MAESTRO: Latest Developments

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MAESTRO: Latest Developments

Collaborators

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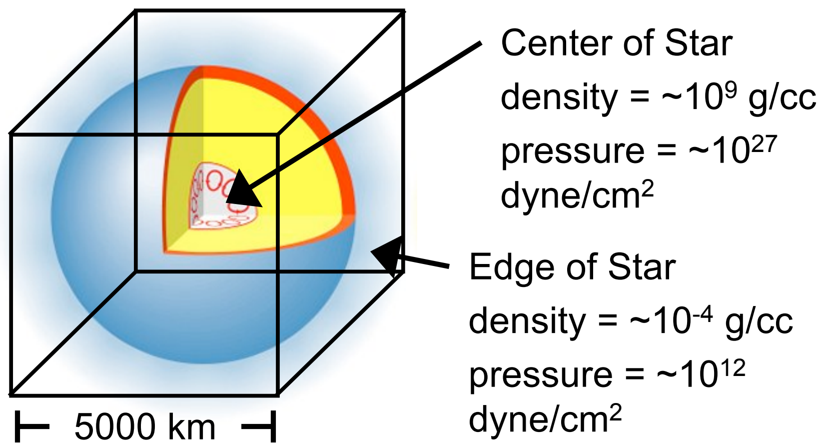
Introduction

- There are a number of problems that are characterized by long-time integration of subsonic flow.
  - Not well-suited for CASTRO

- Motivating examples
  - Type Ia supernovae, convection preceding ignition
  - Type I X-ray bursts, convection preceding outburst
  - Convection in massive stars, oxygen shell burning
  - Classical novae, convection preceding outburst

Type Ia Supernovae

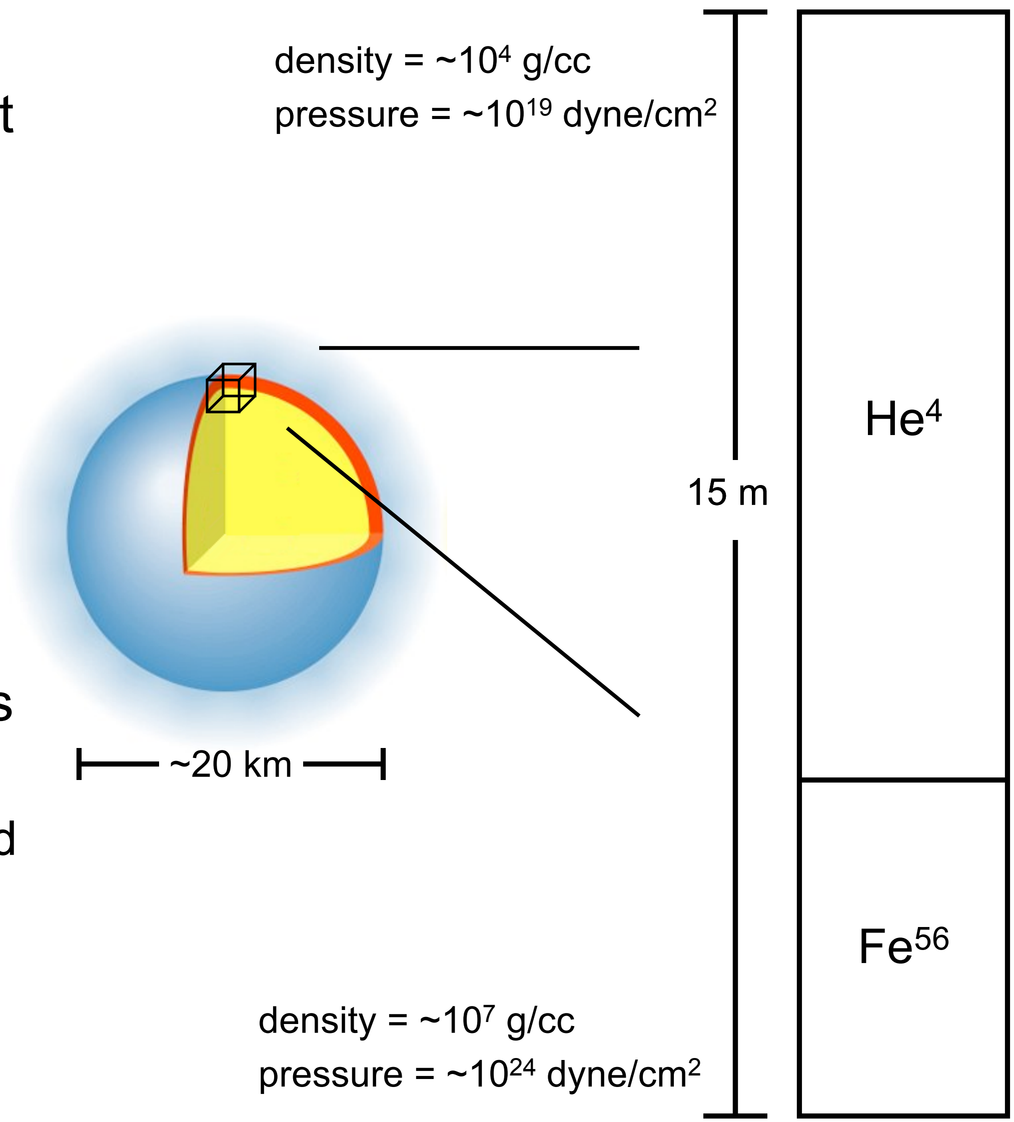
- Last few hours of convection preceding ignition
- Model the entire star in Cartesian geometry
  - Capture full-star dynamics
  - Avoid a singularity at the center of the star



- Highly stratified base state pressure and density
  - Atmosphere expands over time
- We would like to use adaptive mesh refinement (AMR) to focus our computational efforts near the core.
  - Burning drives convection and expansion.
  - We expect ignition to occur near the center of the star.

Type I X-Ray Bursts

- Convection preceding outburst
- Model the surface of the star
- Highly stratified base state expands over time
- We would like to use AMR to focus computational resources near the surface.
  - Burning drives convection and expansion.
  - Fully resolved 3D simulations are infeasible without AMR.



