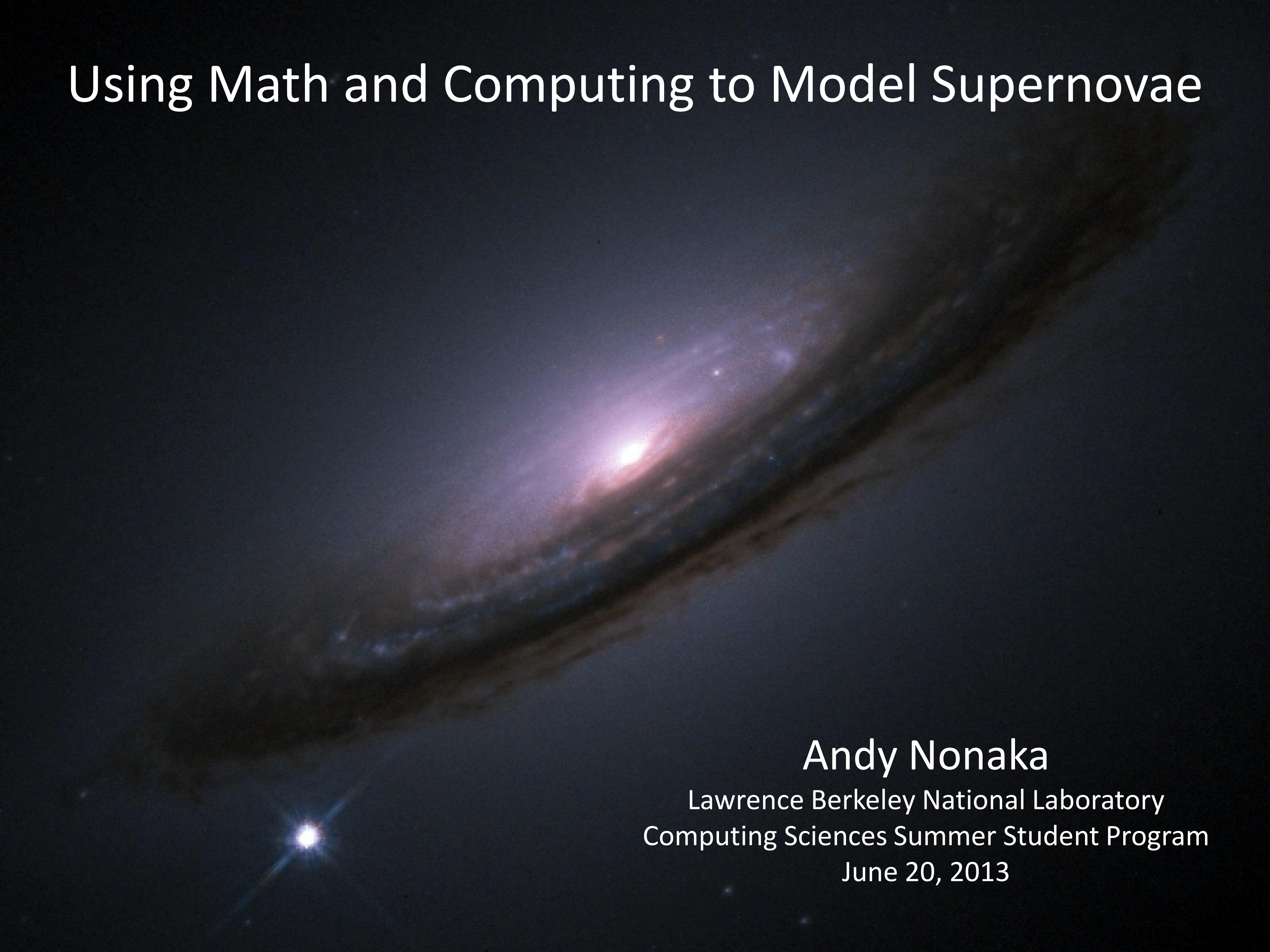
Using Math and Computing to Model Supernovae



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Computing Sciences Summer Student Program
June 20, 2013

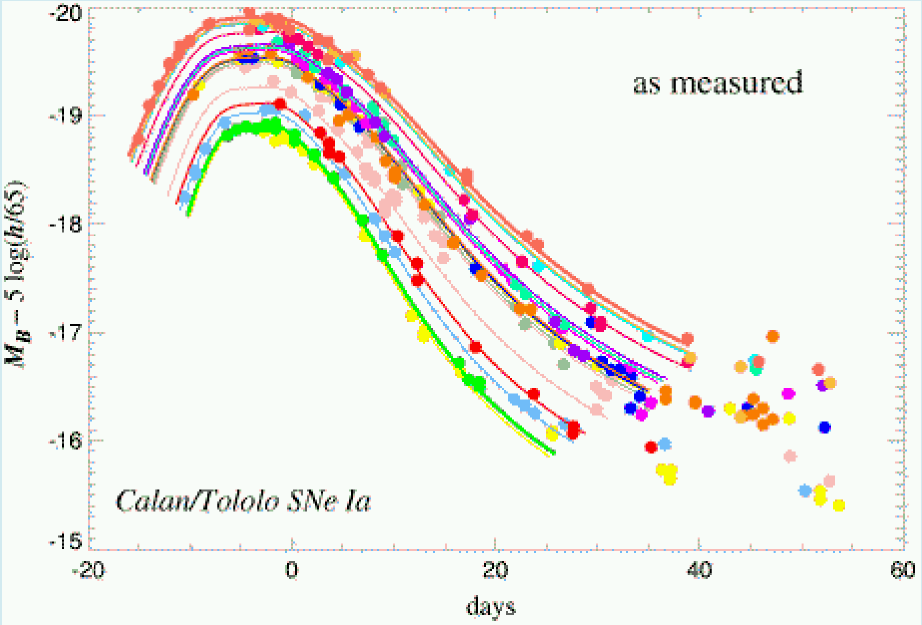
Galaxy NGC 4526 imaged by the Hubble Space Telescope (www.nasa.gov)

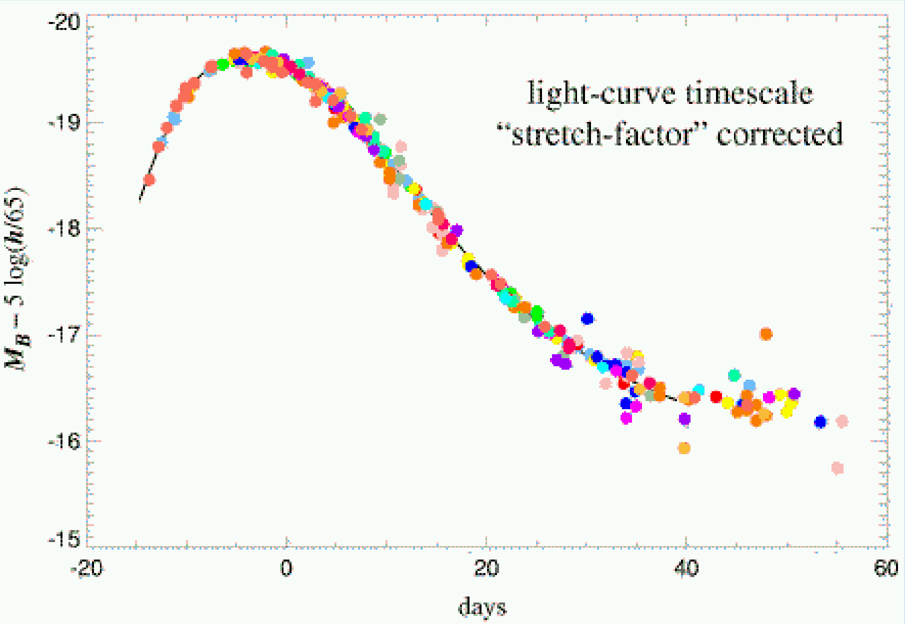
60 million light years away; located in the Virgo constellation

- Why should we care?
- Using modern telescopes, Type Ia supernova light curves can now be observed several hundred times per year.
  - Spectra indicate that oxygen and calcium are present early, where as nickel, cobalt, and iron are present later.

