experimental result
- Periodic boundary conditions on sides- no shock tube in the simulations
- Radiation deposition mechanism not included in the simulations
- Experimental diagnostics do not allow us to determine the correct amount of small scale structure

Rayleigh-Taylor Instabilities

Density schematic:



Multi-mode velocity perturbation:



2.5-5 % sound speed with highest magnitude near the interface

Multi-mode Rayleigh-Taylor

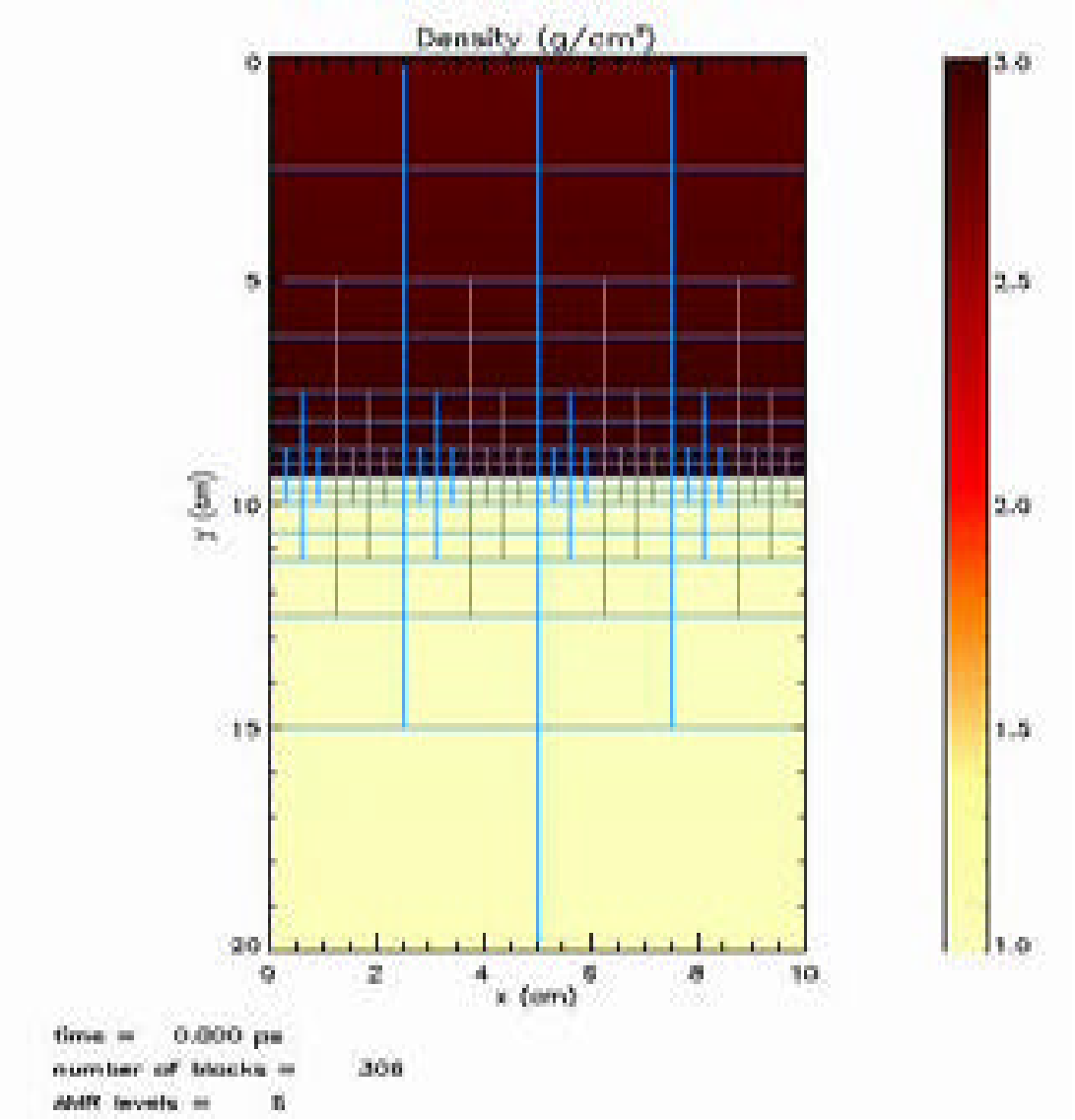
"α-Group" Consortium

