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Verification, Validation and Uncertainty Quantification in Astrophysics

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Sensitivity, Error and Uncertainty Quantification for Atomic, Plasma, and Material Data

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U.S. DEPARTMENT OF ENERGY NASA NSF

Outline

- Introduce problem- stellar explosions known as supernovae
- Validation experiments designed to mimic astrophysical environments.
  - Laser-driven unstable shocks
  - Rayleigh-Taylor Instability
- The lives of stars
  - Hertzsprung-Russel diagram
  - Evolution of stars on H-R diagram
- Uncertainty Quantification Study
  - State of the art MESA simulation code
  - Uncertainty in progenitor of SNe Ia supernovae that are calibrated to be “standard candles”
  - Intrinsic scatter of SNe Ia is large source of uncertainty in observational studies probing dark energy

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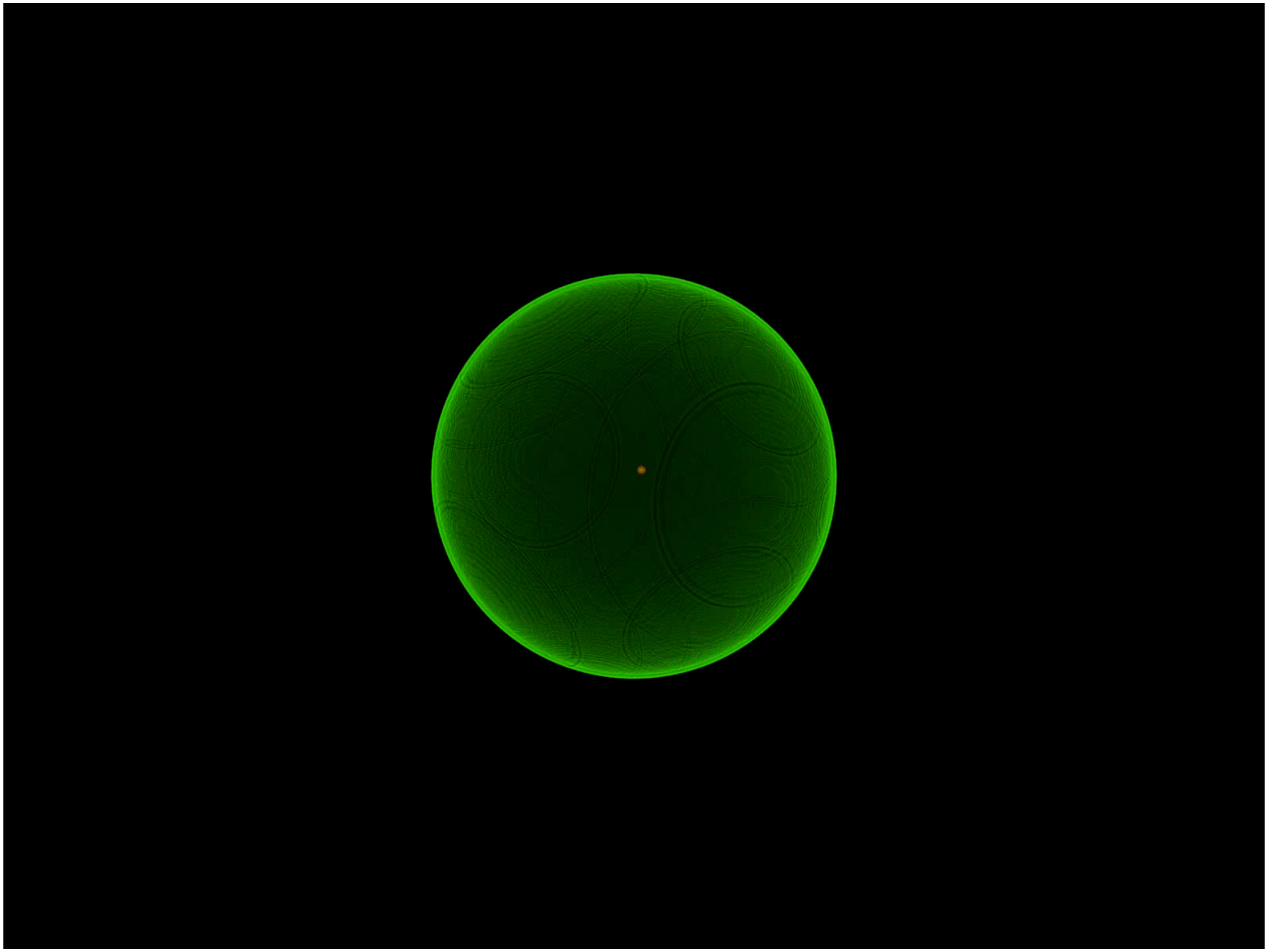
Type Ia Supernova Simulation



Jordan et al. 2008

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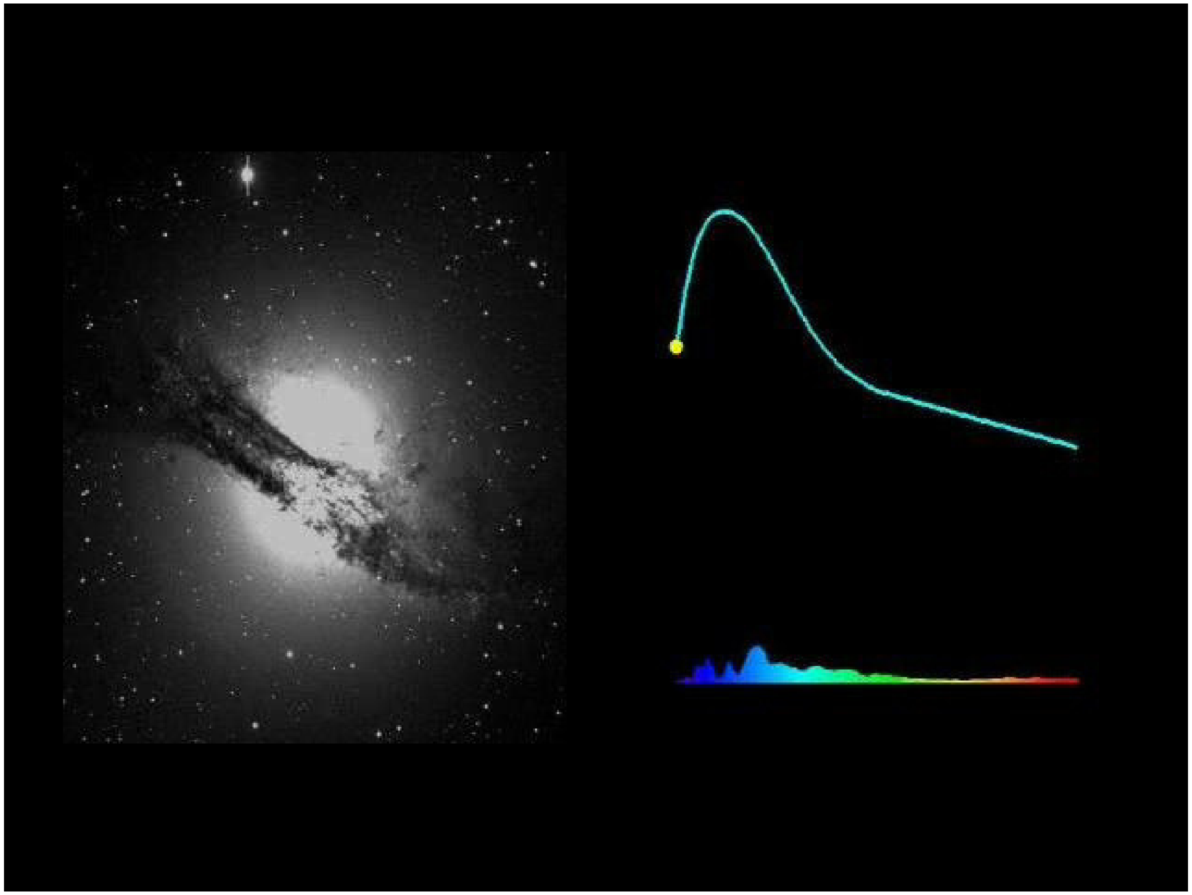
Physics of Type Ia Supernovae

- SN Ia are a multi-scale, multi-physics problem:
  - Reactive Euler equations with self-gravity (multi-dimensional!)
  - Equation of state for degenerate matter
  - Flame model (width/radius < 10^{-9})
  - Nuclear Energetics: $^{12}C+^{12}C$; burn to Nuclear Statistical Quasi-equilibrium (Si group); burn to Nuclear Statistical Equilibrium (Fe group).
  - Emission of ν's result in energy loss, ΔY_e (neutronization)
  - Turbulence-flame interaction.
- Connection to observations
  - Post-process lagrangian tracers with > 200 nuclide network to obtain detailed abundances
  - Mult-frequency radiation transfer to get light curves.
- Realistic models should also include:
  - Rotation
  - Magnetic fields

Astronomical Appearance

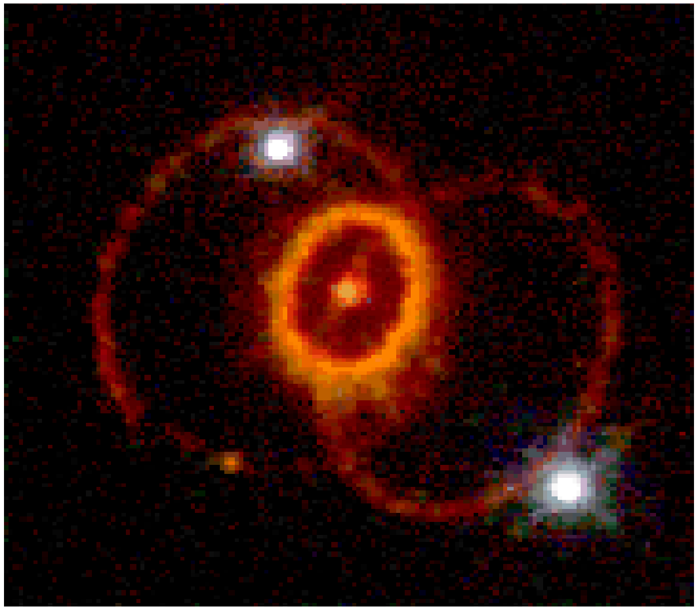


Observations: light curve, the observed intensity of light, and spectrum.

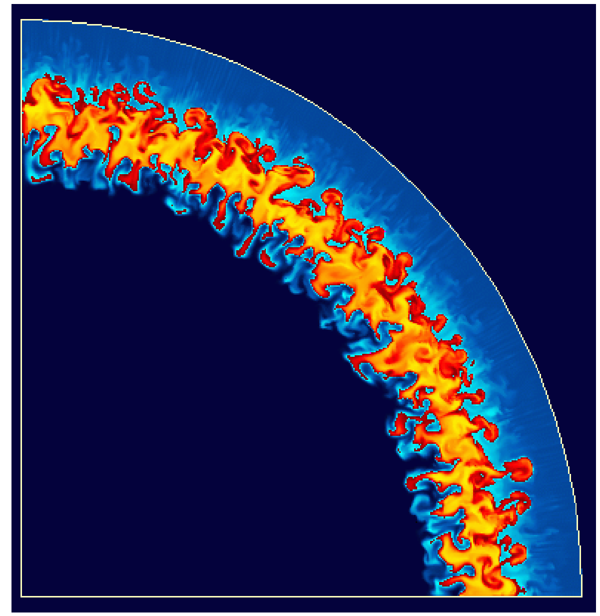
Light curve rises in days, falls off in weeks.