MAESTRO Algorithm Features

- Low Mach number formulation allows for long-time integration of highly subsonic flow
- Time-dependent base state allows for atmospheric expansion
- Retain local compressibility effects (heating, reactions, thermal diffusion)
- General EOS
- General reaction network
- Coordinate systems: 1D Cartesian and spherical, 2D and 3D Cartesian
- AMR (no subcycling in time)

MAESTRO Software Features

- Fortran90
  - BoxLib infrastructure
- Massively parallel using hybrid MPI / OpenMP
  - Scales to 50,000 cores
- Visualization
  - VisIt, amrvis
- Compatible with CASTRO
  - Plotfiles and checkpoint files share the same AMR BoxLib infrastructure
  - Same EOS and reaction network

Mathematical Formulation: Low Mach Model

$$\frac{\partial(\rho X_k)}{\partial t} = -\nabla \cdot (\rho X_k \mathbf{U}) + \rho \dot{\omega}_k$$

$$\frac{\partial(\rho \mathbf{U})}{\partial t} = -\nabla \cdot (\rho \mathbf{U}\mathbf{U}) - (\rho - \rho_0)\mathbf{g} - \nabla \pi$$

$$\frac{\partial(\rho h)}{\partial t} = -\nabla \cdot (\rho h \mathbf{U}) + \frac{D p_0}{D t} + \rho H_{\mathrm{nuc}} + \rho H_{\mathrm{ext}} + \nabla \cdot \kappa \nabla T$$

$$\nabla \cdot (\beta_0 \mathbf{U}) = S - \frac{1}{\overline{\Gamma_1} p_0} \frac{\partial p_0}{\partial t}$$

- Low Mach number equation set
  - Contains no acoustic waves.
  - Appropriate for flows where the Mach number is small (fluid velocity is small compared to the sound speed). Does not enforce that the Mach number is small.
- Time step constrained by the fluid speed, not the sound speed.
  - Time step a factor of ~1/M larger, (Mach number M = U/c)
  - Allows for long-time integration

Mathematical Formulation: Low Mach Model

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$$\nabla \cdot (\beta_0 \mathbf{U}) = S - \frac{1}{\overline{\Gamma_1} p_0} \frac{\partial p_0}{\partial t}$$

- One-dimensional base state density and pressure:
  - Represent the “average” state of the star as a function of radius
  - Constrained by the equation of hydrostatic equilibrium

$$\nabla p_0(r,t) = -\rho_0(r,t) g(r,t)$$

  - Highly stratified and time-dependent

Mathematical Formulation: Low Mach Model

$$\frac{\partial(\rho X_k)}{\partial t} = -\nabla \cdot (\rho X_k \mathbf{U}) + \rho \dot{\omega}_k$$

$$\frac{\partial(\rho \mathbf{U})}{\partial t} = -\nabla \cdot (\rho \mathbf{U}\mathbf{U}) - (\rho - \rho_0)\mathbf{g} - \nabla \pi$$

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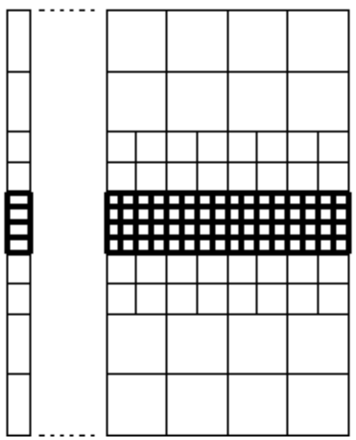
$$\nabla \cdot (\beta_0 \mathbf{U}) = S - \frac{1}{\overline{\Gamma_1} p_0} \frac{\partial p_0}{\partial t}$$

- Dynamic pressure represents perturbations from the background pressure, i.e.,

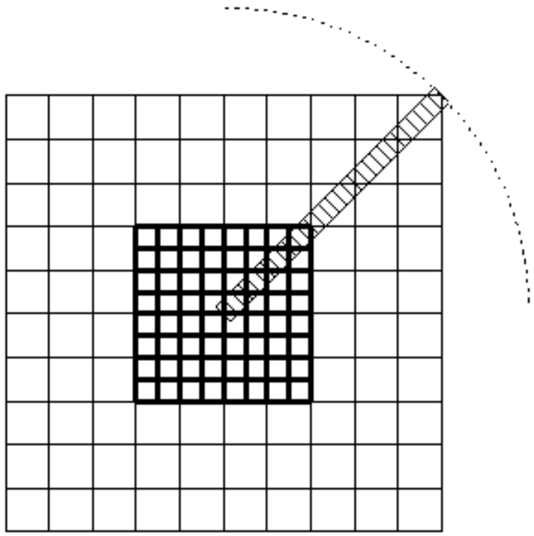
$$p(\mathbf{x}, t) = p_0(r, t) + \pi(\mathbf{x}, t); \quad \pi / p_0 = \mathcal{O}(M^2)$$

Background State Mapping

- Visually, here is how the background state is related to the full state:



"planar" problems



"spherical" problems

- Note that for spherical problems, there is no direct alignment between the 1D background state array and the full state.
  - Requires advanced interpolation stencils

Mathematical Formulation: Low Mach Model

$$\frac{\partial(\rho X_k)}{\partial t} = -\nabla \cdot (\rho X_k \mathbf{U}) + \rho \dot{\omega}_k$$