Type Ia Supernovae are Distance Indicators

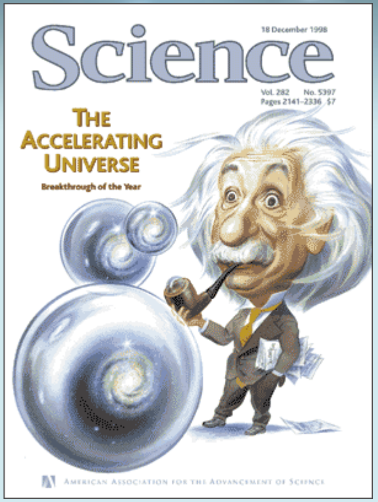
- By observing Type Ia supernovae Ia at known, nearby distances, scientists have established a width-luminosity relationship; wider = brighter.





- Theory: by observing the peak luminosity and decay rate, we can determine the distance to a host galaxy.
  - Particularly useful for mapping distant galaxies since they are so bright!

Type Ia Supernovae are Speed Indicators



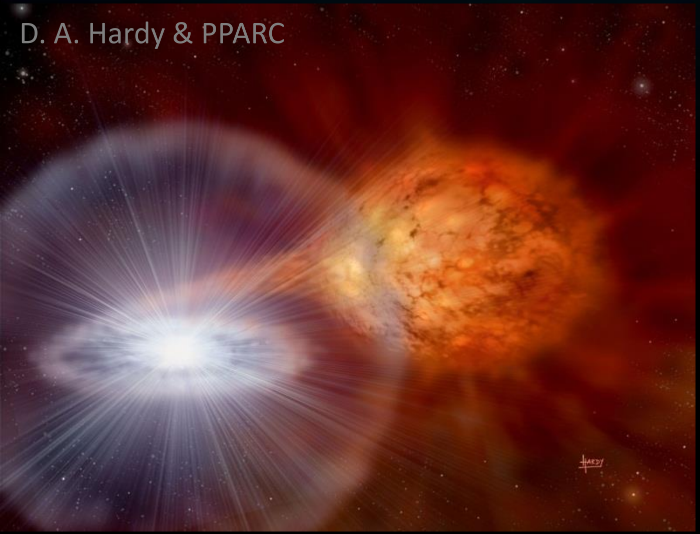
- Due to the observed redshift, we know the speed at which the host galaxy is moving away from us.
  - Led to discovery of the acceleration of the expansion of the universe in 1998
  - 2011 Physics Nobel Prize (Perlmutter, LBNL)
- Problem: We don't know how well the width-luminosity relationship holds for distant Type Ia supernovae
  - Farther away = earlier in the life of the universe
  - Composition of stars was different back then…
  - Not even sure if accepted models properly describe nearby events…

Studying Type Ia Supernovae

- How can we study this problem using computers?

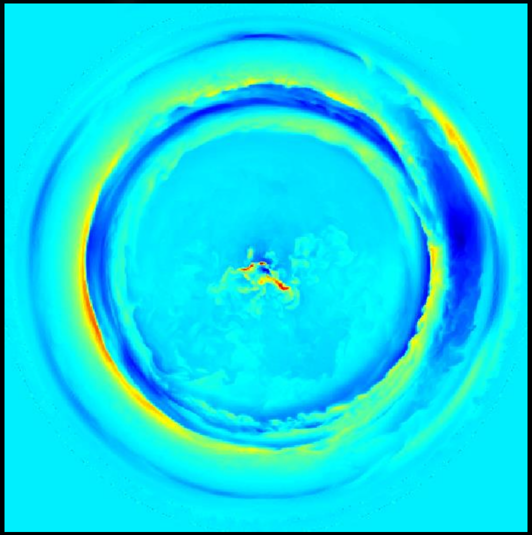
- We can develop mathematical models and the associated numerical methods for simulating such events on supercomputers.
  - Requires expertise in applied math and computer science.
  - Requires expertise in astrophysics (collaborate with experts in the field).

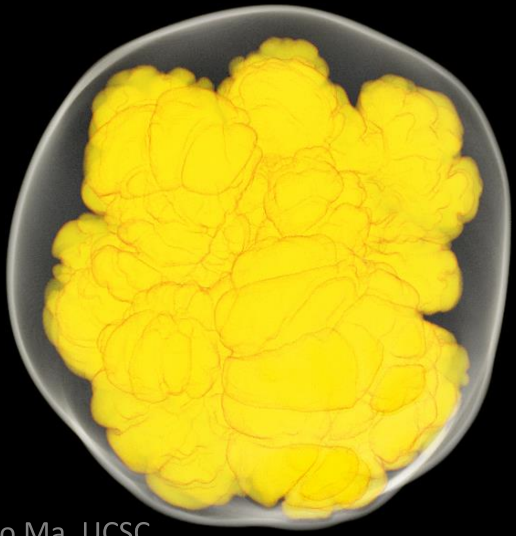
The Phases of Type Ia Supernovae: Single Degenerate Model



A white dwarf accretes matter from a binary companion over millions of years.

Smoldering phase characterized by subsonic convection and gradual temperature rise lasts hundreds of years.





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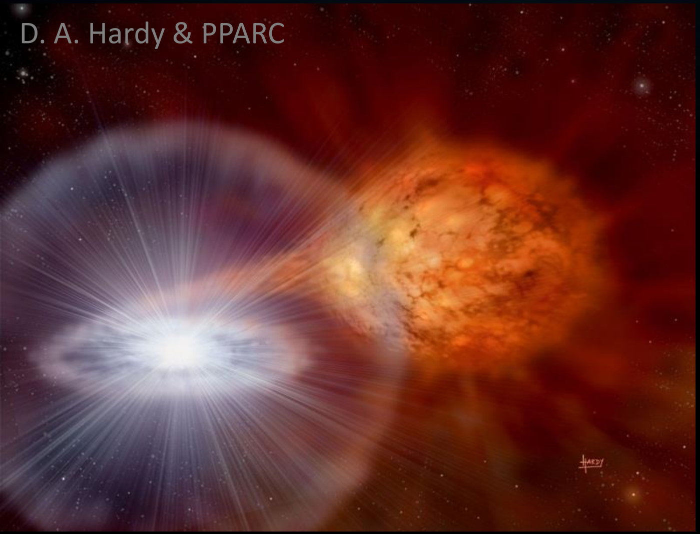
Flame (possibly) transitions to a detonation, causing the star to explode within two seconds.

The resulting event is visible from Earth for weeks to months.