- Organized by G. Dimonte (Oct. 1998)
- Purpose – to determine if the t^2 scaling law holds for the growth of the R-T mixing layer, and if so, to determine the value of α
  - simulation - experiment comparisons
  - inter-simulation comparisons

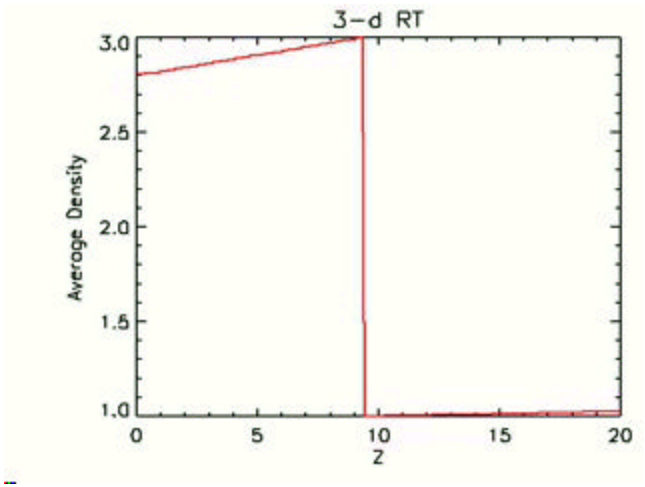
$$h_{b,s} = \alpha_{b,s}\, gAt^2, \text{ where } A = (\rho_2 - \rho_1)/(\rho_2 + \rho_1)$$

- Definition of standard problem set (D. Youngs)

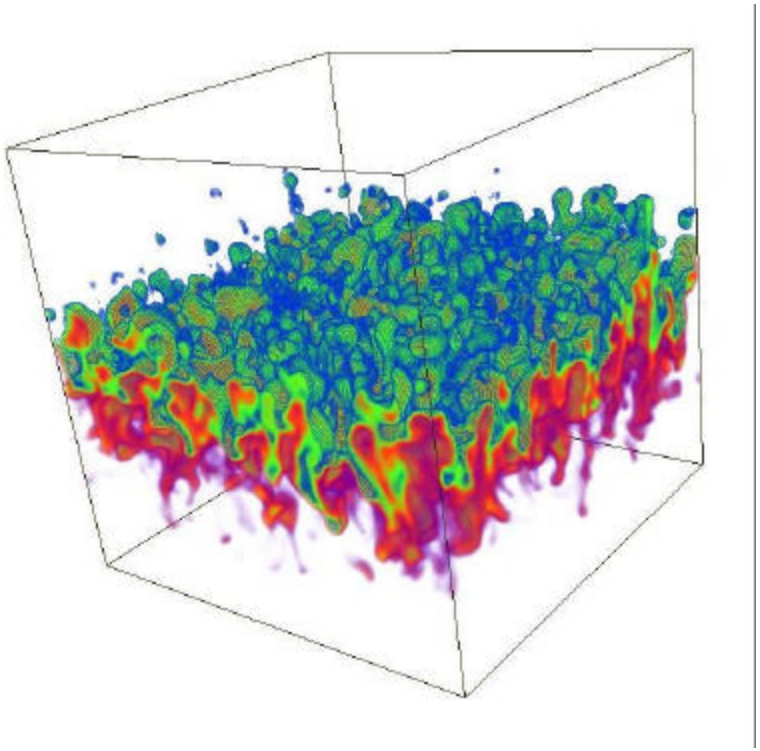
Multi-mode Rayleigh-Taylor: 2-d Simulation