P. Nugent (LBNL)

Fluid Instabilities in Astrophysics



STScI



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

Validation experiments probing fluid instabilities

- Two experiments in environments similar to the interiors or stars.
- Similar, but not the same.

- Note- validation study came about under DOE ASC program.

Multi-mode Rayleigh-Taylor

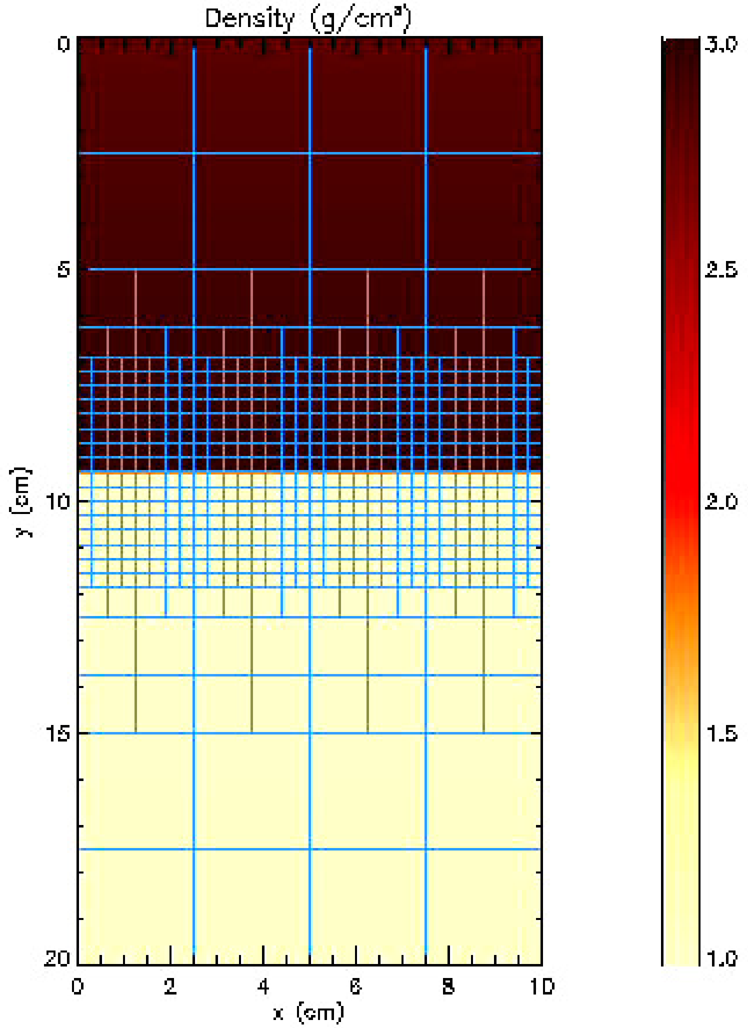
"α-Group" Consortium

- 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 a
  - simulation - experiment comparisons
  - inter-simulation comparisons

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

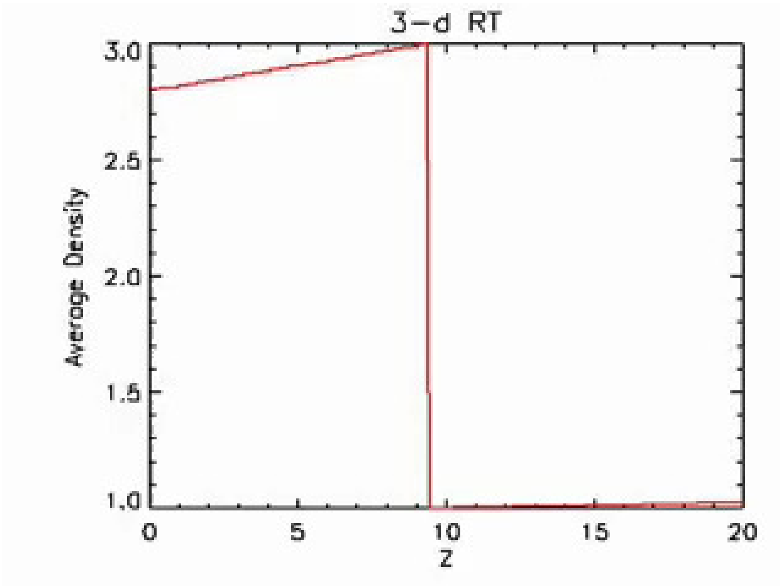
- Definition of standard problem set (D. Youngs)

Multi-mode Rayleigh-Taylor: 2-d Simulation

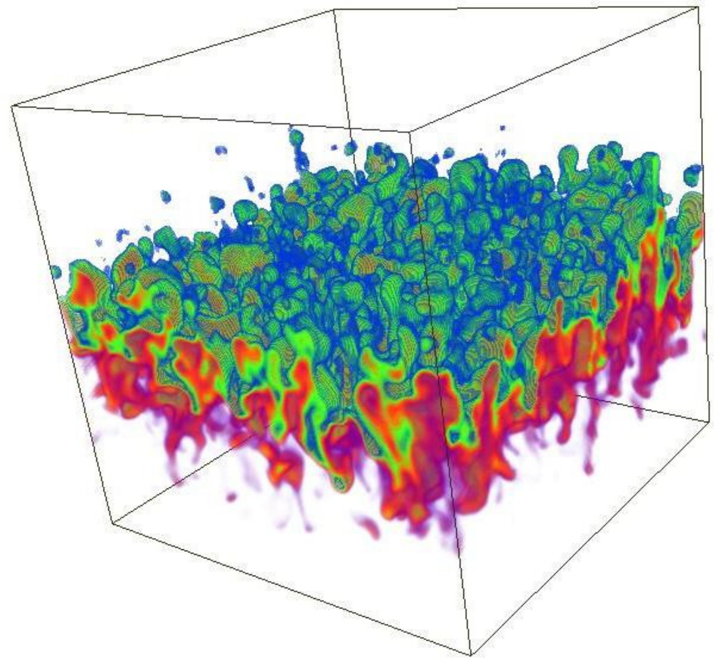


time = 0.000 ps
number of blocks = 778
AMR levels = 6

Multi-mode Rayleigh-Taylor: 3-d Simulation



Horizontally Averaged Density



Modes 32-64 perturbed

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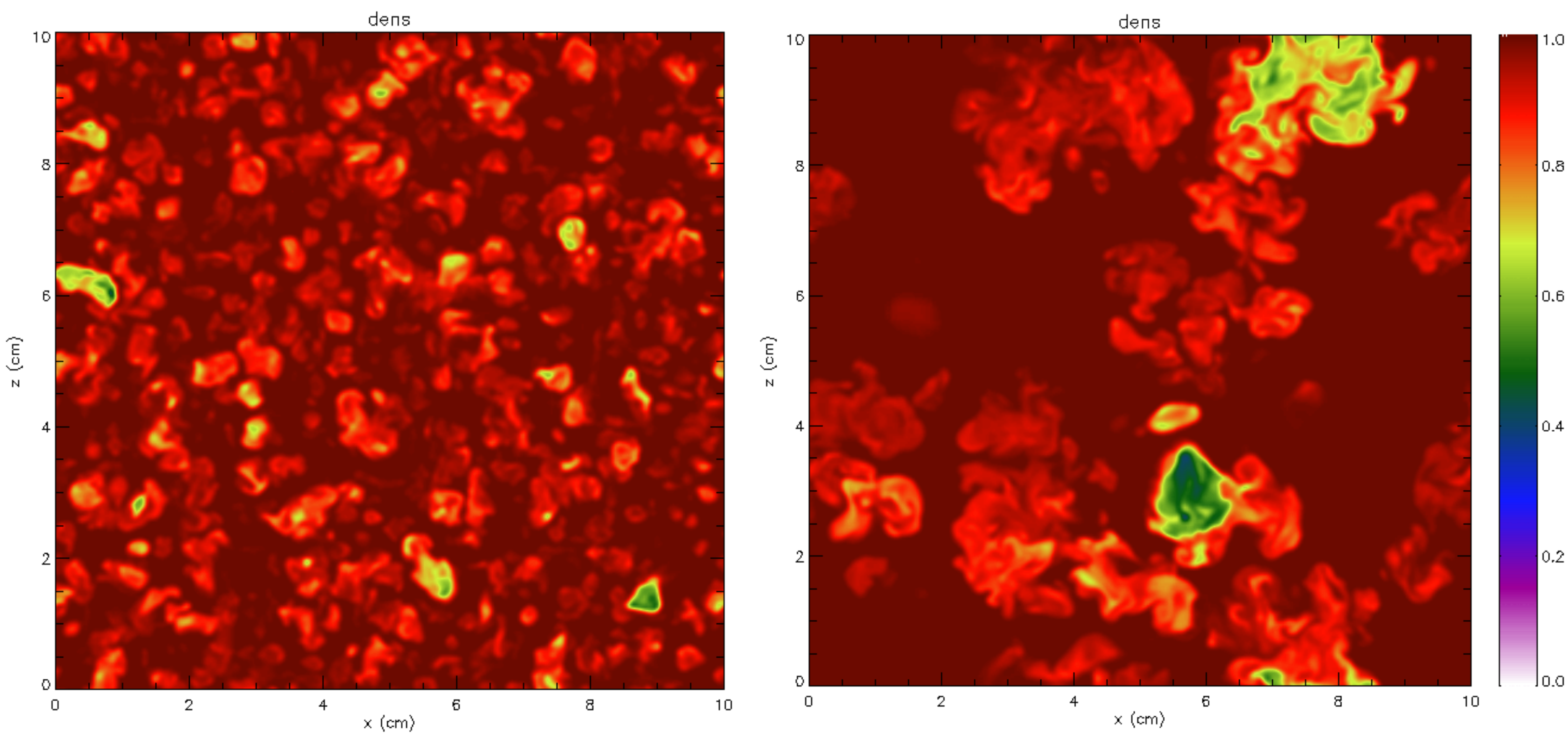
Multi-mode Rayleigh-Taylor: Inverse Cascade