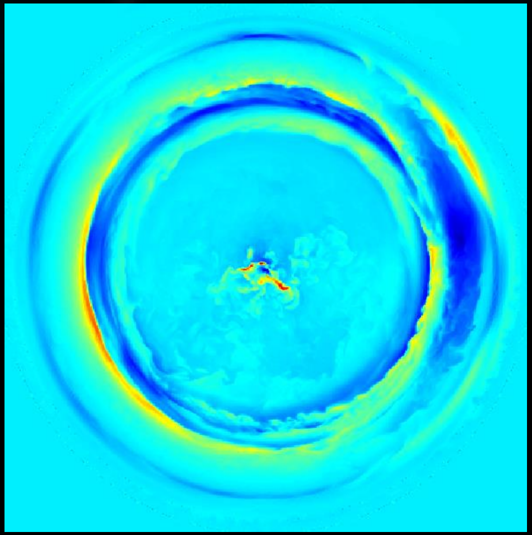
SN 1994D (High-Z SN Search team)

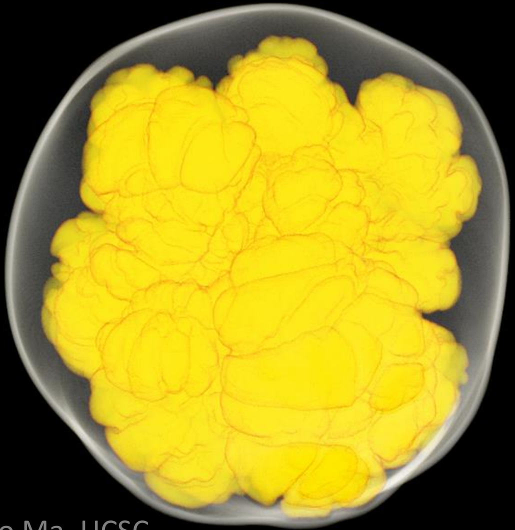
Each Phase has Different Computational Requirements



KEPLER
(Woosley, UCSC)

MAESTRO
(LBNL)





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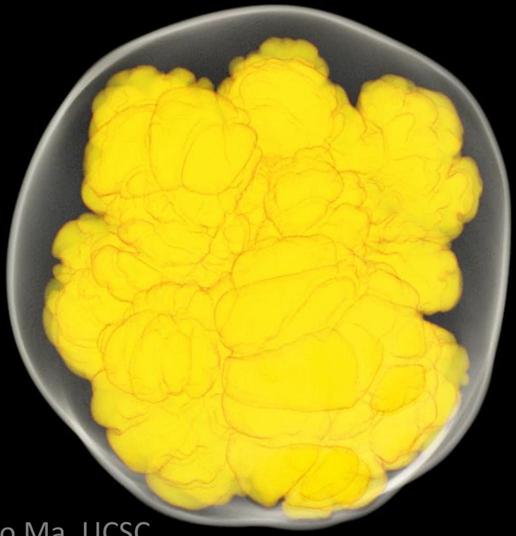
CASTRO (LBNL)

SEDONA
(Kasen, Thomas, Nugent, LBNL)

SN 1994D (High-Z SN Search team)

Computing the Explosion Phase

- Over the past decade, many have performed studies of the explosion phase using supercomputers.
  - Governed by well-understood (both theoretically and numerically) compressible fluid equations.
  - A supercomputer can model this system in a few weeks or months, depending on spatial resolution.



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Basic Solution Methodology

- Mathematical model (compressible fluid equations)

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

$$\frac{\partial(\rho \mathbf{u})}{\partial t} = -\nabla \cdot (\rho \mathbf{u}\mathbf{u}) - \nabla p + \rho \mathbf{g}$$ conservation of momentum

$$\frac{\partial(\rho E)}{\partial t} = -\nabla \cdot (\rho \mathbf{u} E + p \mathbf{u}) + \rho H + \rho \mathbf{u} \cdot \mathbf{g}$$ conservation of energy

---

ρ	density	E	total energy per unit mass
$\mathbf{u}$	velocity	$\mathbf{g}$	gravity
X_k	mass fraction of species “k”	H	energy release due to reactions
$\dot{\omega}_k$	reaction rate of species “k”	p	pressure

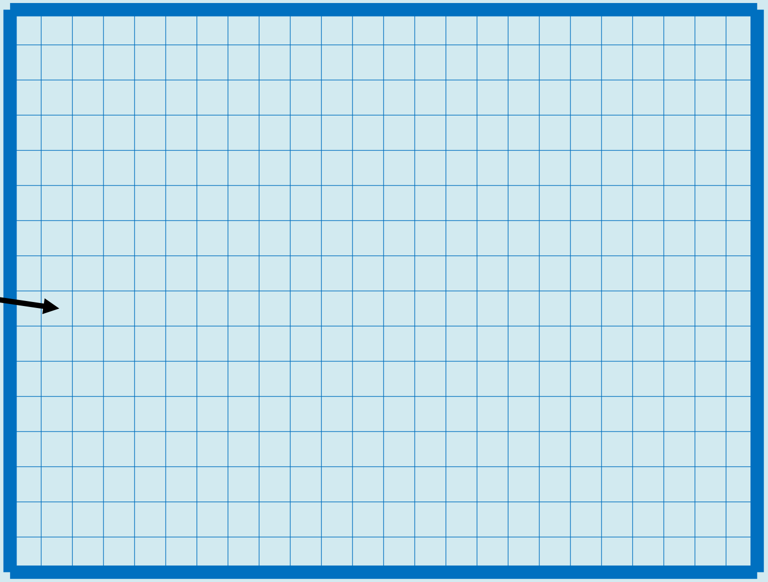
Basic Solution Methodology

- Mathematical model (compressible fluid equations)

$$
\begin{aligned}
\frac{\partial(\rho X_k)}{\partial t} &= -\nabla\cdot(\rho \mathbf{u} X_k) + \rho\dot{\omega}_k && \text{conservation of mass} \\
\frac{\partial(\rho \mathbf{u})}{\partial t} &= -\nabla\cdot(\rho \mathbf{u}\mathbf{u}) - \nabla p + \rho\mathbf{g} && \text{conservation of momentum} \\
\frac{\partial(\rho E)}{\partial t} &= -\nabla\cdot(\rho \mathbf{u} E + p\mathbf{u}) + \rho H + \rho\mathbf{u}\cdot\mathbf{g} && \text{conservation of energy}
\end{aligned}
$$

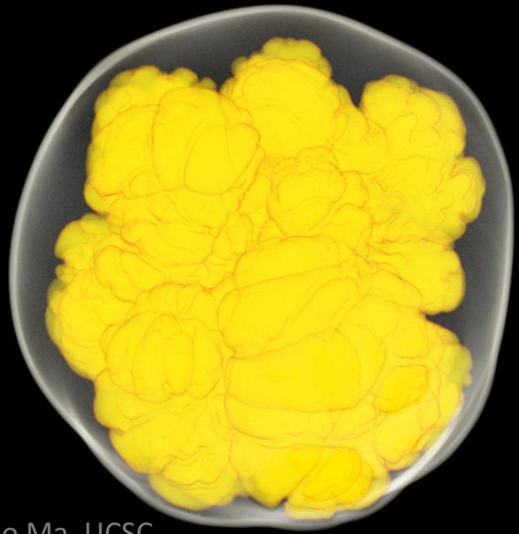
- Finite volume approach.
  - Divide problem into grid cells

$$\rho, \mathbf{U}, p, E, \cdots$$



  - Advance solution in time using numerical methods.

Computing the Explosion Phase

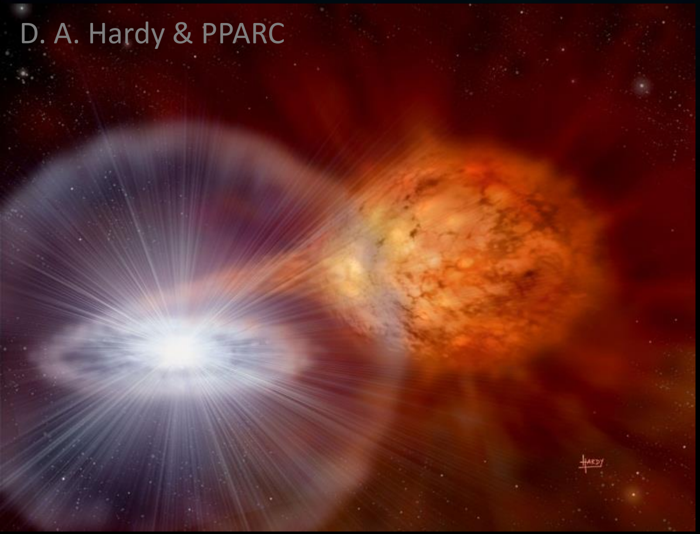


Haitao Ma, UCSC

A major problem are the initial conditions, which have been based on “guesses”.