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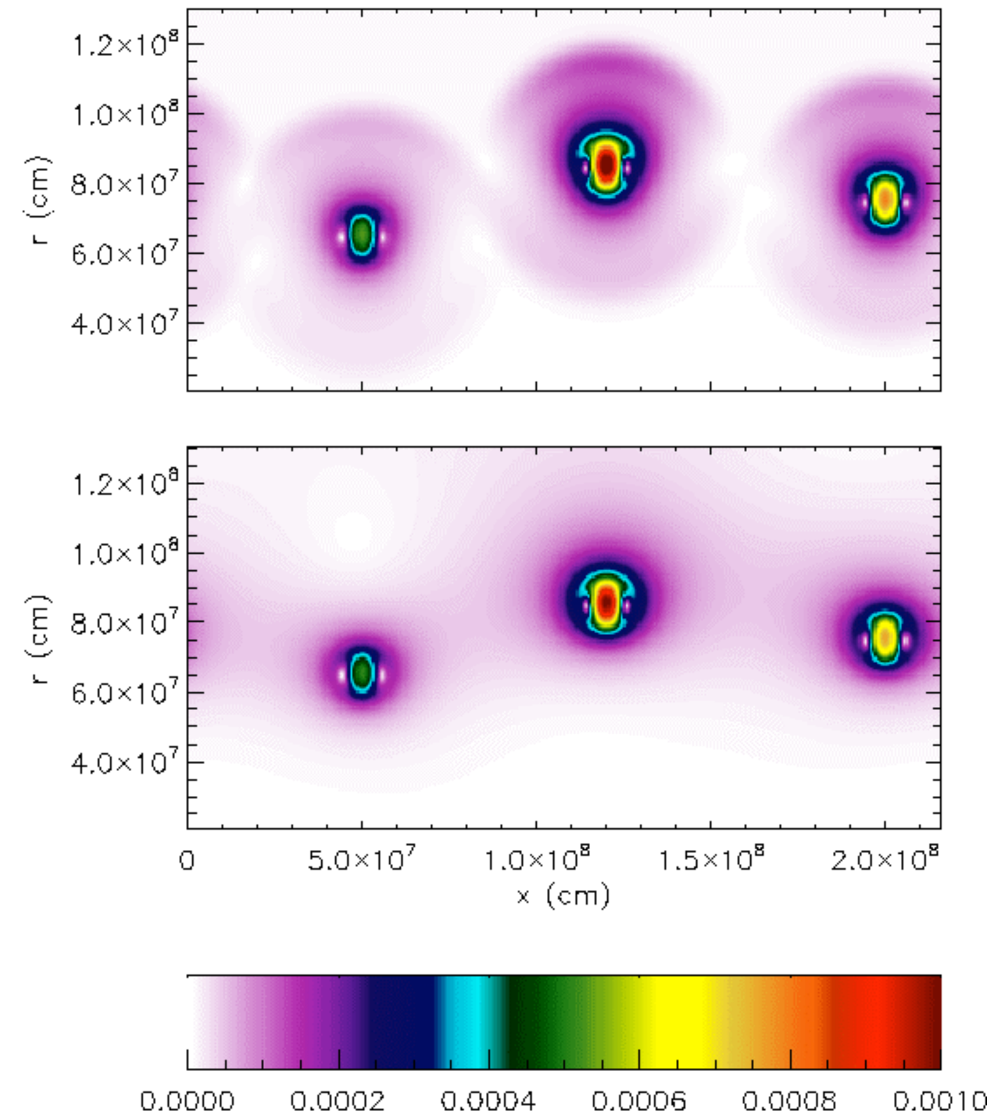
$$\nabla \cdot (\beta_0 \mathbf{U}) = S - \frac{1}{\overline{\Gamma_1} p_0} \frac{\partial p_0}{\partial t}$$

- Conservation of mass and momentum are exact – no approximations.
- Base state pressure is used in the enthalpy equation and to constrain the thermodynamics.
- An elliptic constraint on velocity represents instantaneous acoustic equilibration.

Acoustic Equilibration



- Plot of Mach number for a set of reacting, rising bubbles in a white dwarf environment.
  - Compressible (above)
  - Low Mach (below)

Mathematical Formulation: Low Mach Model

- Elliptic constraint captures effects of background stratification….

$$\nabla \cdot (\beta_0 \mathrm{U}) = S - \frac{1}{\overline{\overline{\Gamma_1}} p_0} \frac{\partial p_0}{\partial t}$$

Mathematical Formulation: Low Mach Model

- Elliptic constraint captures effects of background stratification….

$$\nabla \cdot (\beta_0 \mathbf{U}) = S - \frac{1}{\overline{\Gamma}_1 p_0} \frac{\partial p_0}{\partial t}$$

…while also capturing local compressibility effects:

compositional changes

$$S = -\sigma \sum_k (\xi_k + q_k)\dot{\omega}_k + \frac{1}{\rho p_\rho} \sum_k p_{X_k} \dot{\omega}_k + \frac{\sigma}{\rho} \nabla \cdot \kappa \nabla T$$

reaction heating

thermal diffusion

Numerical Approach

- Fractional step scheme
  - Unsplit PPM integrator for hydrodynamics
  - Strang-splitting for reaction, heating, and thermal diffusion terms
  - Multigrid for elliptic solve and pressure update

$$\frac{\partial(\rho X_k)}{\partial t} = -\nabla \cdot (\rho X_k \mathbf{U}) + \rho \dot{\omega}_k$$