Multi-mode Rayleigh-Taylor: 3-d Simulation



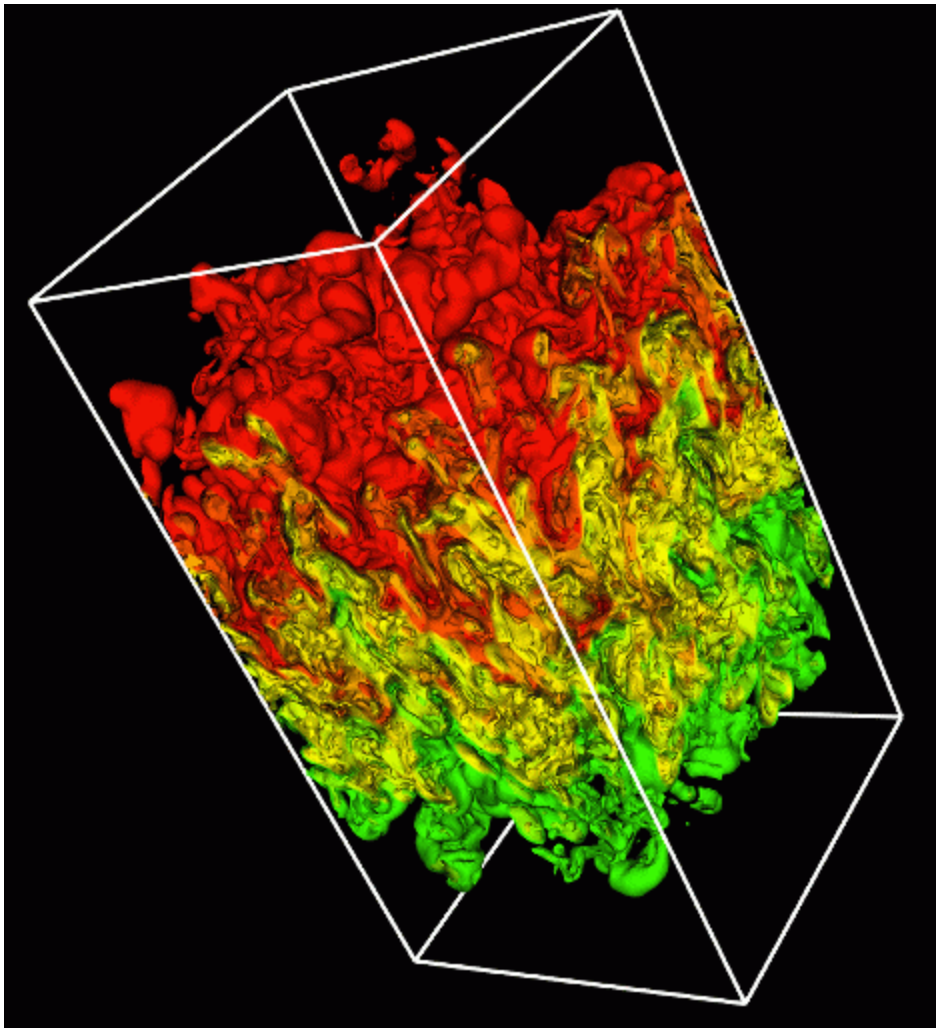
Horizontally Averaged Density