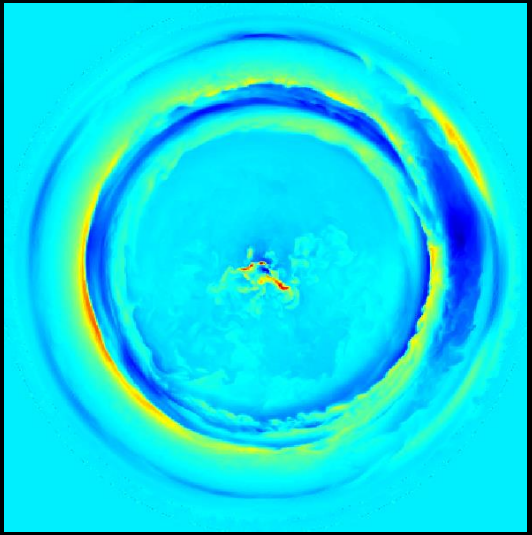
What is the initial state of the star?
Where are the first flames?
How many are there?

Each Phase has Different Computational Requirements



KEPLER
(Woosley, UCSC)

MAESTRO
(LBNL)



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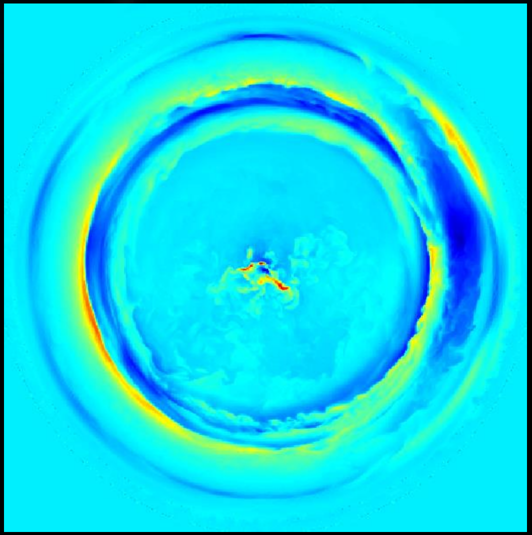
CASTRO (LBNL)

SEDONA
(Kasen, Thomas, Nugent, LBNL)

SN 1994D (High-Z SN Search team)

Computing the Convective Phase



MAESTRO
(LBNL)

- We begin with a discussion of the last few hours of convection up to the point of ignition.
- We use MAESTRO to determine the initial conditions for the post-ignition phase for CASTRO

What is MAESTRO?

- Long-time integration infeasible using fully compressible approach
- Having access to hundreds of thousands of CPUs is great, but still not enough to solve this problem. We must also utilize specialized mathematical models to solve this problem.

- “Low Mach Number” system - fluid speed small compared to sound speed (~1%)
- Effects of acoustic wave propagation unimportant
  – Can we take advantage of this?

Low Mach Number Equation Set

- Derive new equations/model using low Mach number asymptotics
  - Mach number: M = U/c
  - Looks similar to the standard equations of compressible flow, but sound waves have been analytically removed
    - Enables time steps constrained by the fluid velocity CFL, not the sound speed CFL:

$$\Delta t_{\text{compressible}} < \frac{\Delta x}{|u| + c} \qquad \Delta t_{\text{lowMach}} < \frac{\Delta x}{|u|}$$

    - Low Mach time step is a factor of 1/M larger than a compressible time step, enabling long-time integration!

Low Mach Number Equation Set

- Derived from fully compressible equation set

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

conservation of mass

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

conservation of momentum

$$\frac{\partial(\rho h)}{\partial t} = -\nabla \cdot (\rho h \mathbf{u}) + \rho H$$

conservation of energy

ρ	density	h	specific enthalpy
$\mathbf{u}$	velocity	$\mathbf{g}$	gravity
X_k	mass fraction of species “k”	H	energy release due to reactions
$\dot{\omega}_k$	reaction rate of species “k”	π	deviation from ambient pressure

Low Mach Number Equation Set

- Our system is closed with an equation of state, which keeps system in thermodynamic equilibrium.
  - Differentiate equation of state along particle paths to represent as a divergence constraint:

$$\nabla \cdot (\beta_0 \mathbf{u}) = \beta_0 S$$

$\beta_0 \rightarrow$ captures expansion/contraction of fluid due to changes in altitude

$S \rightarrow$ captures local compressibility effects due to reactions and thermal diffusion

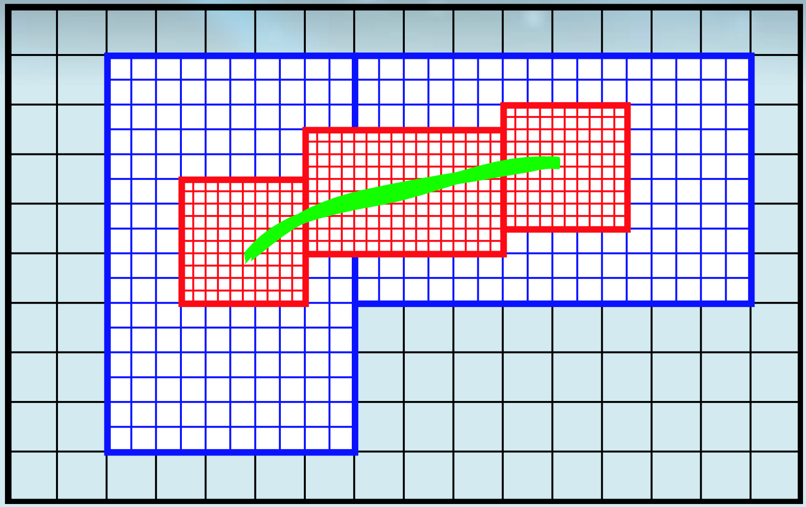
- Numerical enforcement of divergence constraint requires large linear algebra solvers that are computationally expensive and will dominate the simulation time.

Computational Efficiency

- In our white dwarf simulations, the peak Mach number is $O(10^{-2})$
  - The low Mach number time step is a factor of **<u>70</u>** greater than a compressible time step
  - However, a low Mach number time step takes approximately 2.5 times longer to compute, mostly due to the linear algebra
  - Thus, to advance the solution to the final time, MAESTRO is a factor of (70 / 2.5) ≈ 28 more efficient than a compressible algorithm, given the same number of computational resources for this problem