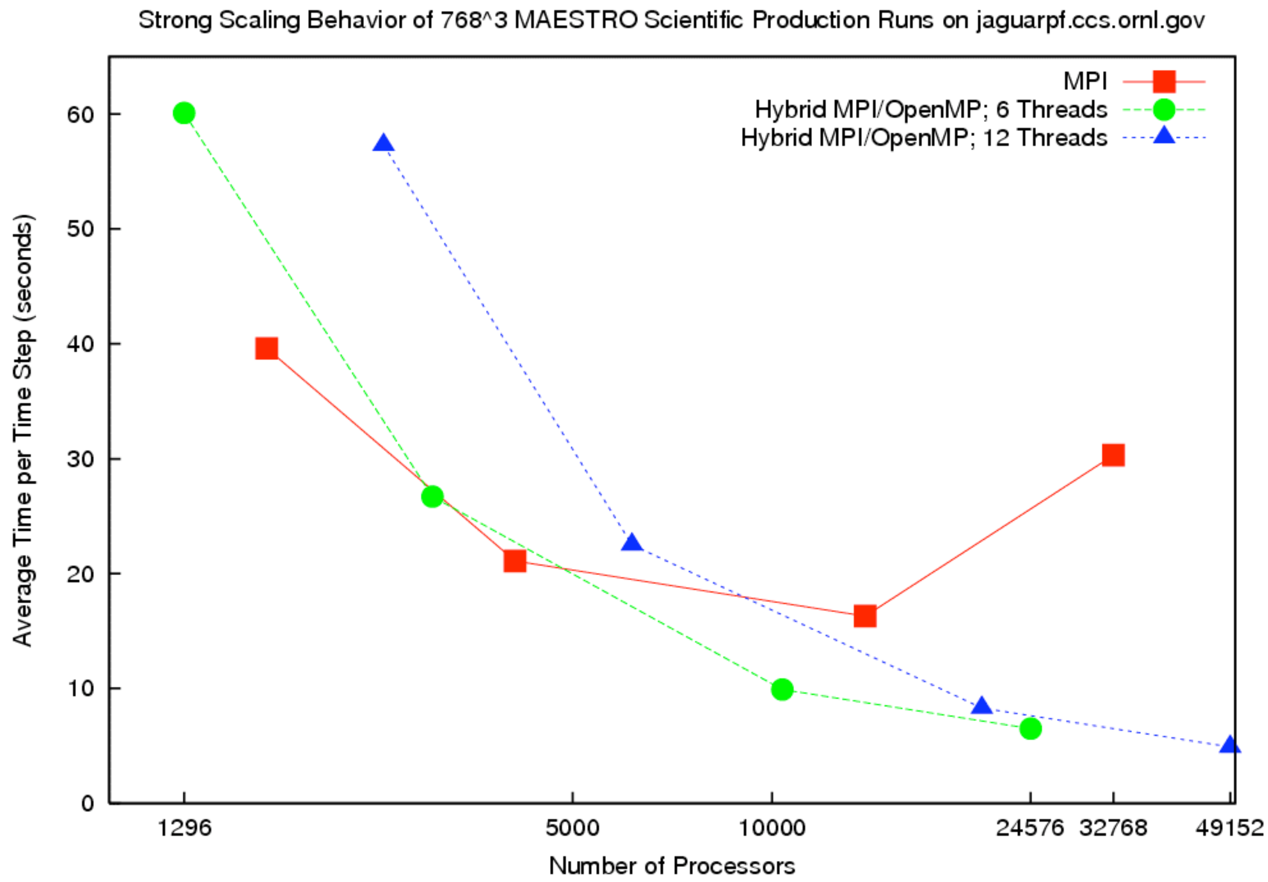
$$\frac{\partial(\rho \mathbf{U})}{\partial t} = -\nabla \cdot (\rho \mathbf{U}\mathbf{U}) - (\rho - \rho_0)\mathbf{g} - \nabla \pi$$

$$\frac{\partial(\rho h)}{\partial t} = -\nabla \cdot (\rho h \mathbf{U}) + \frac{Dp_0}{Dt} + \rho H_{\mathrm{nuc}} + \rho H_{\mathrm{ext}} + \nabla \cdot \kappa \nabla T$$

$$\nabla \cdot (\beta_0 \mathbf{U}) = S - \frac{1}{\overline{\Gamma_1} p_0} \frac{\partial p_0}{\partial t}$$