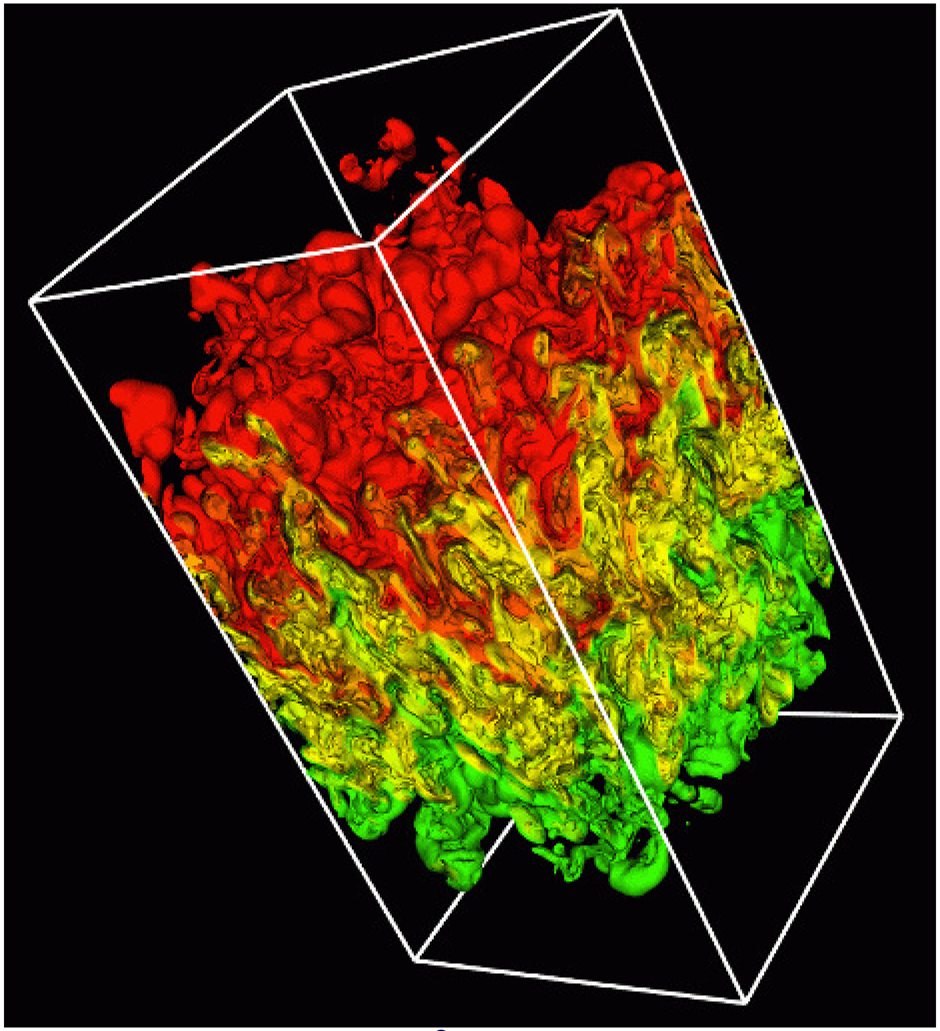
Bubbles of the lighter fluid in the denser fluid



t = 7.00 sec t = 14.75 sec

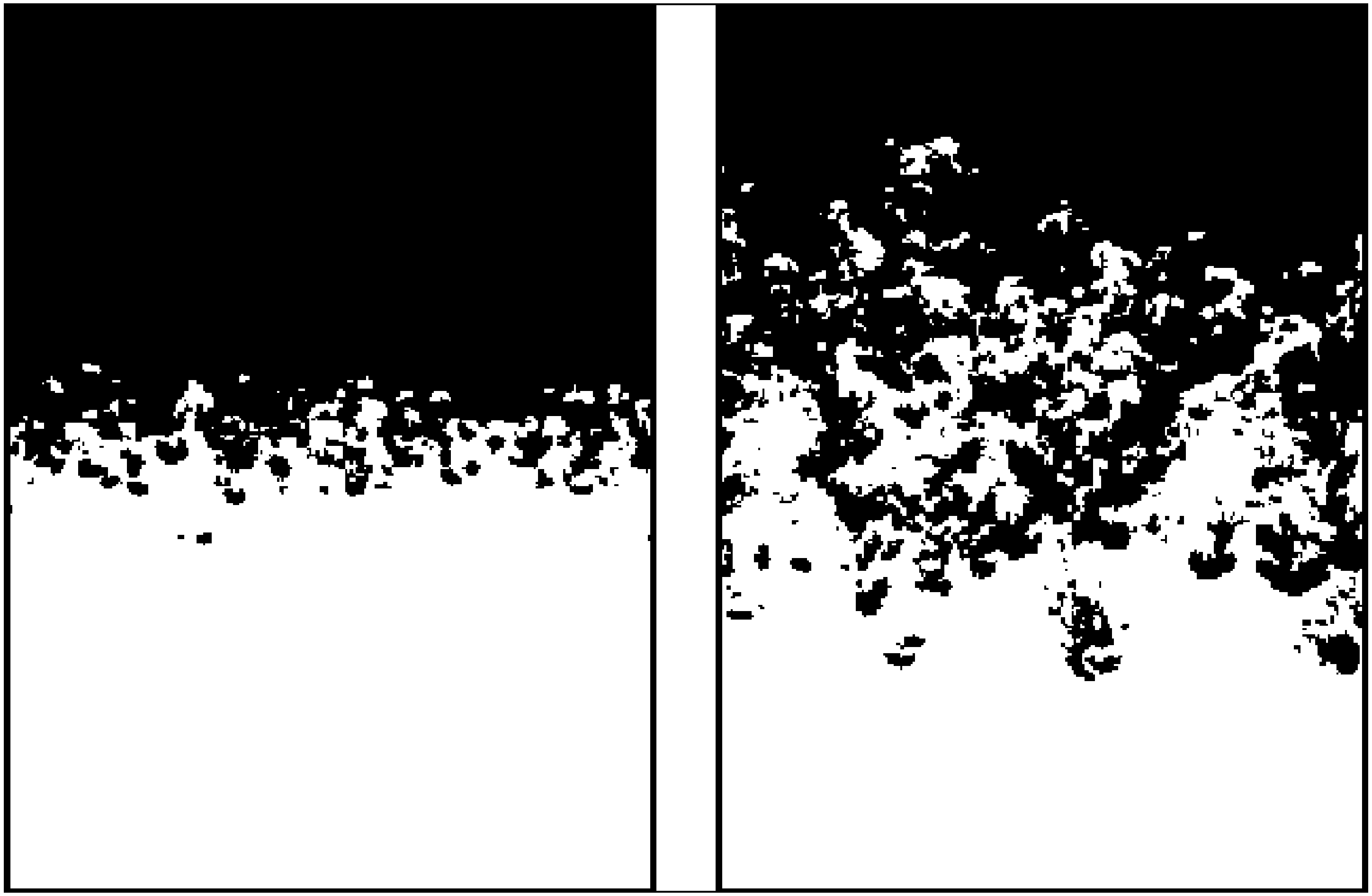
Multi-mode Rayleigh-Taylor

Rendering of
Mixing Zone



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

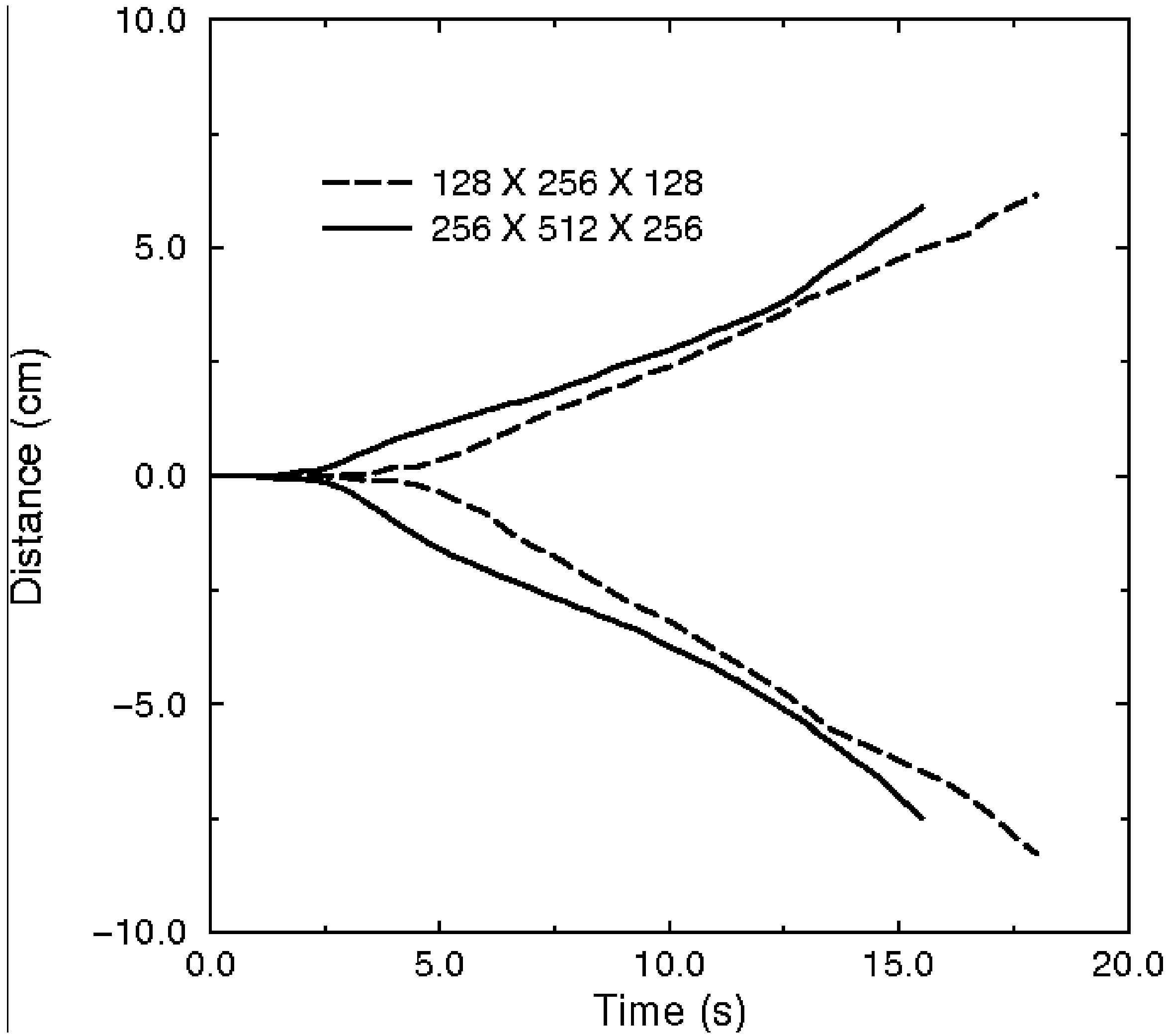
Multi-mode R-T Experimental LIF Image



It looks similar to the simulation…..