Modes 32-64 perturbed

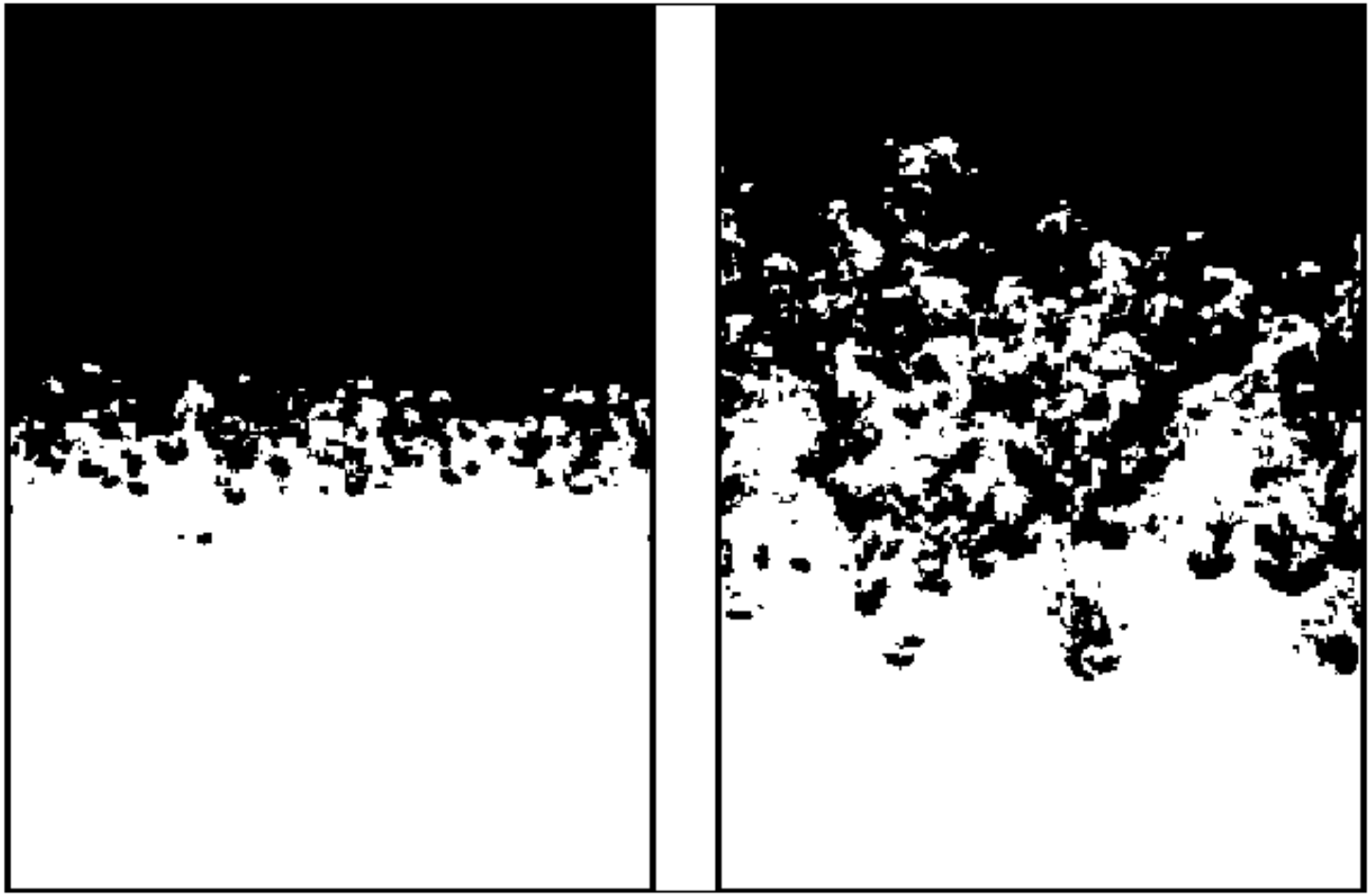
Multi-mode Rayleigh-Taylor

Rendering of Mixing Zone