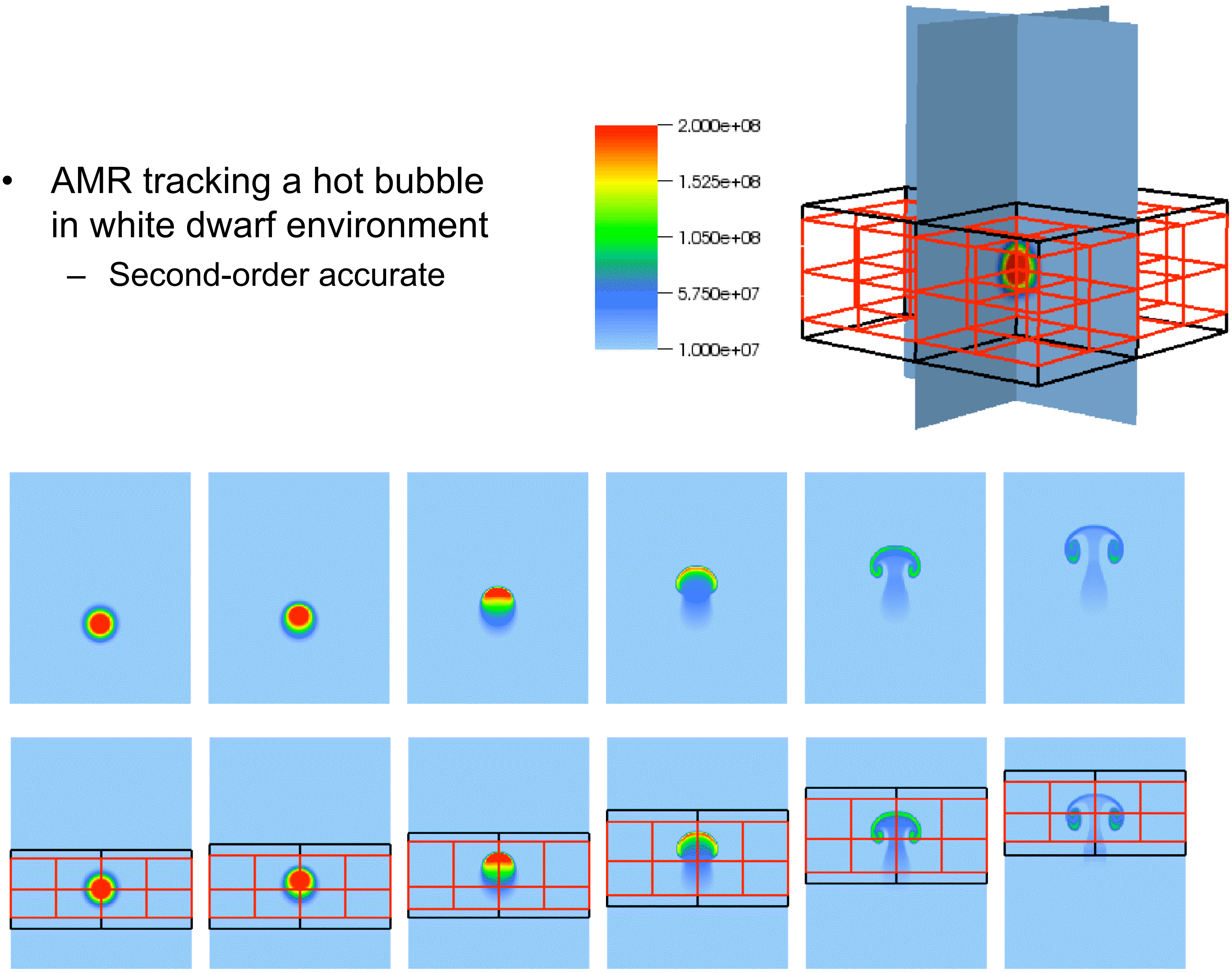
Parallel Performance

- We have recently adopted a hybrid programming approach.
  - MPI with OpenMP
  - Code scales to 50,000 processors



Validation

- AMR tracking a hot bubble in white dwarf environment
  - Second-order accurate

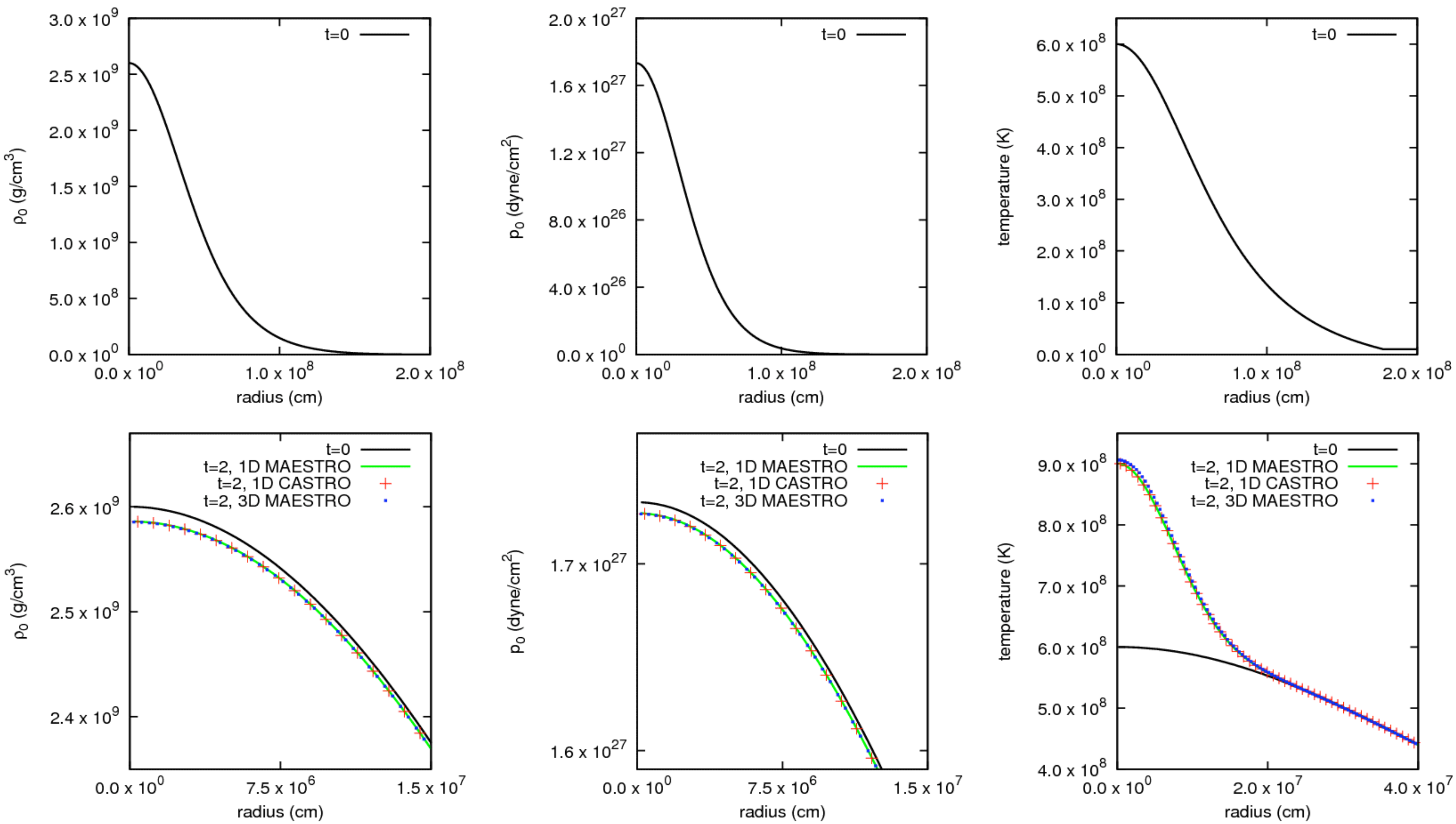


- Expansion of a full star subjected to external heating at the core
  - 3D MAESTRO, 1D MAESTRO, and 1D CASTRO compare well