Multi-mode Rayleigh-Taylor

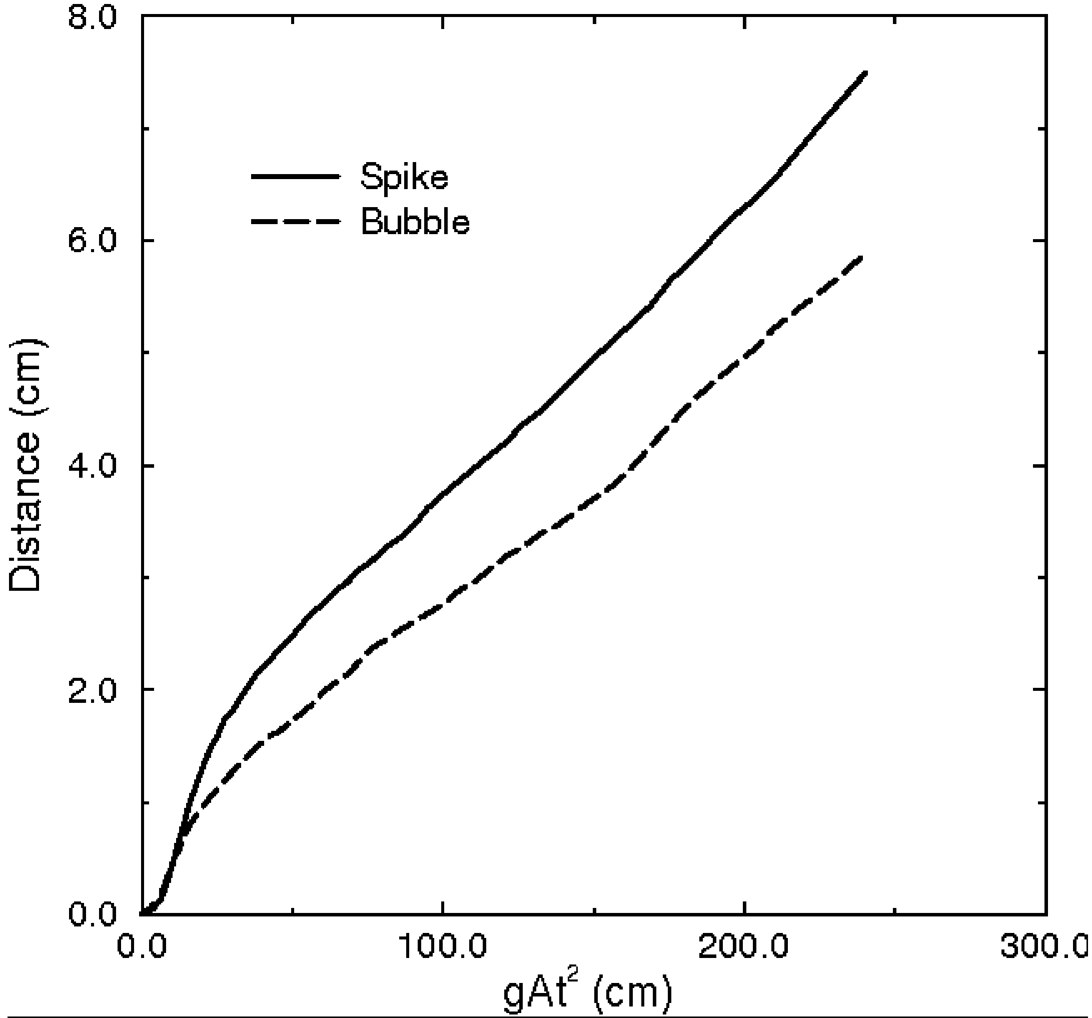
FLASH Simulation



Are we adequately resolved?