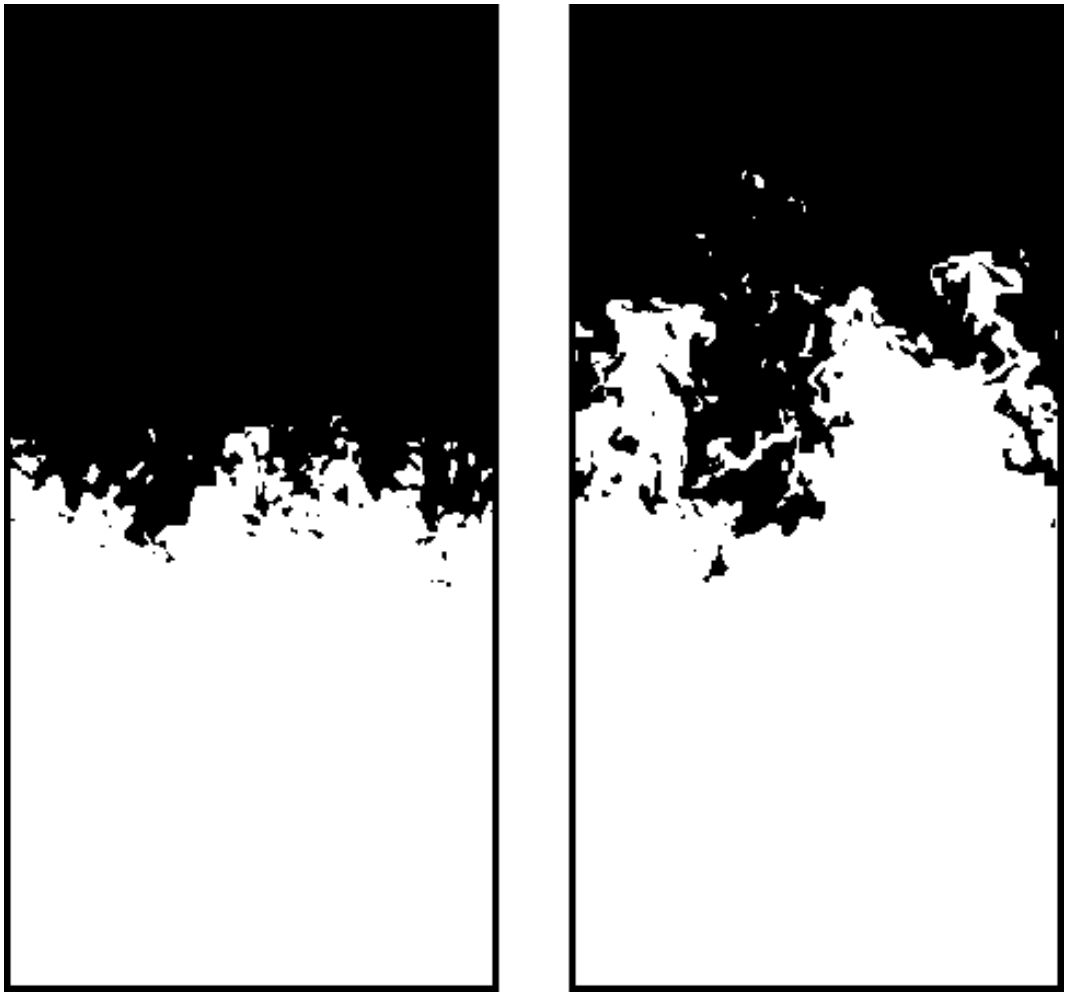


Density (g/cm^3) at t = 14.75 sec

Multi-mode R-T Experimental LIF Image