density | pressure | temperature

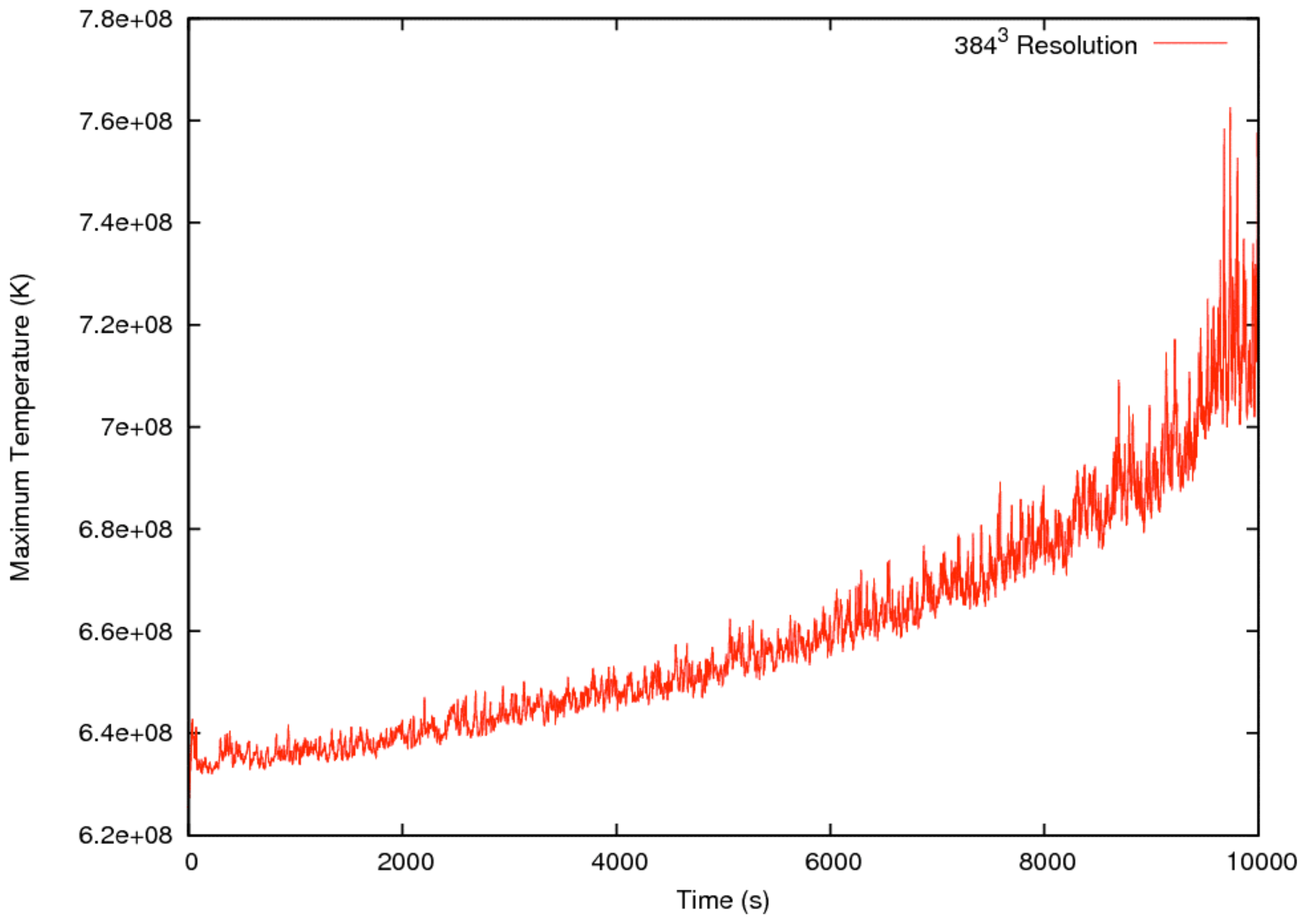
t=0

t=2 s



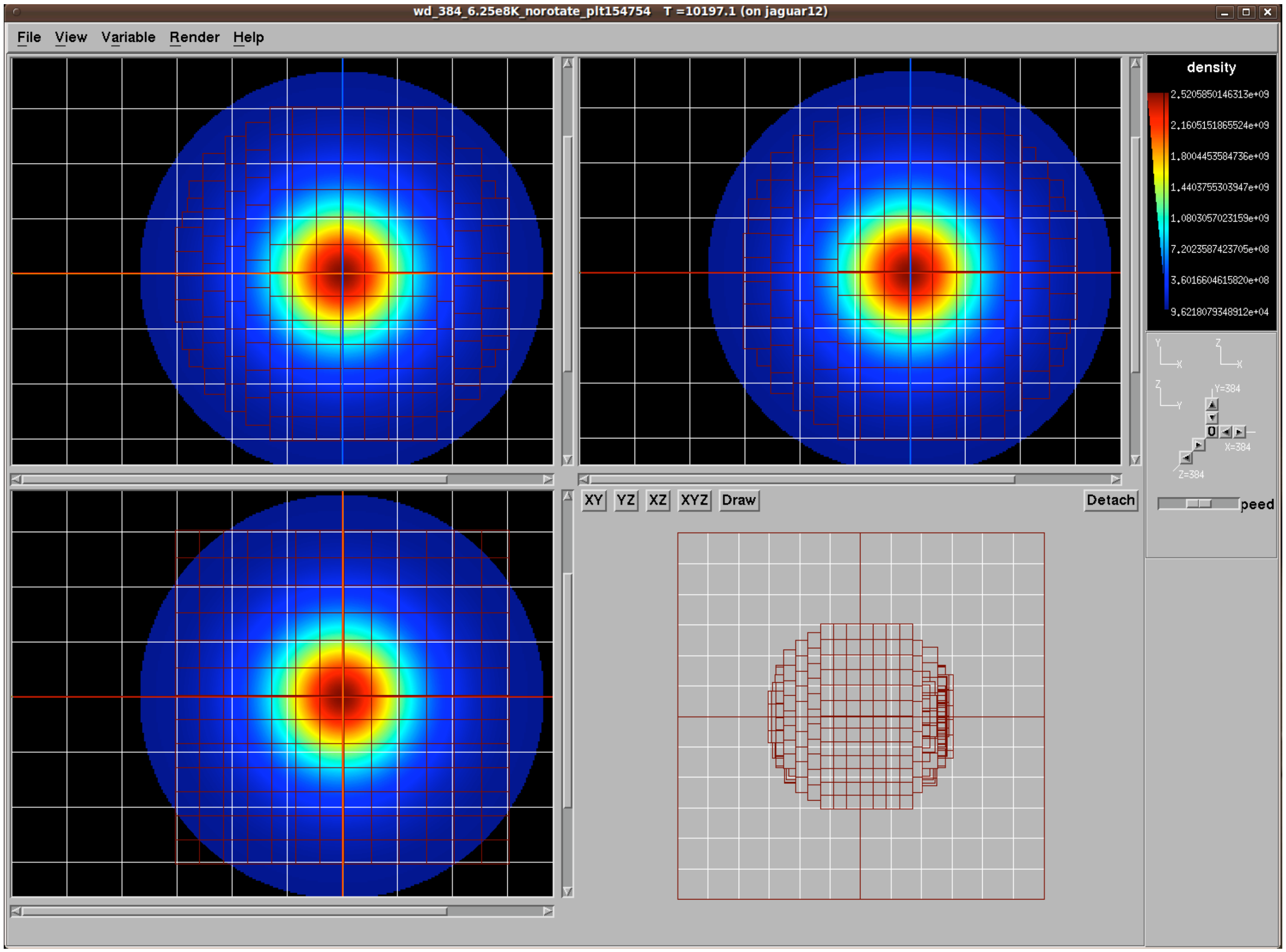
Full-Star Simulation

- Preview of results from Type Ia ignition study (more in Zingale's talk)
  - Tracking temperature of hot spot as a function of time.