Adaptive Mesh Refinement

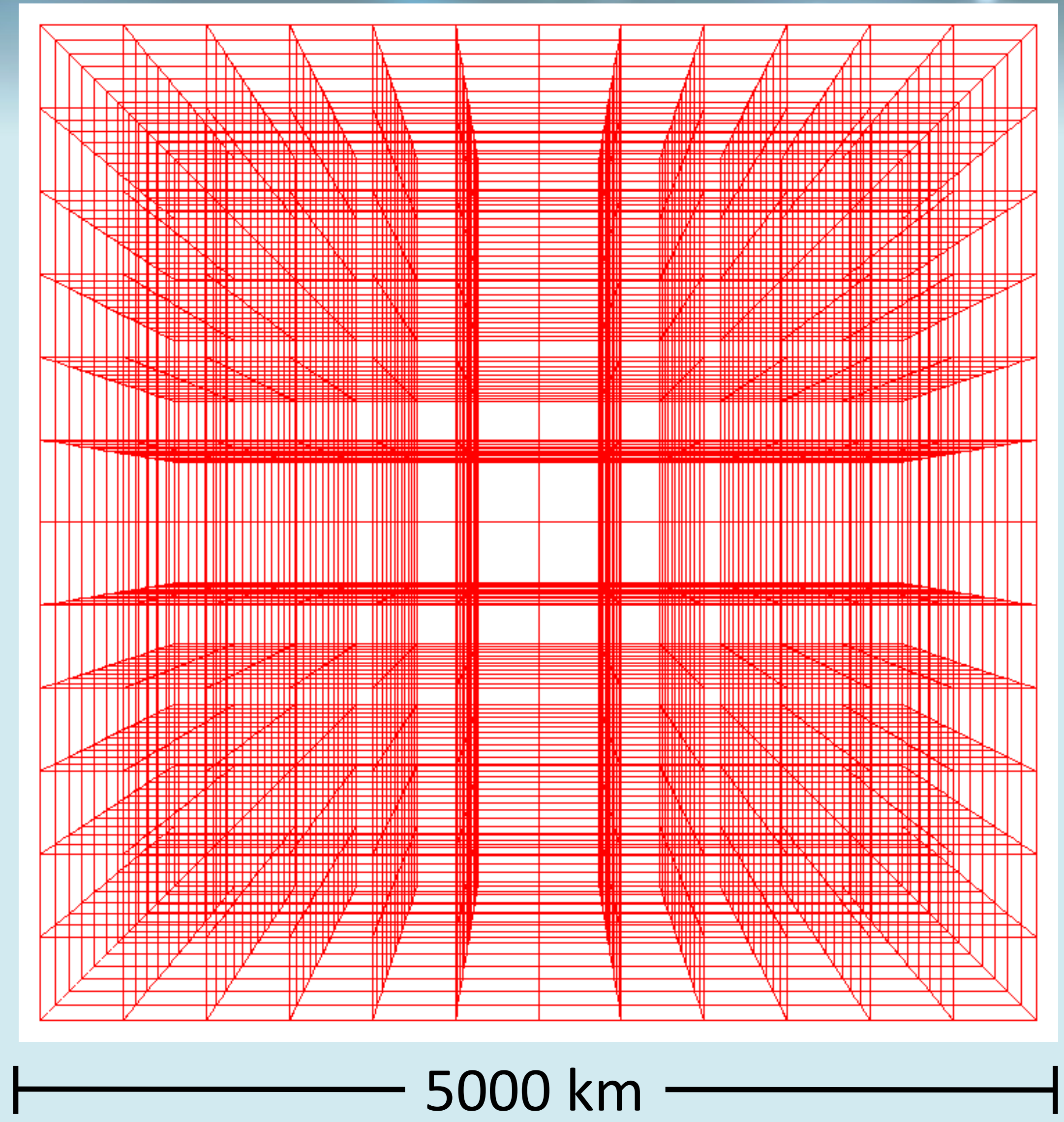
- Incorporate AMR using established techniques
  - Advance each level independently and synchronize solution between levels to maintain conservation



- For the full star problem, we need to consider our refinement criteria
  - Burning occurs near core, driving flow in the inner-convective region of the star.
  - We expect ignition point(s) to be near the center of the star

Adaptive Mesh Refinement

- 576^3 (8.7 km)
  - $1728 \cdot 48^3$ grids
  - 191 Million Cells



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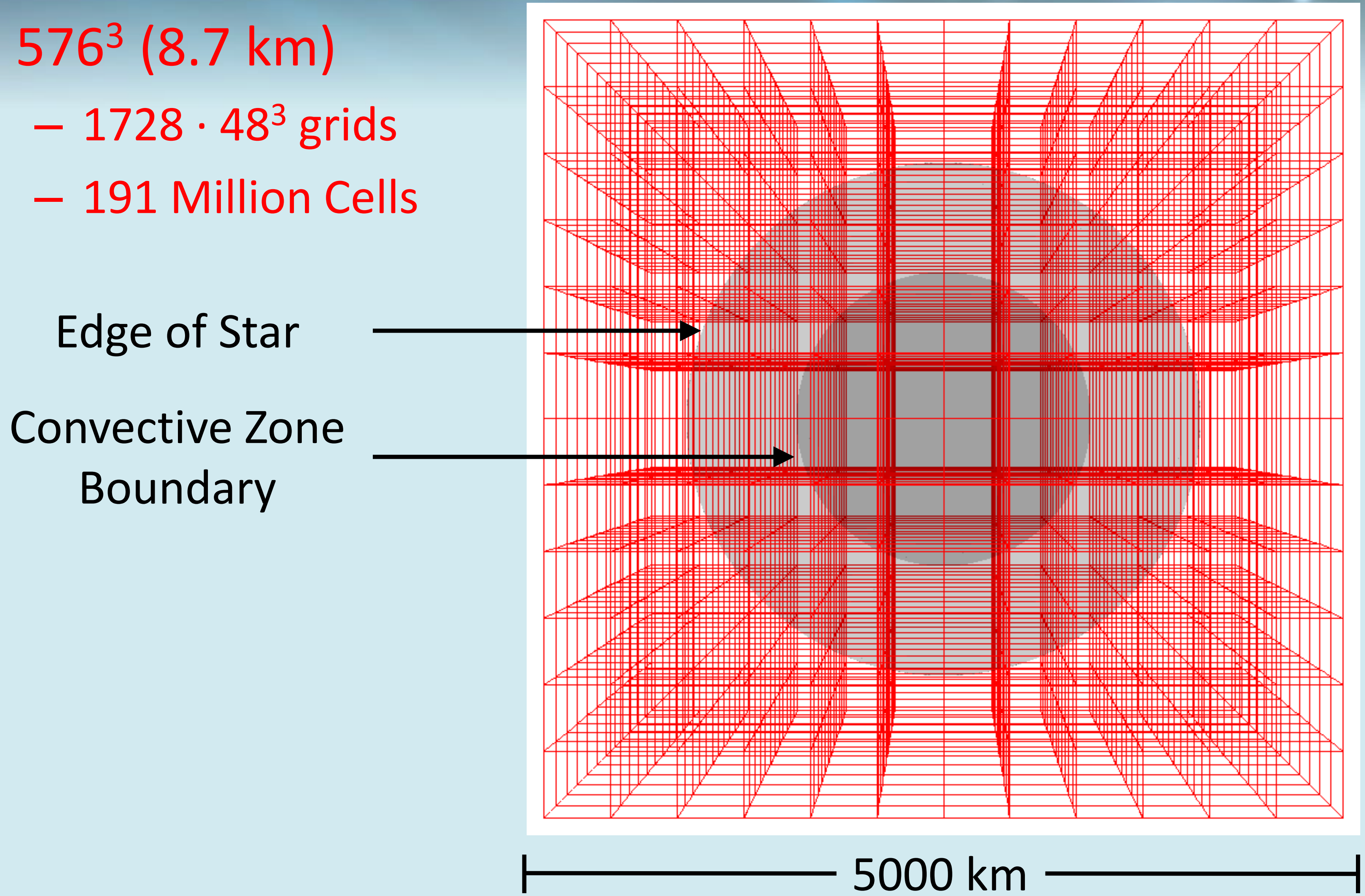