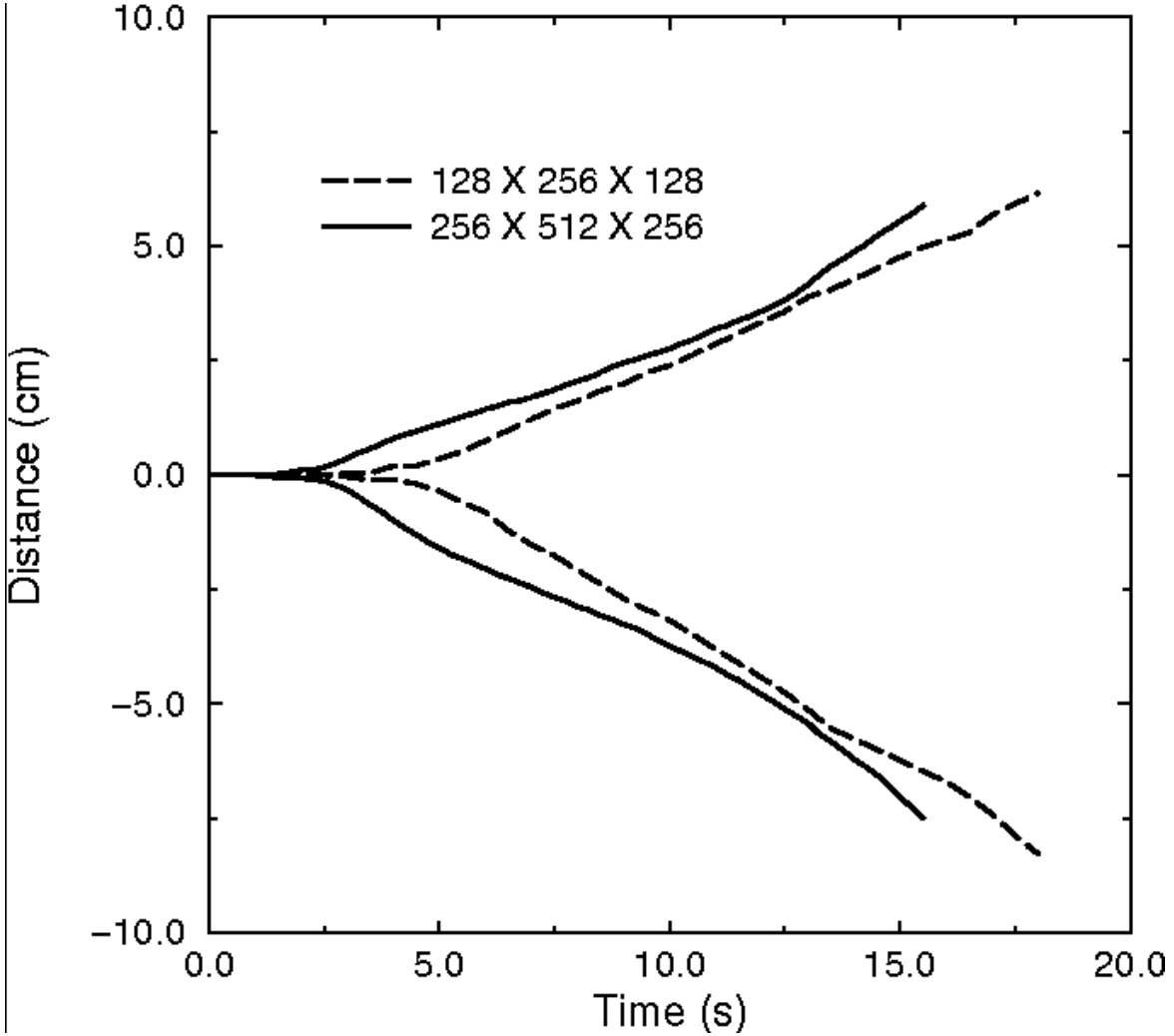
Multi-mode R-T Simulated LIF Image



It looks similar to the experiment…..