  - No AMR



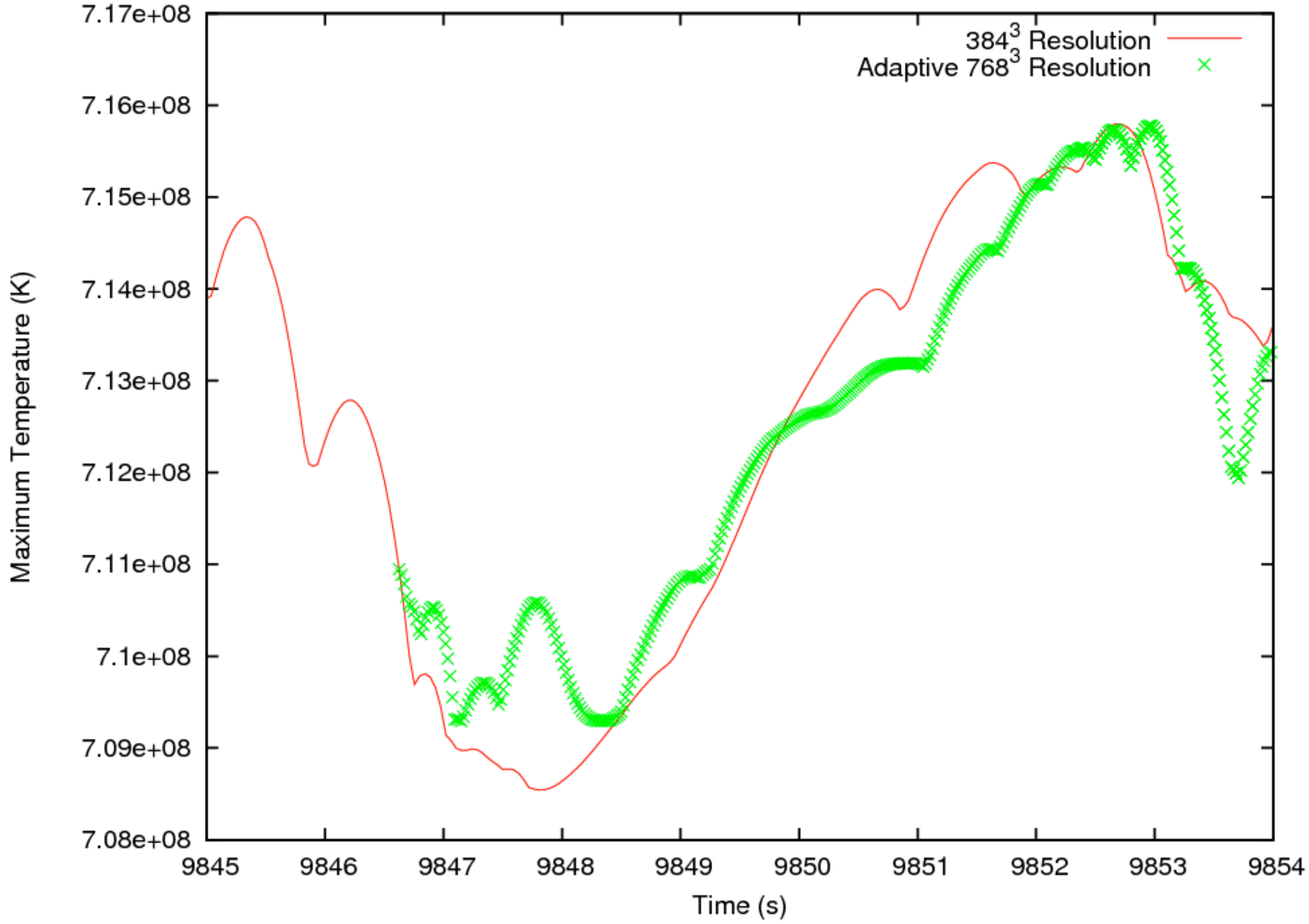
Verification: Full-Star AMR

- Then we refine the innermost ~10% of the star.



Verification: Full-Star AMR

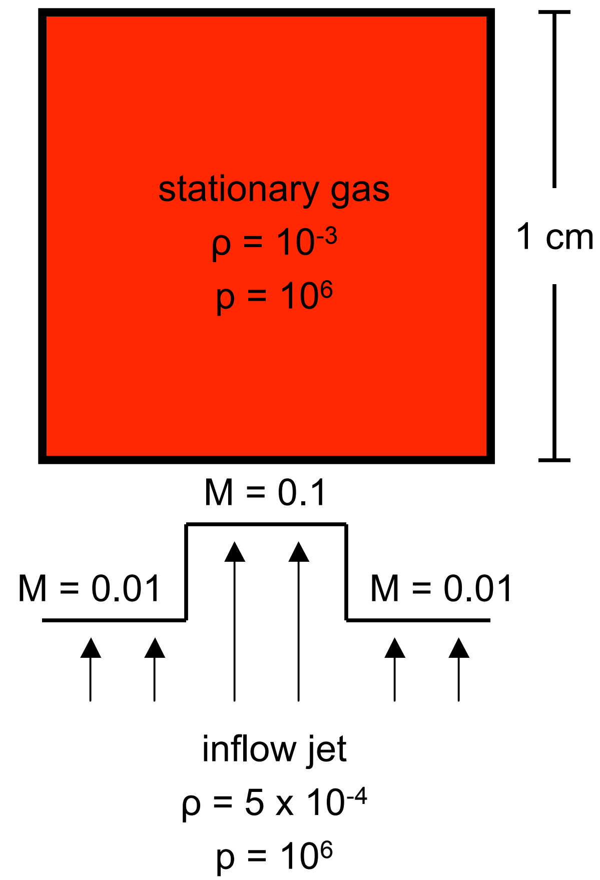
- Zoom-in of temperature plot after adding refinement.