Multi-mode Rayleigh-Taylor

FLASH Simulation

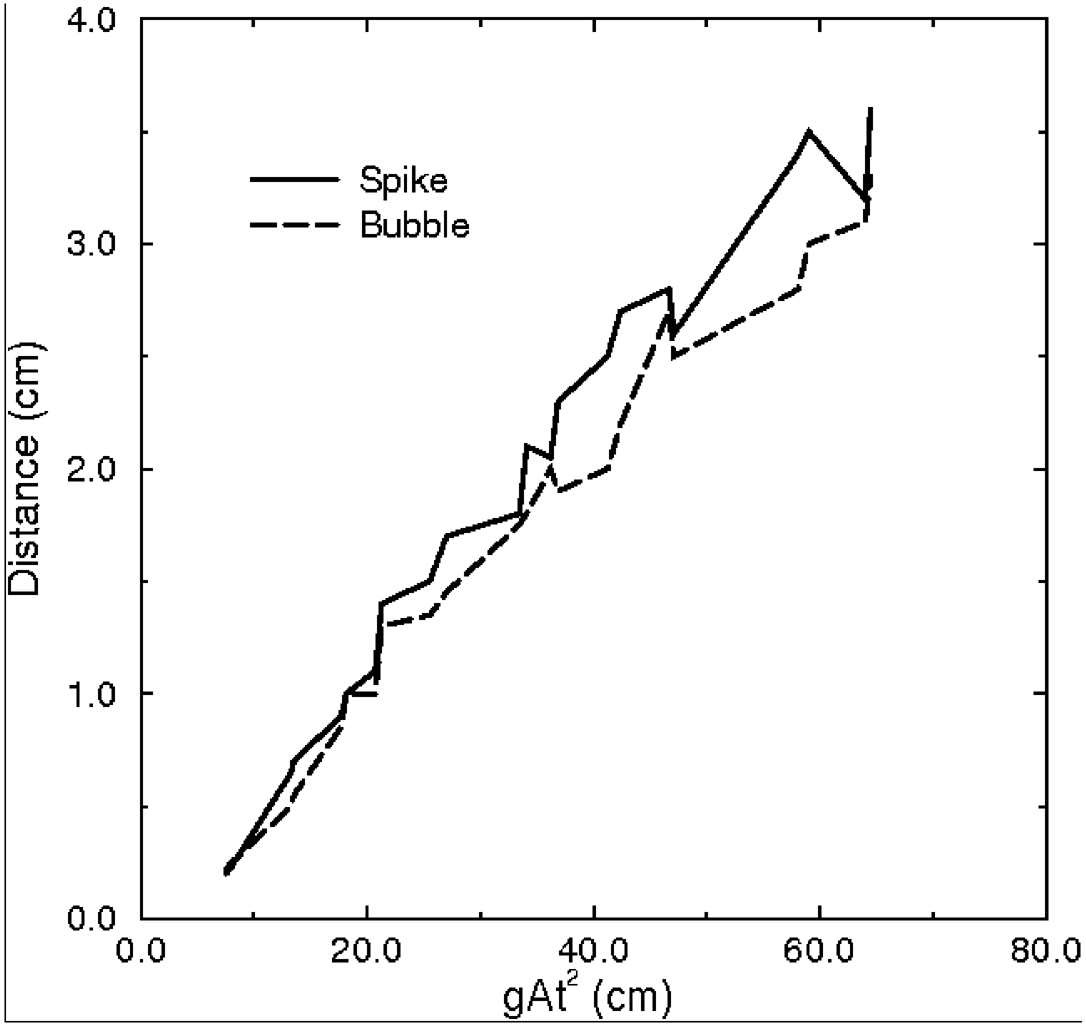


$\alpha_{spike} = 0.026$

$\alpha_{bubble} = 0.021$

Multi-mode Rayleigh-Taylor

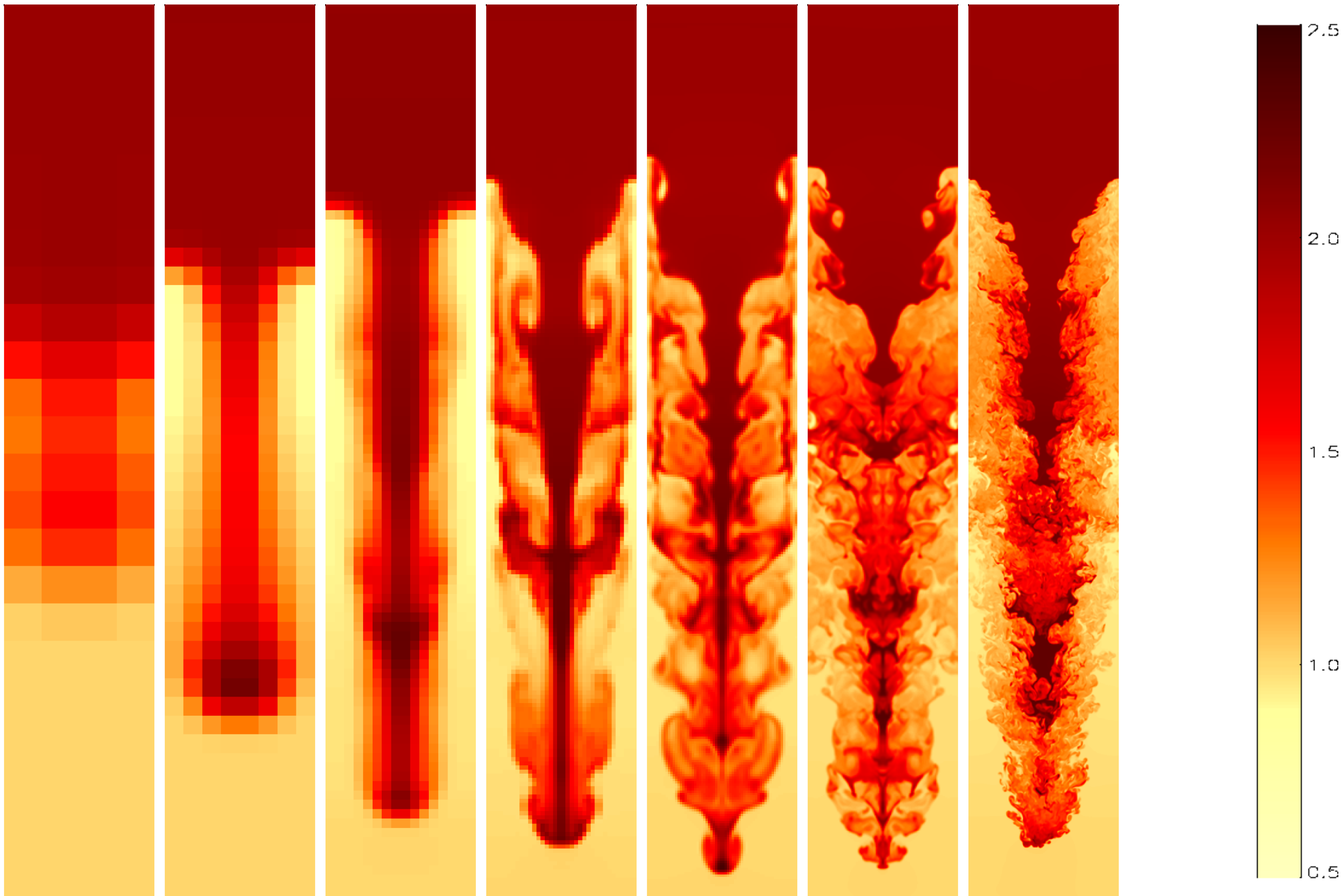
Experiment



$\alpha_{spike} = 0.058$

$\alpha_{bubble} = 0.052$

Single-mode 3-D Rayleigh-Taylor



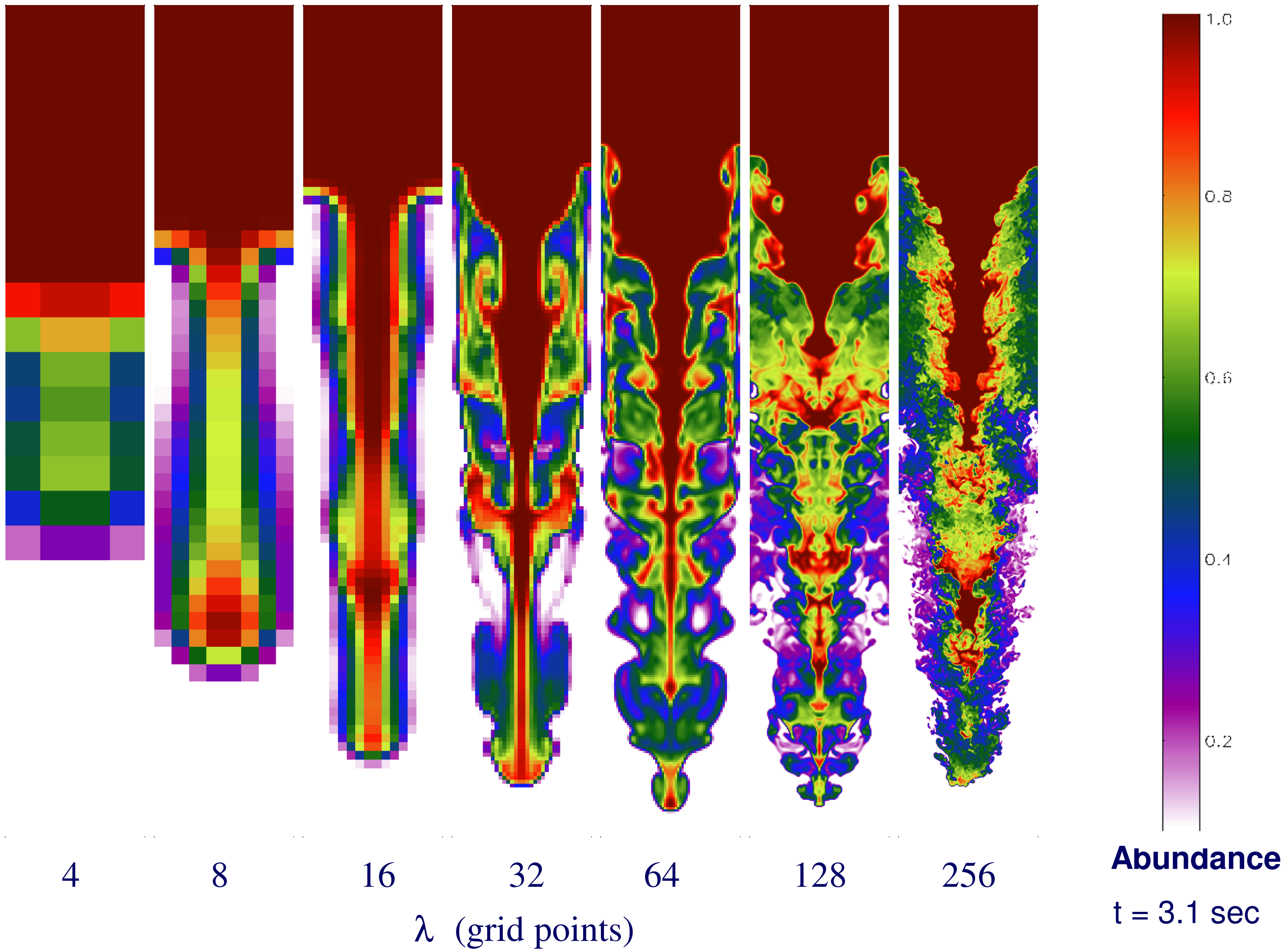
4 8 16 32 64 128 256

λ (grid points)

Density (g/cc)

t = 3.1 sec

Single-mode 3-D Rayleigh-Taylor



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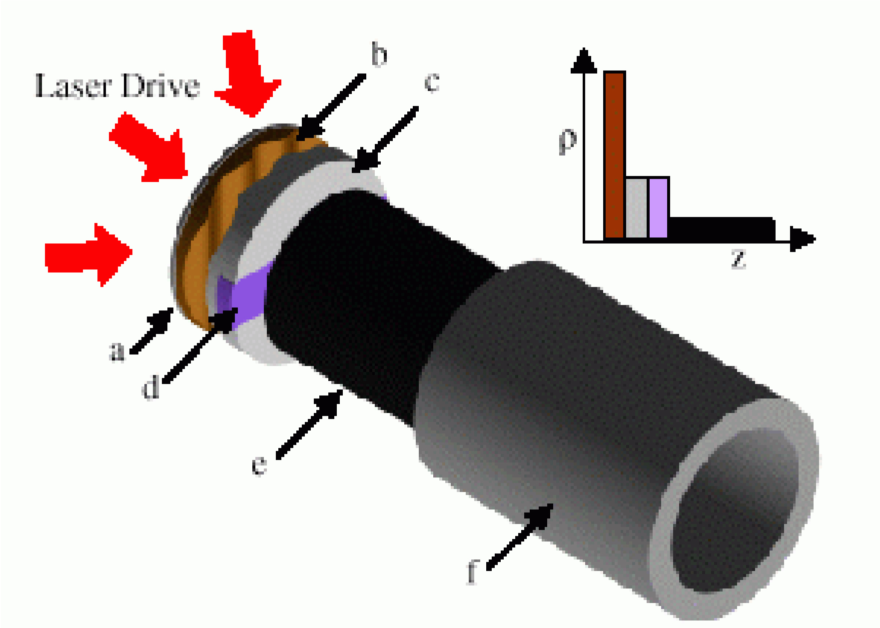
Validated?

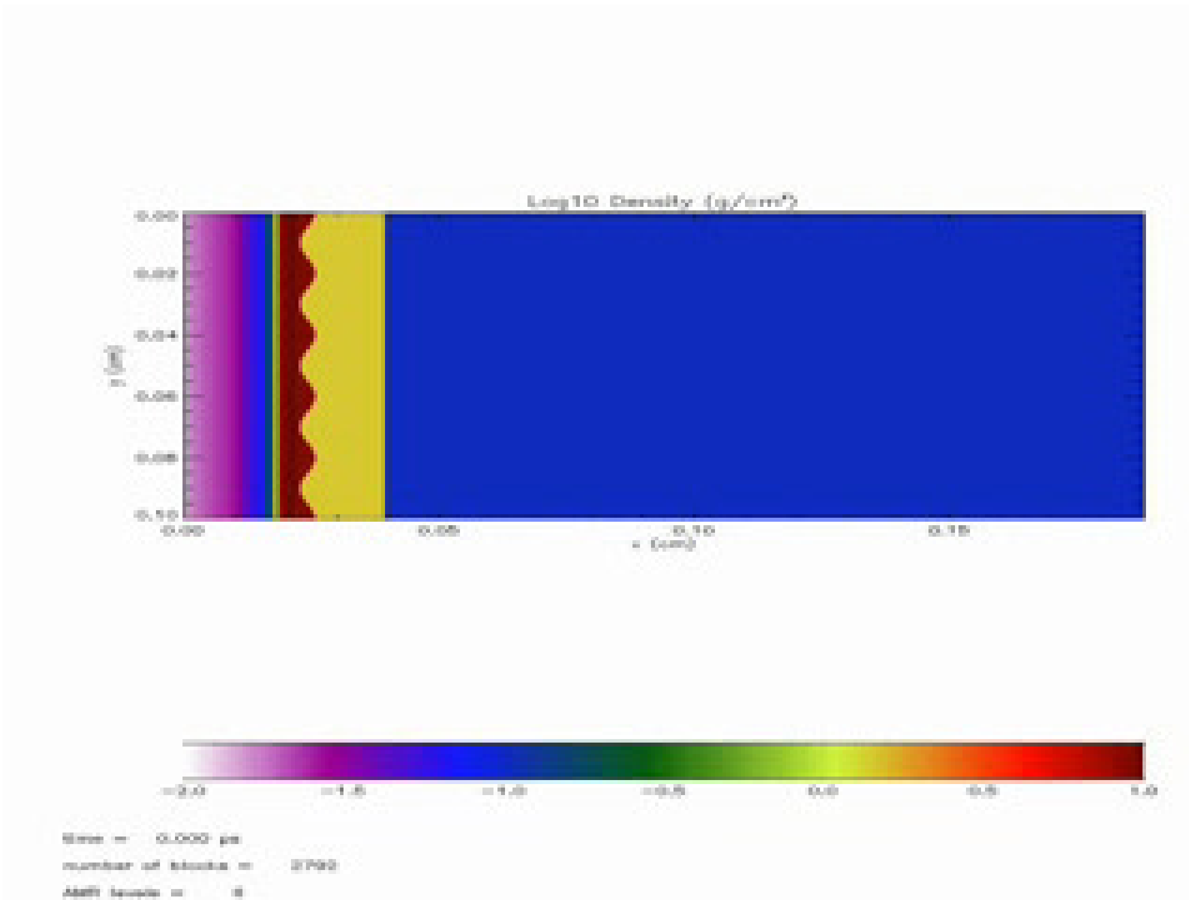
- Simulations disagreed with experiment.
- Simulations agreed with simulations by others in the α-group.
  - Utility of code-code comparisons?
- Experimentalist was skeptical of his own data.
- Summary- learned a vast amount, but did not validate.

Three-layer Shock Imprint Experiment



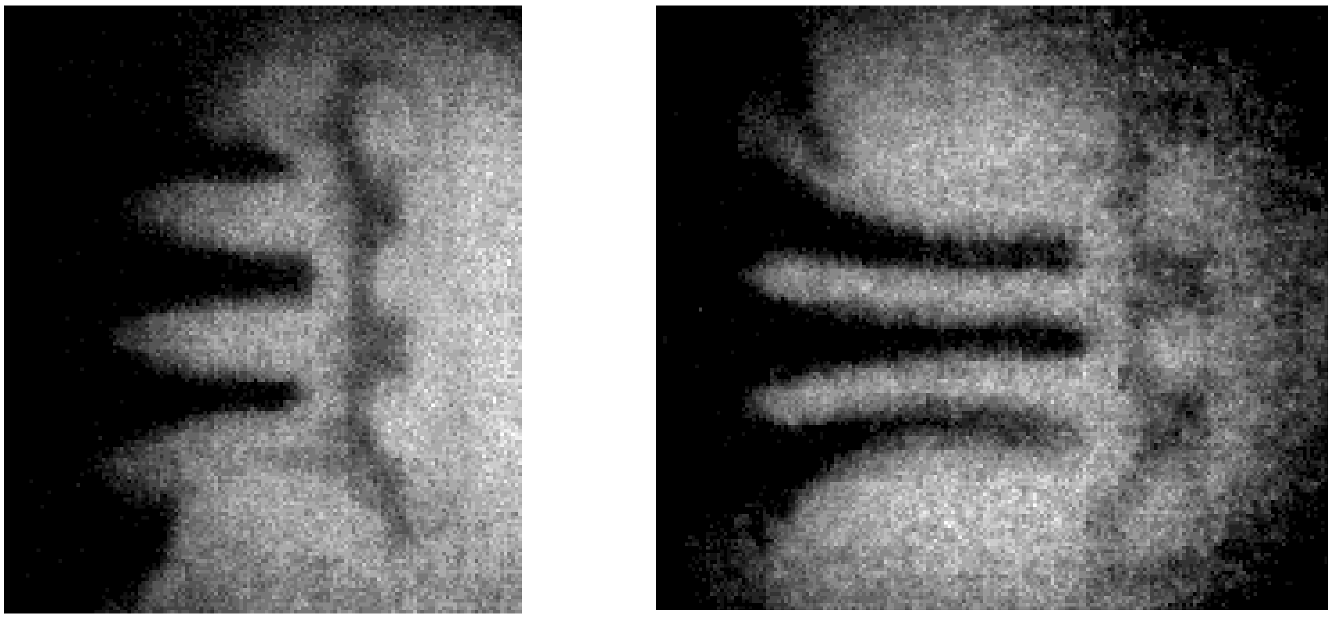
- Performed at the Rochester Omega laser facility
- Strong shock driven through a planar, copper-plastic-foam three-layer target
- Rayleigh-Taylor and Richtmyer-Meshkov instabilities