Multi-mode Rayleigh-Taylor

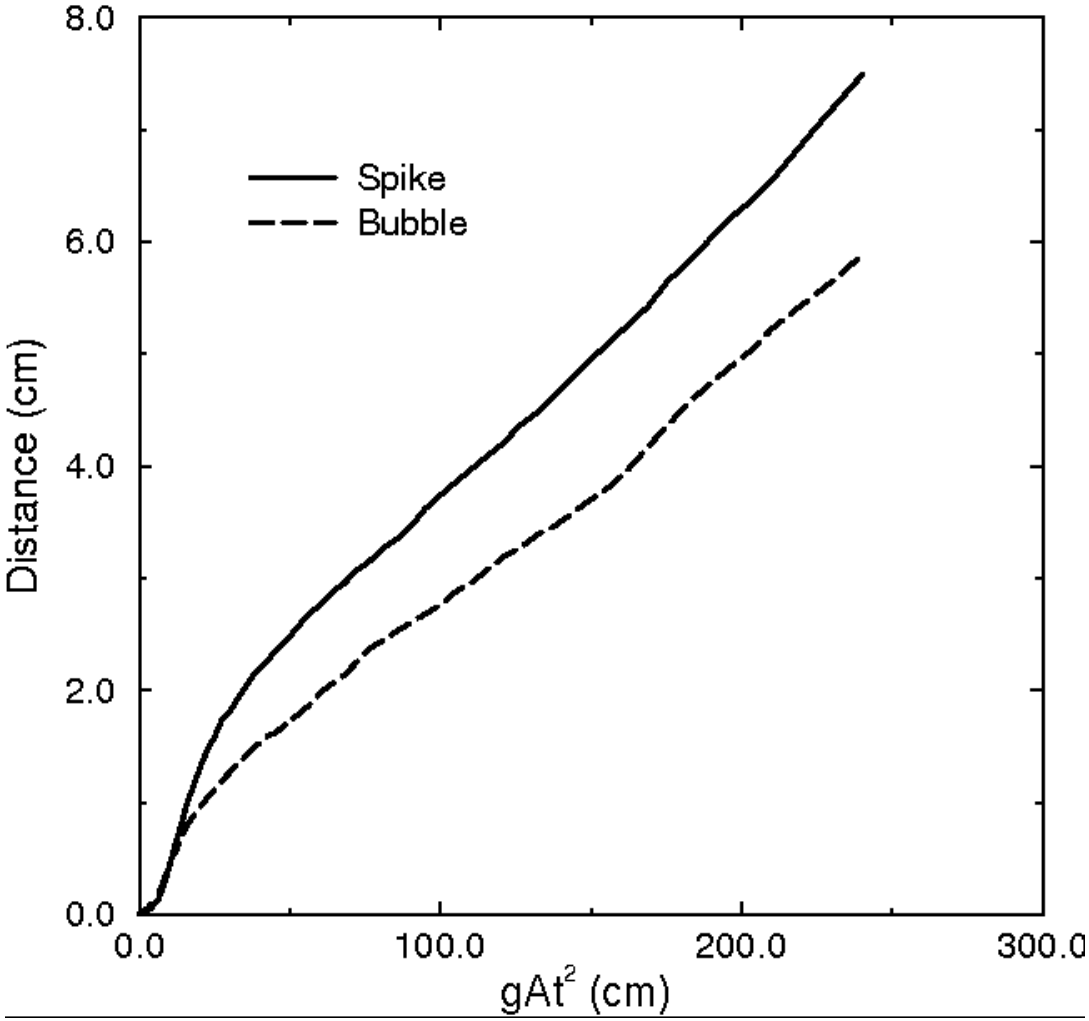
FLASH Simulation



Are we adequately resolved?