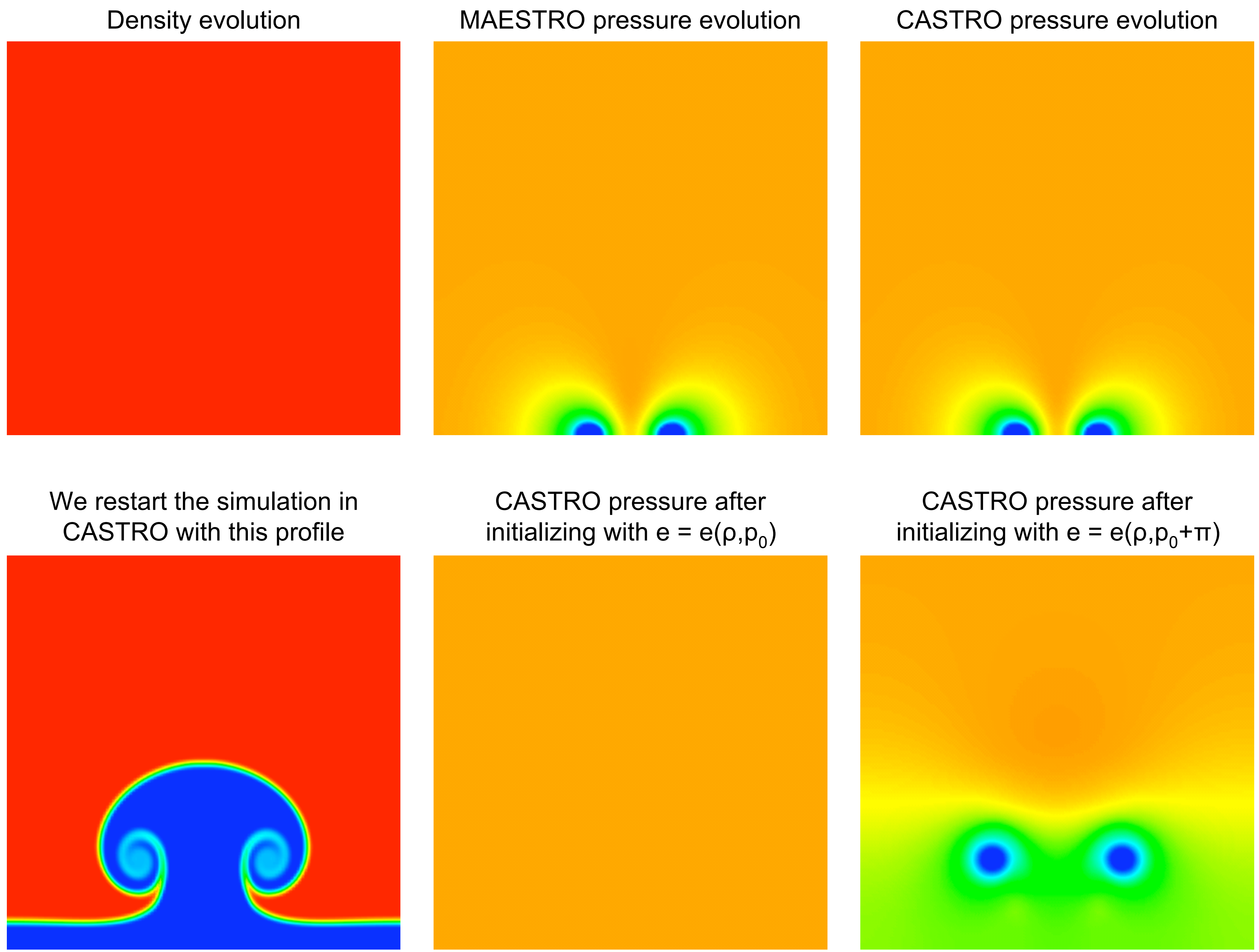


MAESTRO / CASTRO Transition

- Study the effects of using a MAESTRO dataset to initialize a CASTRO simulation
  - Different initialization algorithms
  - Mach number dependency
  - EOS dependency

- Test problem description
  - Gamma-law gas, terrestrial conditions
  - Subsonic inflow jet with lower density




Density evolution
MAESTRO pressure evolution
CASTRO pressure evolution
We restart the simulation in CASTRO with this profile
CASTRO pressure after initializing with e = e(ρ,p0)
CASTRO pressure after initializing with e = e(ρ,p0+π)

References

- Theoretical and algorithmic developments:
  - Almgren et al., ApJ 637, 2006 (hydrodynamics)
  - Almgren et al., ApJ 649, 2006 (heating)
  - Almgren et al., ApJ 684, 2008 (reactions)
  - Zingale et al., ApJ 704, 2009 (full-star problems)
  - Nonaka et al., ApJS 188, 2010 (time-dependent base state w/AMR)

- Current studies in progress:
  - Type Ia supernovae, convection preceding ignition (Zingale)
  - Type I X-ray bursts, convection preceding outburst (Malone)
  - Convection in massive stars, oxygen shell burning (Gilet)
  - Classical novae, convection preceding outburst (Brendan Krueger, SBU)
  - Type Ia supernovae, post ignition dynamics (Almgren, Bell, Zingale)