Three-layer Target Simulation



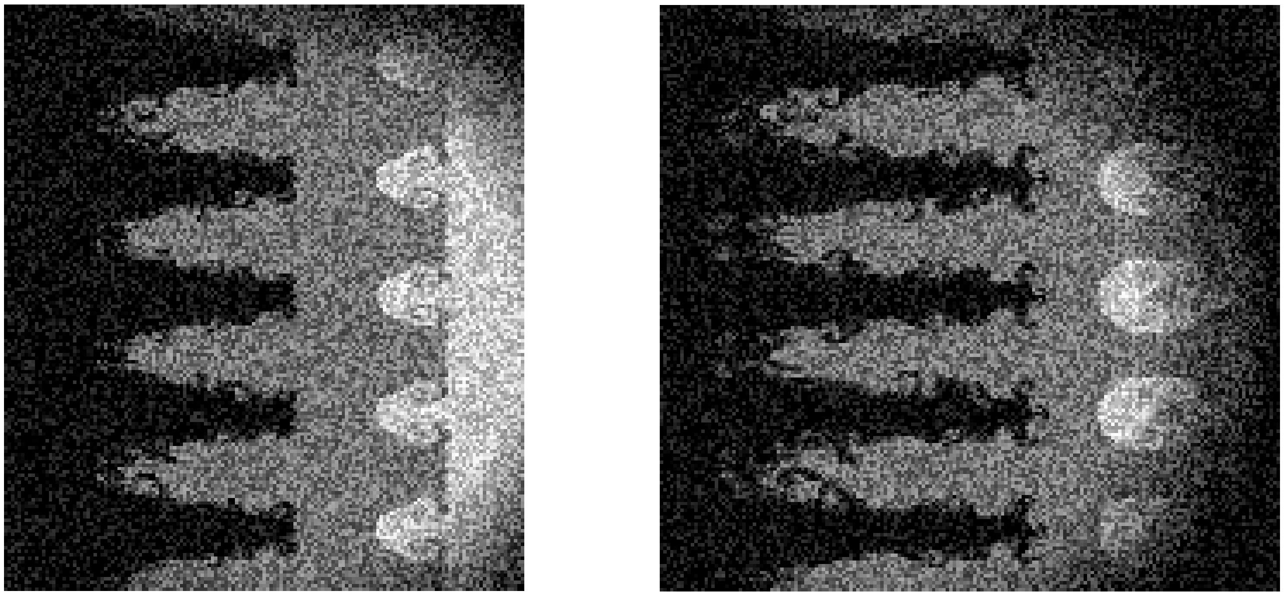
Movie

Three-layer Target Simulation



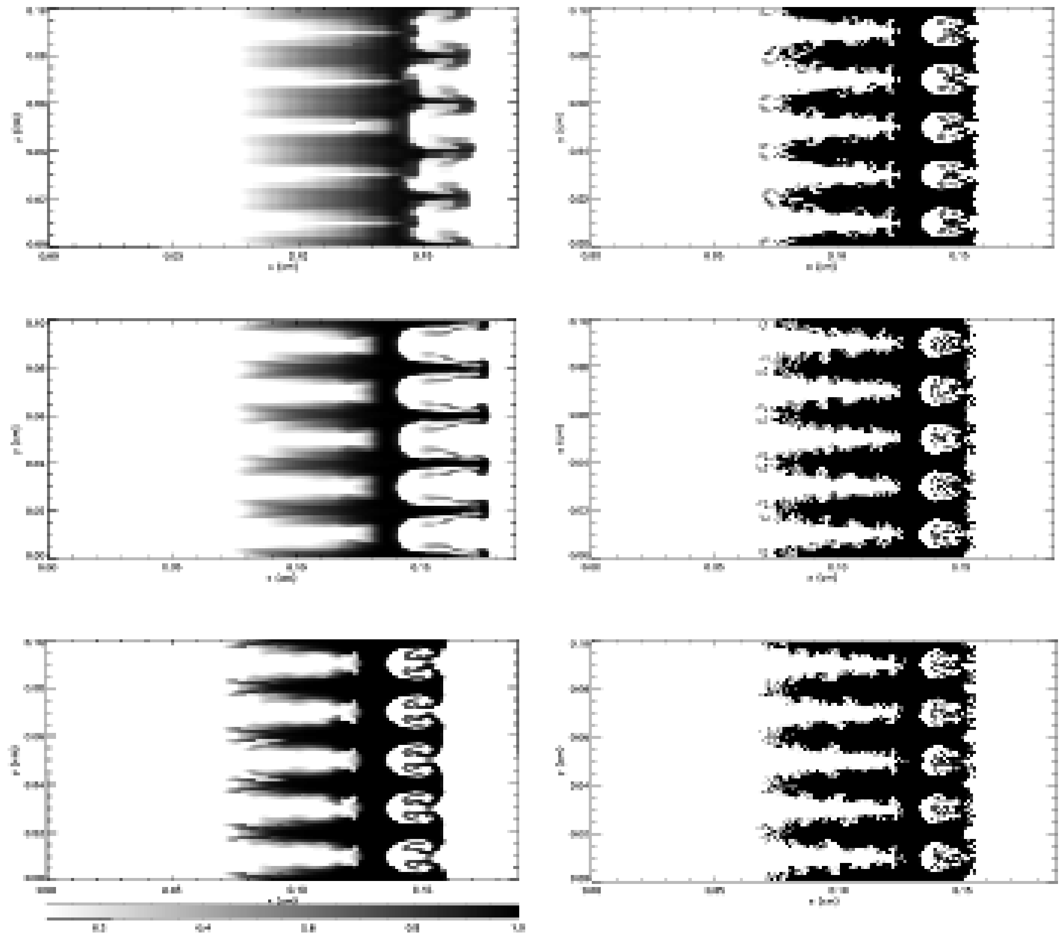
Images from the experiment

Three-layer Target Simulation



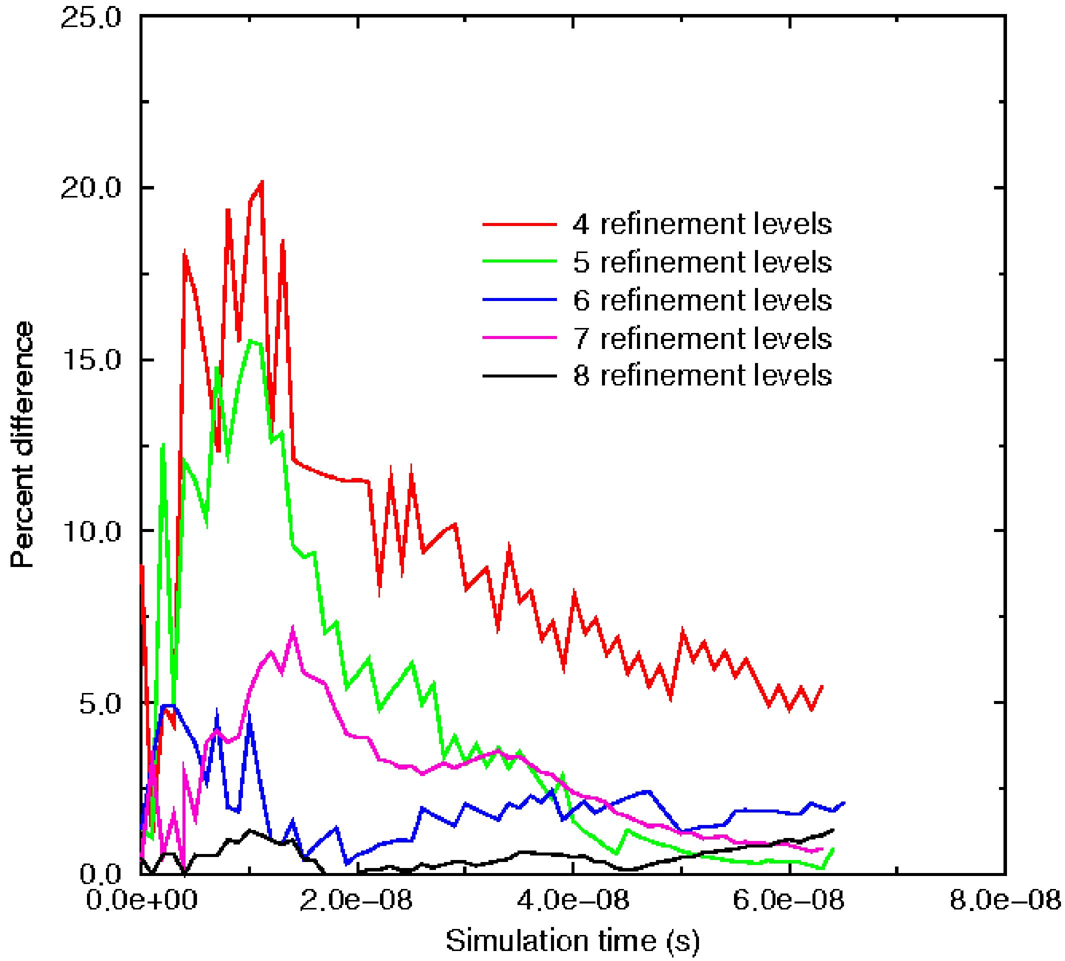
Simulated radiographs

Three-layer Target Simulation



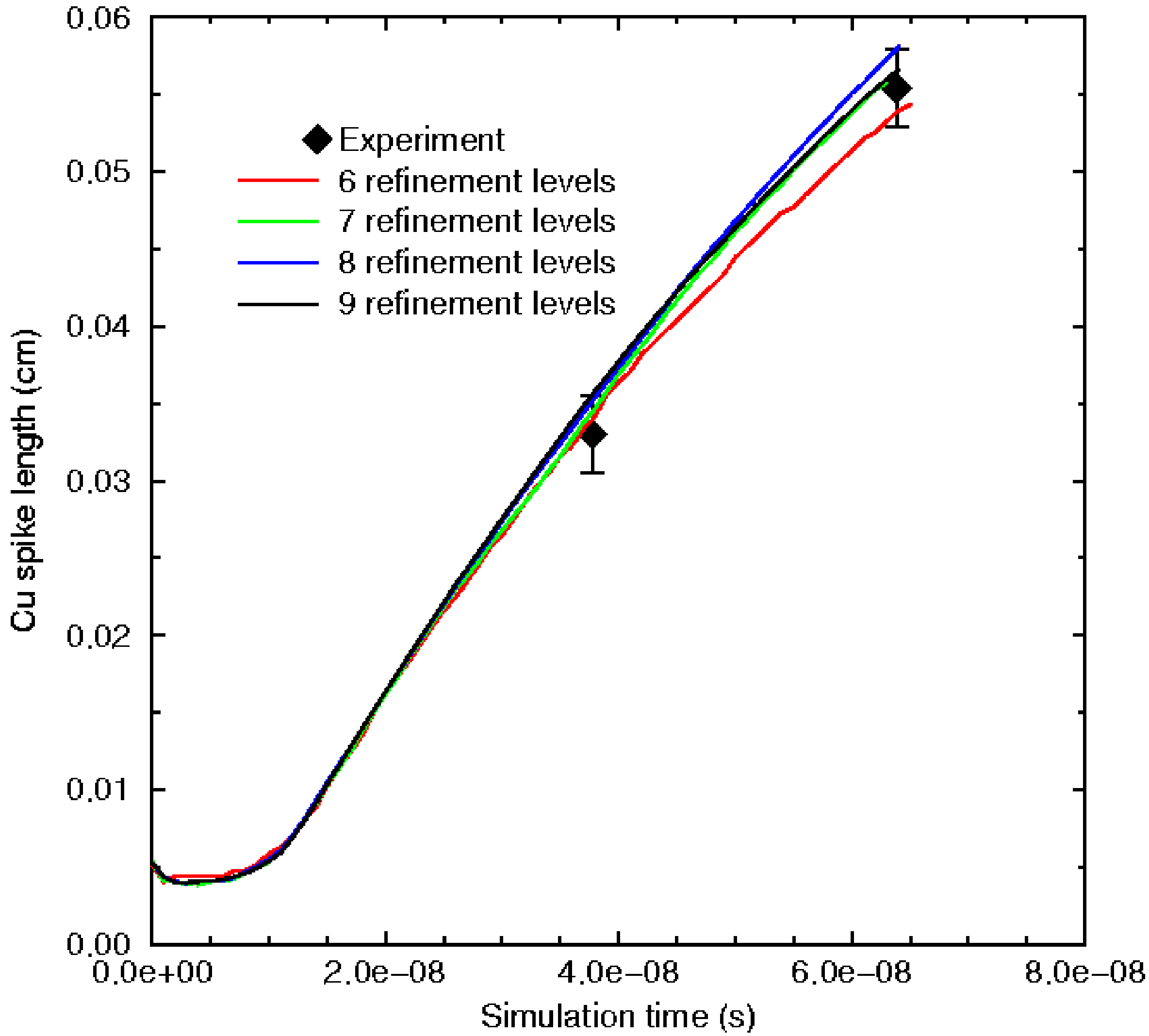
Resolution Study

Three-layer Target Simulation



Convergence results: percent difference

Three-layer Target Simulation



Validated? Incomplete Physics

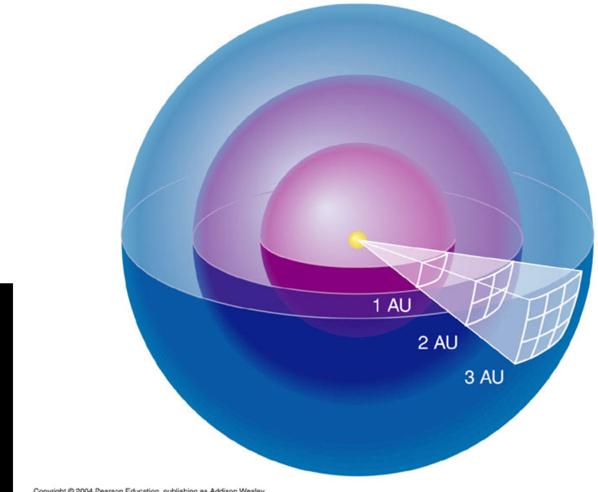
- Simulations used a gamma-law EOS, $P = (\gamma - 1)\rho\varepsilon$, with choice of gamma to match experimental result
- Periodic boundary conditions on sides- no shock tube in the simulations
- Radiation deposition mechanism not included in the simulations
- Experimental diagnostics do not allow us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

What is a supernova?

- Bright stellar explosion
- Type Ia- thermonuclear incineration of a compact star
- Converts lower-mass elements to higher-mass elements.
- Binding energy release powers the explosion
- Display powered by radioactive decay of ^{56}Ni

http://apod.nasa.gov/apod/ap150531.html

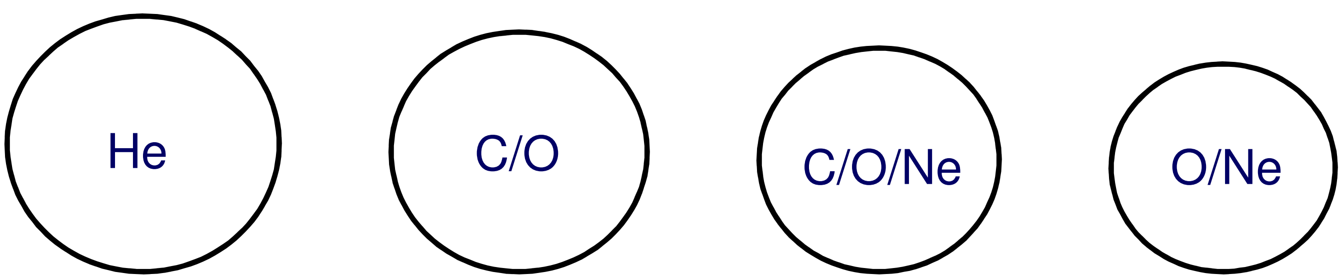
Exploding Stars as Standard Candles