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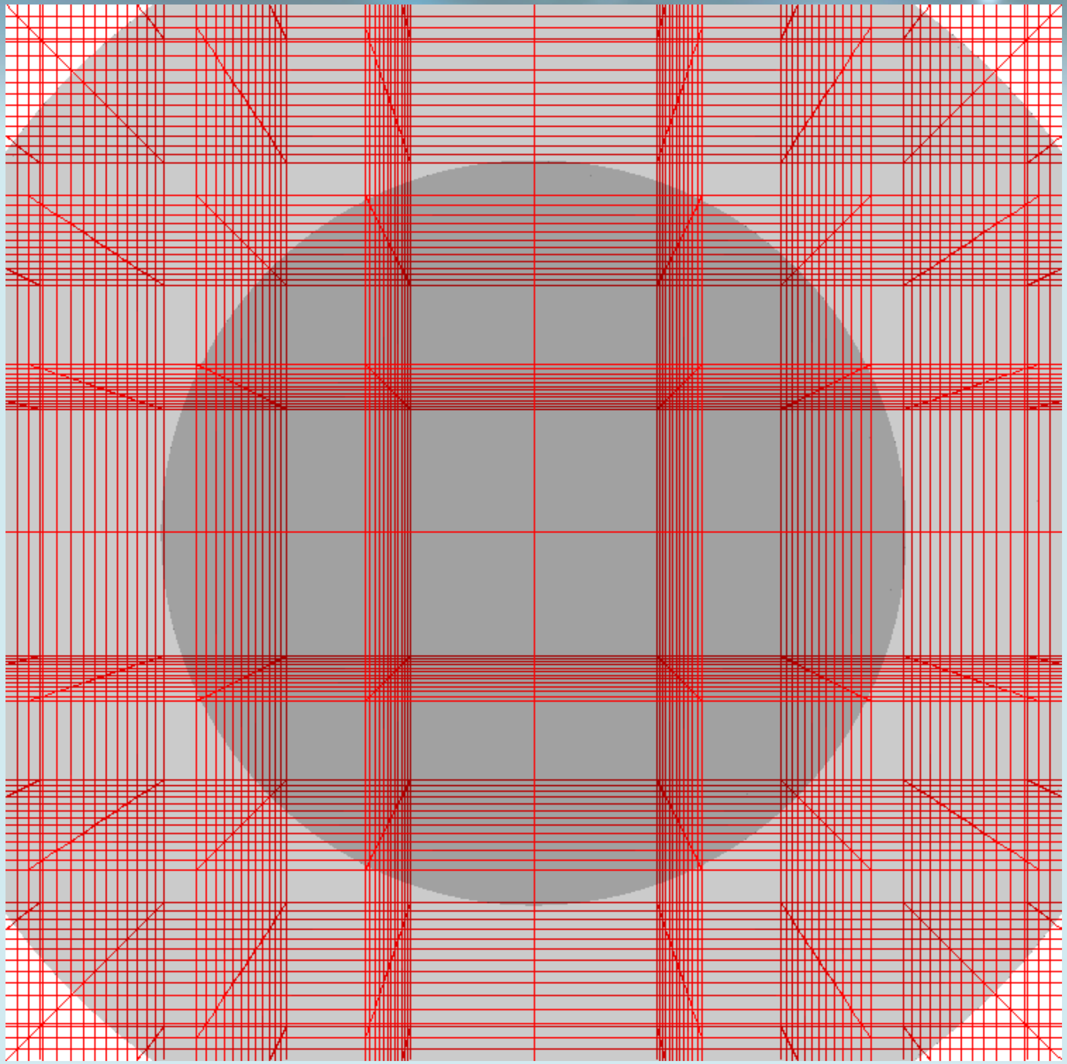
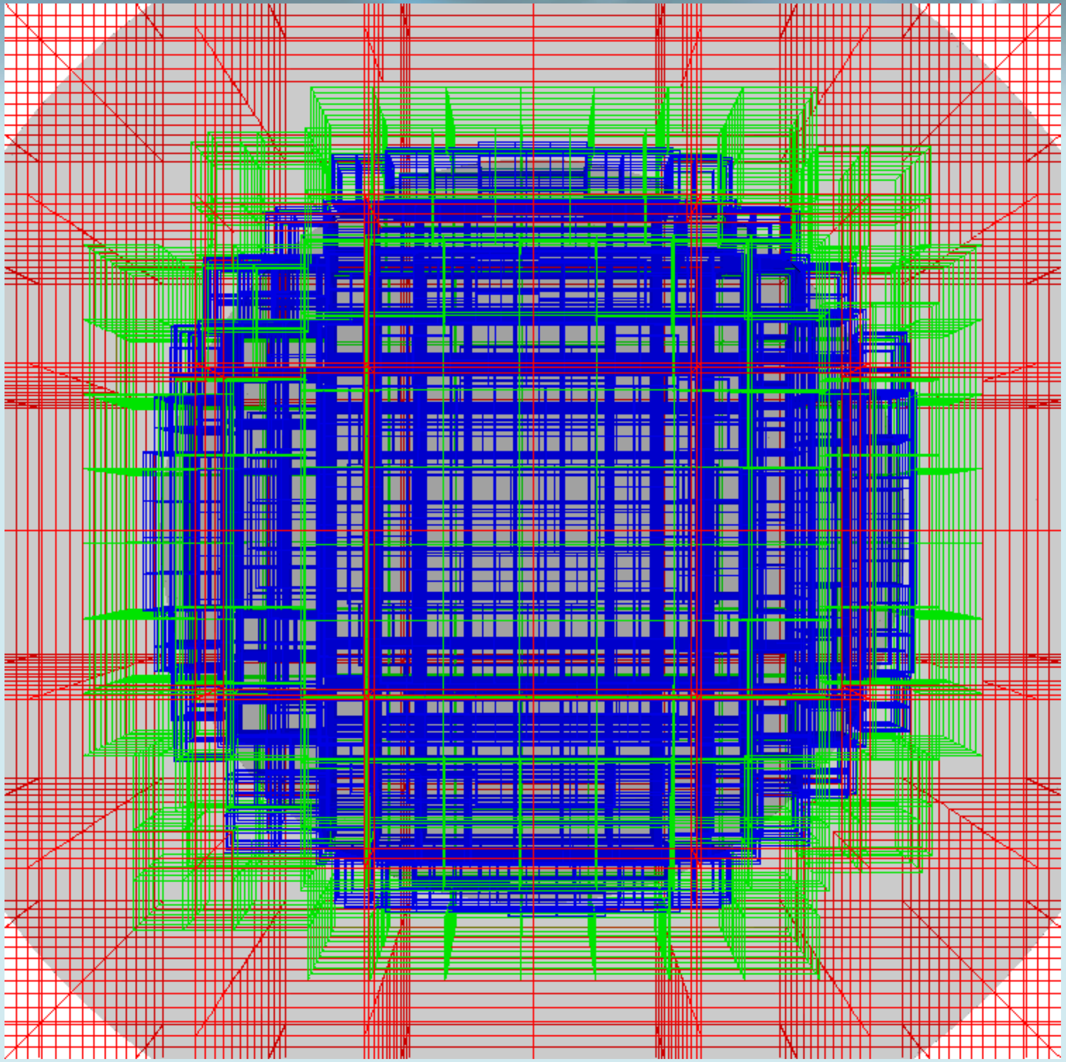