Multi-mode Rayleigh-Taylor

FLASH Simulation

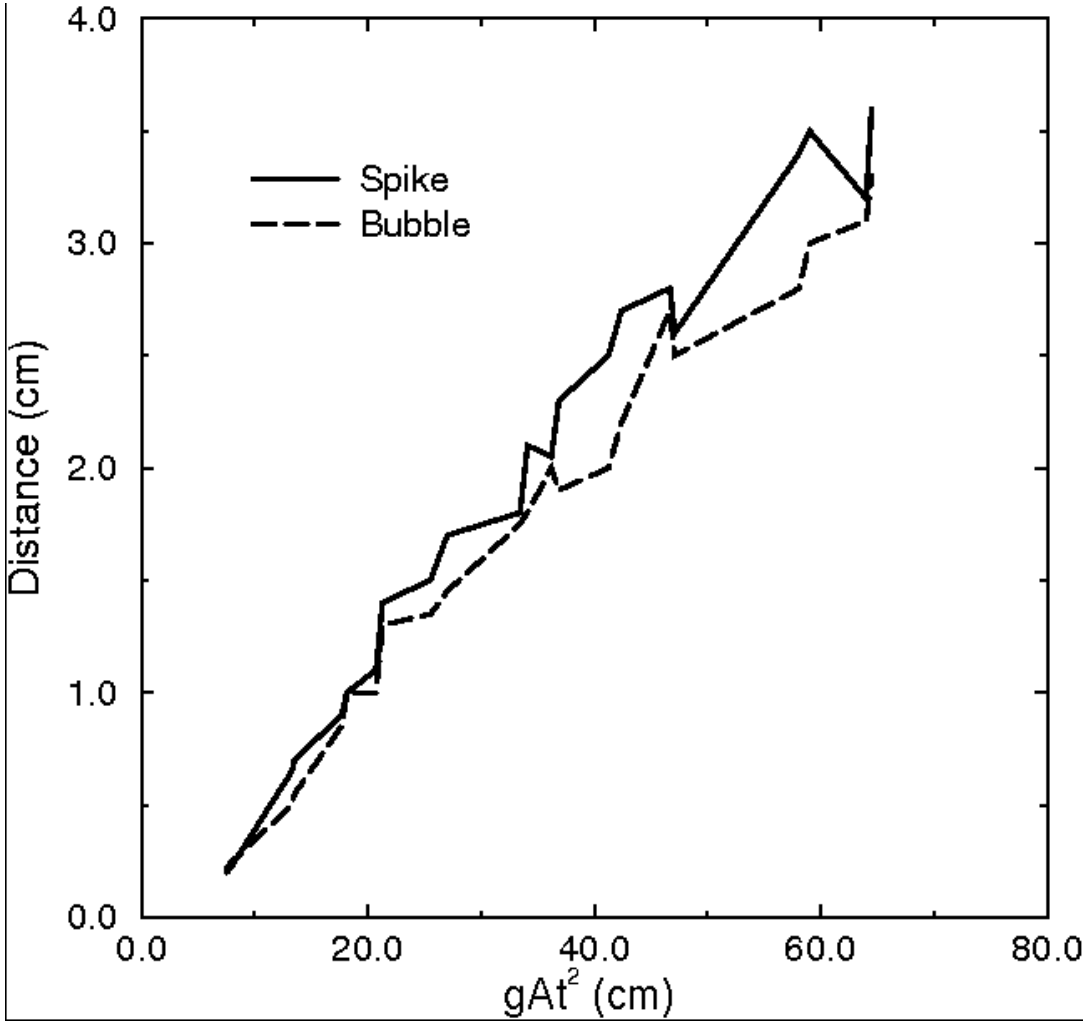


$\alpha_{spike} = 0.026$

$\alpha_{bubble} = 0.021$

Multi-mode Rayleigh-Taylor

Experiment



$\alpha_{spike} = 0.058$

$\alpha_{bubble} = 0.052$

Summary of Results

- Verification tests: Pass!
- Validation tests: 50/50 split
  - Three-layer targets- Good agreement with experiment
    - Incomplete physics
    - Additional work won't improve astrophysical simulations
  - Multi-Mode Rayleigh-Taylor- Poor agreement with experiment
    - Several reasons proposed: resolution, initial conditions
    - Single-mode study under way

Lessons Learned

- R-T, R-M problems are a challenge!
- Good collaboration with experimentalists is essential!
  - Access to experimental results and error/uncertainty assessment
  - Comparison to other simulations
  - Benefits theorists and experimentalists
- Increased confidence in Flash results
  - We are learning how to establish the limits of validity of Flash
  - We are establishing a methodology for systematic comparisons between experiments and simulations
- We are learning about R-T and R-M instability

Bibliography

Flash Code:

Fryxell et al., ApJS, 131, 273

Calder et al., in Proc. Supercomputing 2000, sc2000.org/proceedings

Validation:

Calder et al., ApJS, in press

Calder et al. CiSE submitted