sorrisoblu.blogspot.com

Key Points

- A successful explosion requires a WD composition with a significant fraction of C.
- Composition follows principally from initial mass of main sequence star.
- Additional mass gained from accretion from companion.
- Question- what range of initial masses produce enough C? How are initial masses distributed and can we relate that host galaxy properties?



Mass of WD →

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Overarching Goal of UQ Study

- Question- how does one do UQ with a “black box” code in general if one can't assume linearity of the outputs from changes in the inputs, or more generally, if one can't even estimate the dependence?
- Big picture is the uncertainty in the “pipeline” to simulate an astrophysical event.
  - Can’t do end-to-end simulations, so work in stages with different technology for each.
  - Create hierarchy in which some simulations serve as sub-grid-scale models for others.
- Our problem- evolution of star from birth to explosive death to quantify uncertainty in the observed outburst.
- Want a language of uncertainty in astrophysics and hope to contribute to methodology.

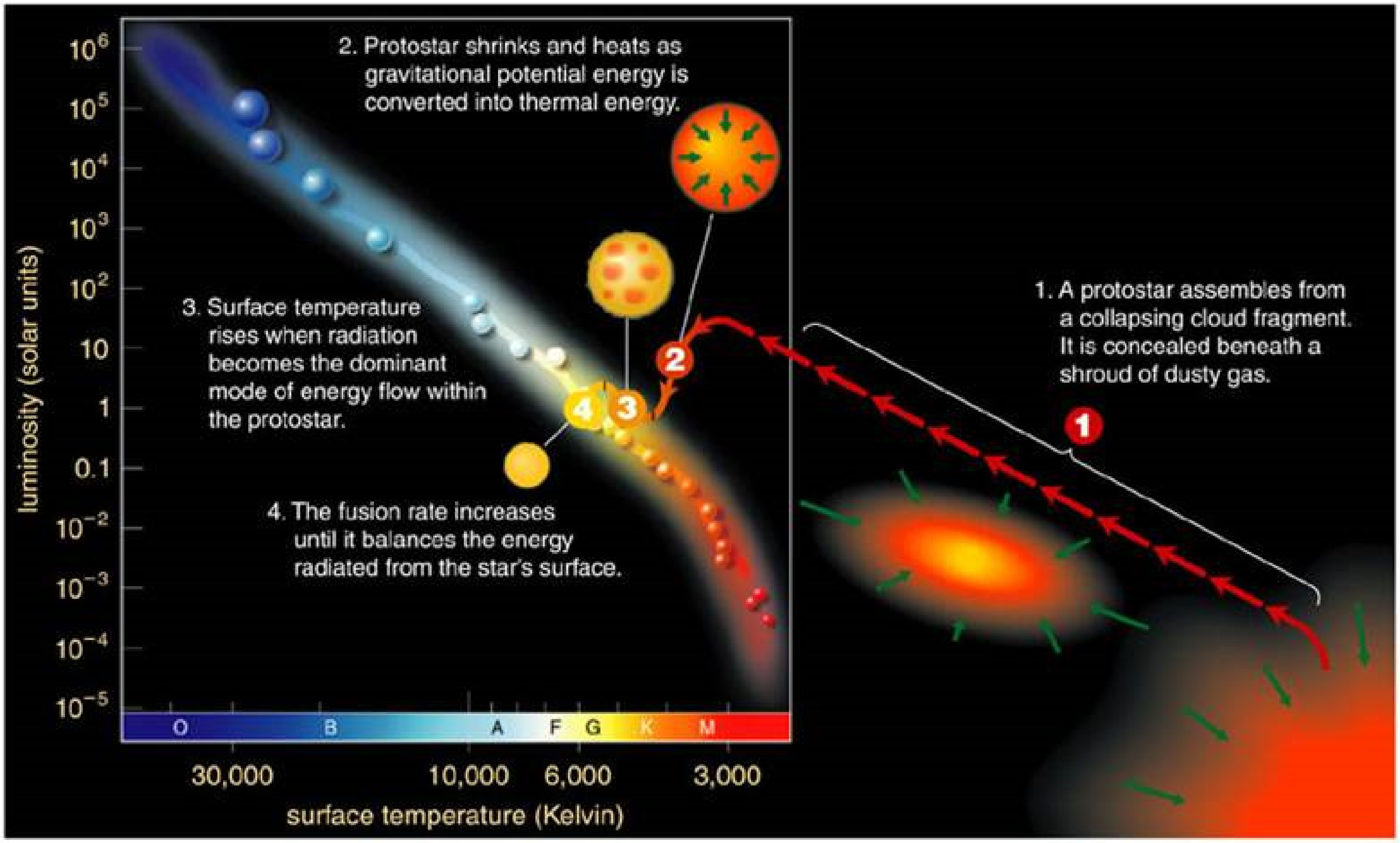
MESA stellar evolution code

- Modules for Experiments in Stellar Astrophysics (mesa.sourceforge.net)