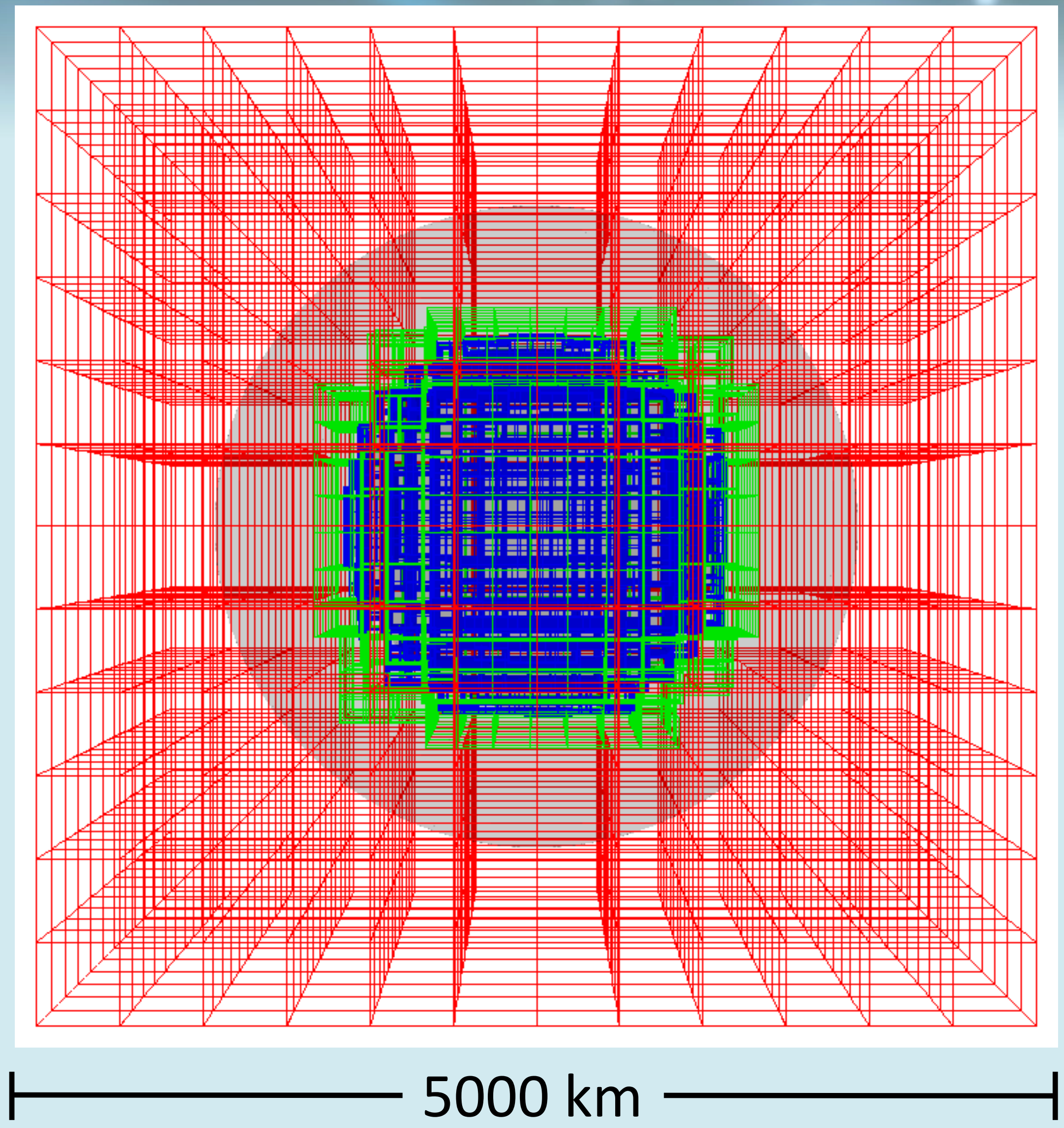
Adaptive Mesh Refinement

- 576^3 (8.7 km)
  - 1728 · 48^3 grids
  - 191 million cells
- 1152^3 (4.3 km)
  - 1684 grids
  - 148 million cells
  - 9.7% of domain
- 2304^3 (2.2 km)
  - 3604 grids
  - 664 million cells
  - 5.4% of domain



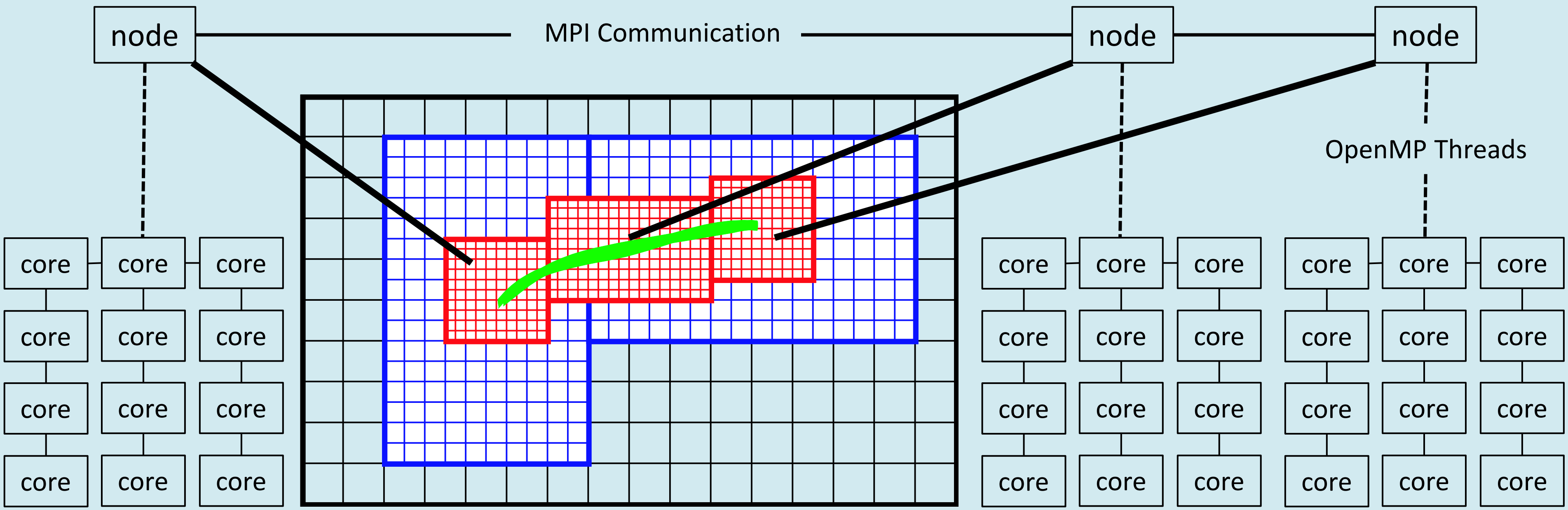
Adaptive Mesh Refinement

- A 2304^3 simulation with no AMR would contain 12.2 billion cells.
- Our simulation contains a total of 1.0 billion cells, requiring a factor of 12 less work.
  - Excluding AMR overhead, which is a few percent



Parallelization Strategy

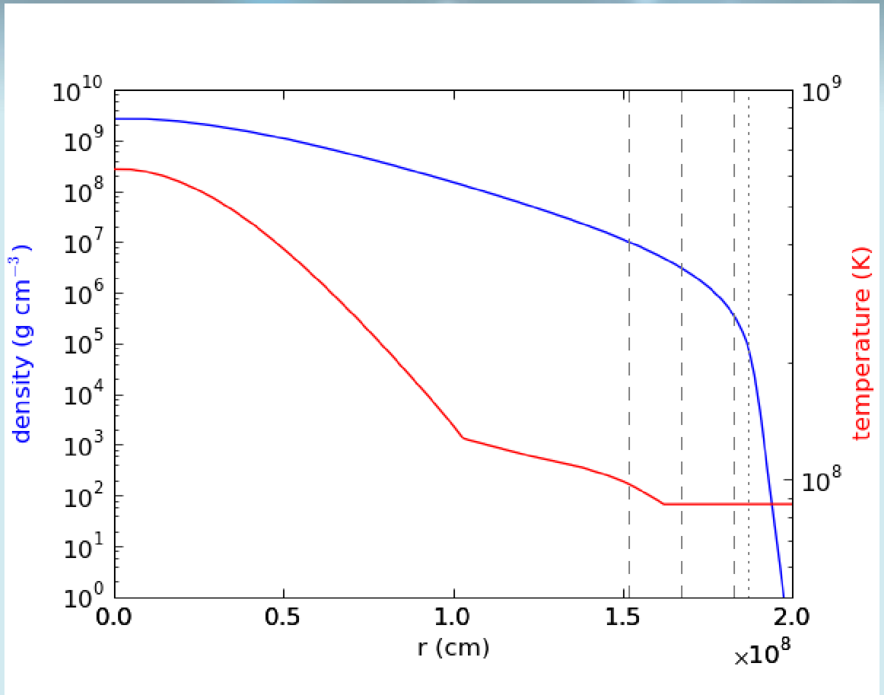
- Hybrid MPI/OpenMP approach to parallelization.
  - Nodes assigned to grids, threads spawned on cores to work on grids