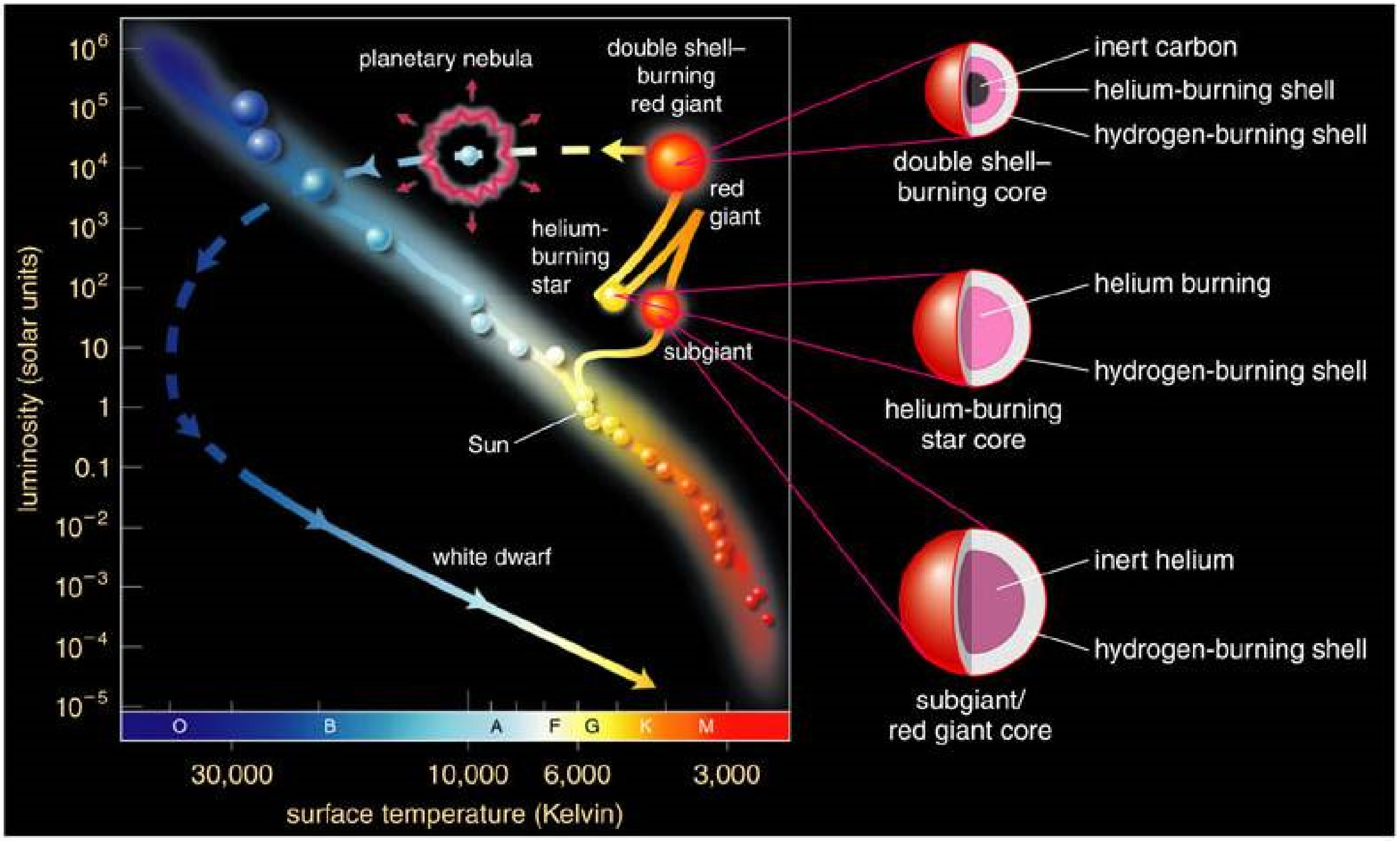
- 1-d hydrodynamics coupled to additional physics (reactions and diffusion)
  - Simultaneously solves fully coupled structure and composition equations.
  - Independently usable modules:
    - EOS
    - opacity
    - nuclear reaction rates
    - atmosphere boundary conditions

- Many of the issues with turbulent dynamical systems apply
  - Non-linear evolution equations
  - Large parameter space
  - Wide range of energy, length, and time scales
  - Possibly discontinuous results

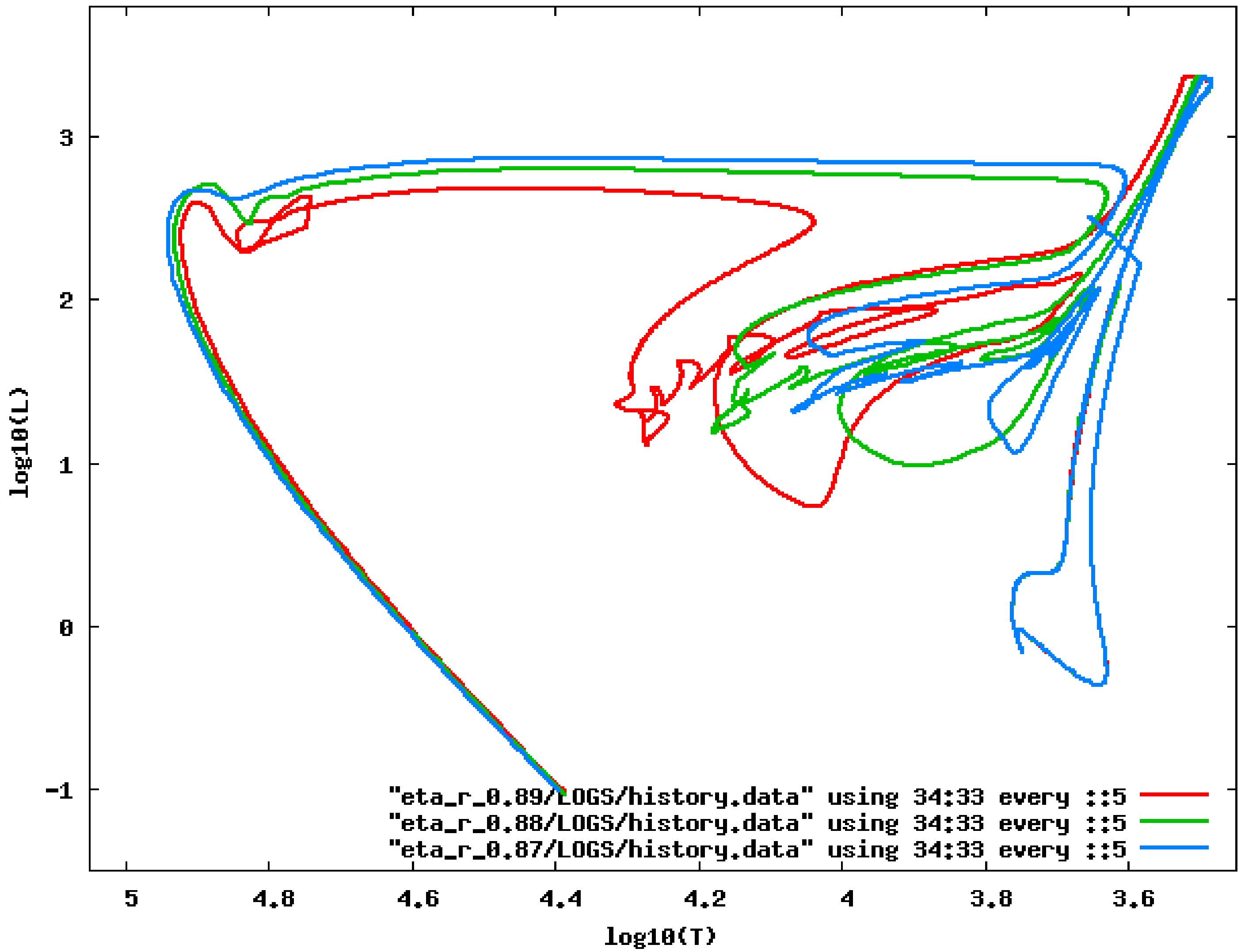
Low-mass stellar evolution as we teach it



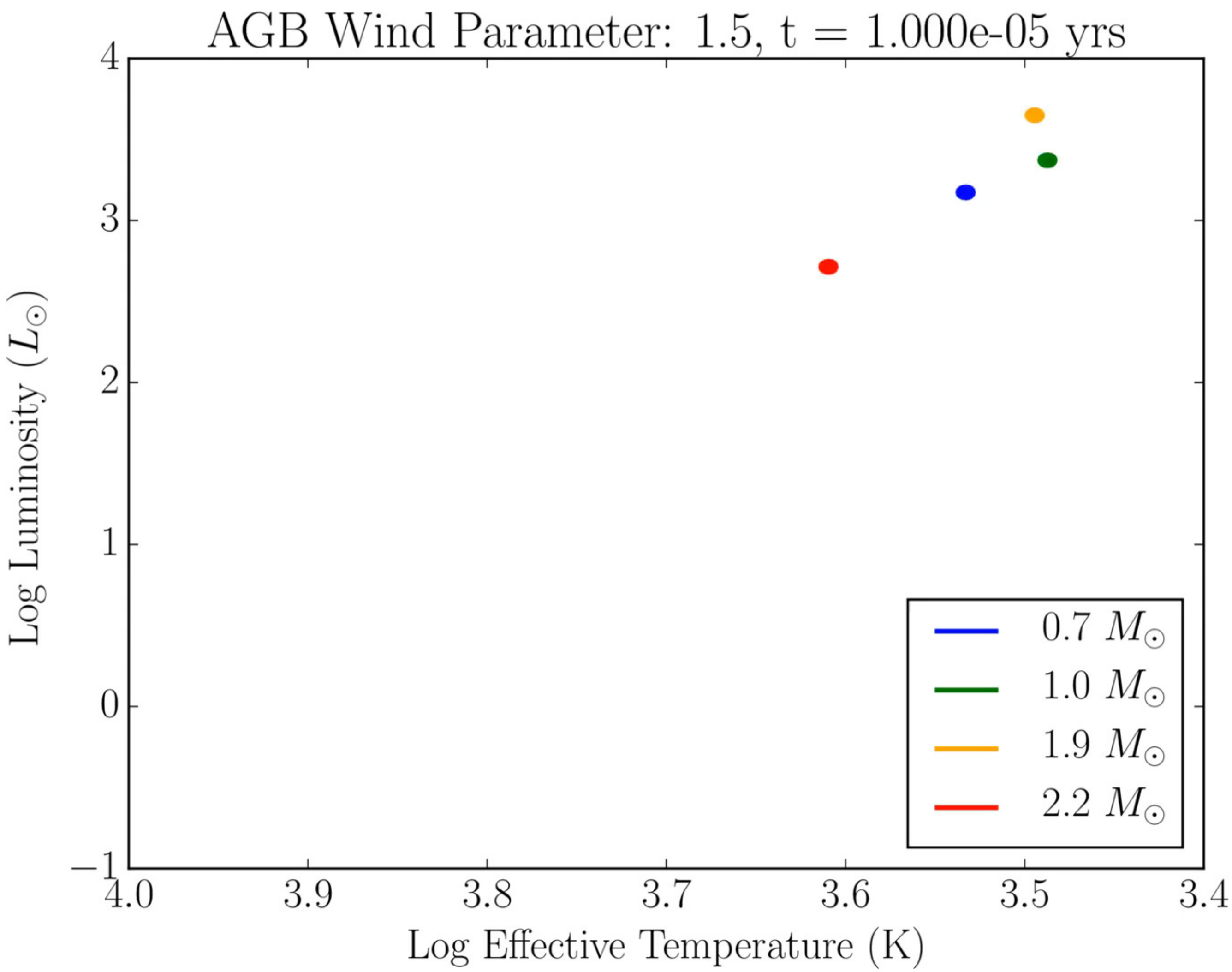
Low-mass stellar evolution as we teach it



Low-mass Stellar Evolution



Evolution of Different Mass Stars



Status

- Really after intrinsic scatter of Type Ia brightness to improve precision of cosmological results.

- Identified parameters of interest
  - Initial mass and composition (aleatory uncertainty or variability)
  - Stellar wind (epistemic uncertainty or incertitude)

- Performing sensitivity analysis:
  - Uniform march through model parameters
  - Cauchy deviates to bound results
  - Monte Carlo
  - Simulations from a distribution of physical parameters

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…and that leads us to

QUESTIONS AND DISCUSSION

Please send comments or ideas to alan.calder@stonybrook.edu

Bibliography

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  - Kreinovich and Ferson, Texas CS report UTEP-CS-02-28a, Reliable Engineering and Systems Safety 85, 267 (2004)
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