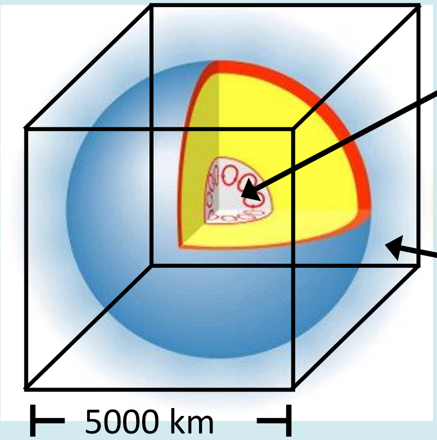


- We are able to efficiently run our codes on 100,000+ processors using this approach.

White Dwarf Convection: Initial Conditions

- Initial conditions
  - 1D KEPLER model mapped onto Cartesian grid
  - Random velocity perturbation added to prevent initial nuclear runaway





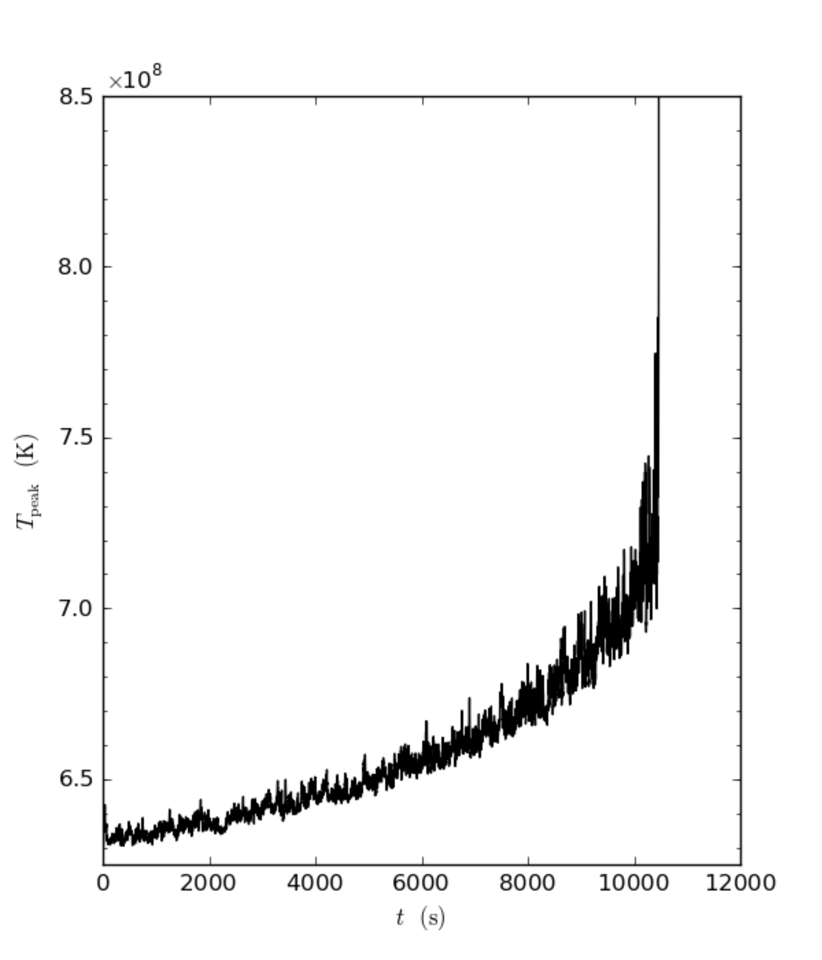
Center of Star
density = 2.6 x 10^9 g/cc
Temperature = 6.25 x 10^8 K

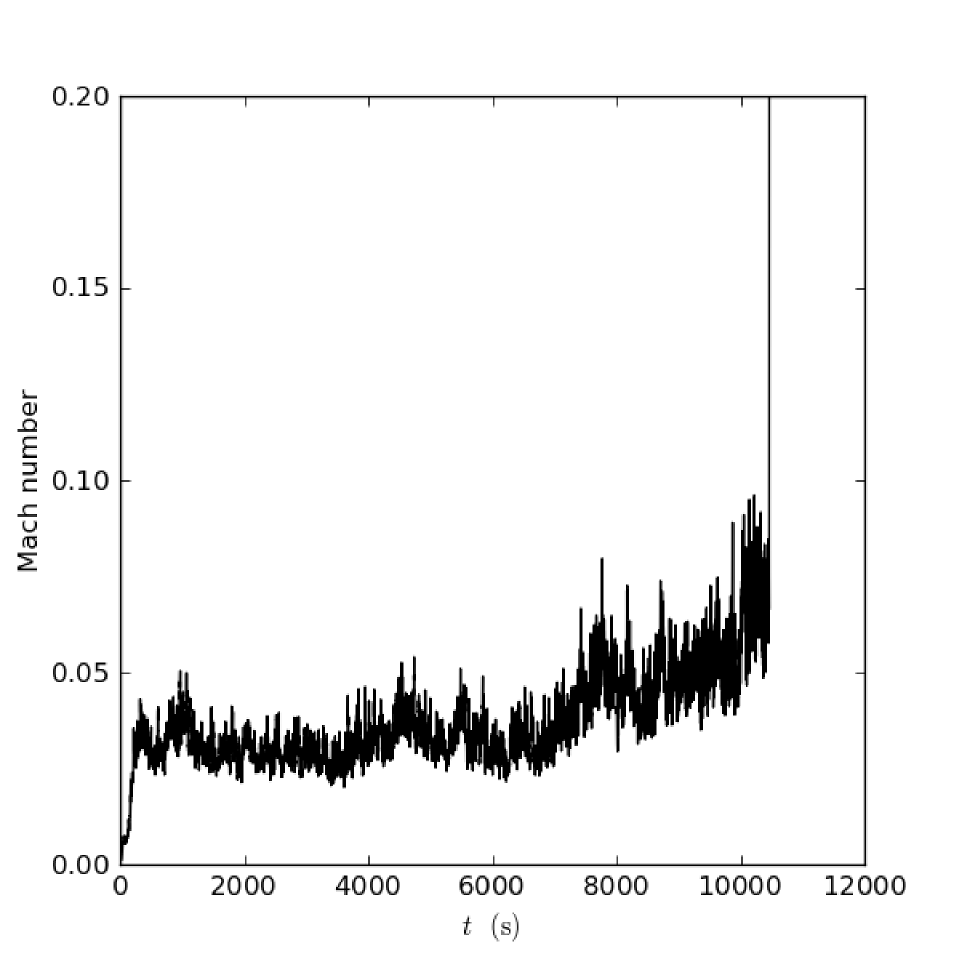
Edge of Star
density = 10^{-4} g/cc

- Use 10K cores for 40 days (10 million CPU hours) to run effective 1152^3 resolution (4.3km zones) to ignition

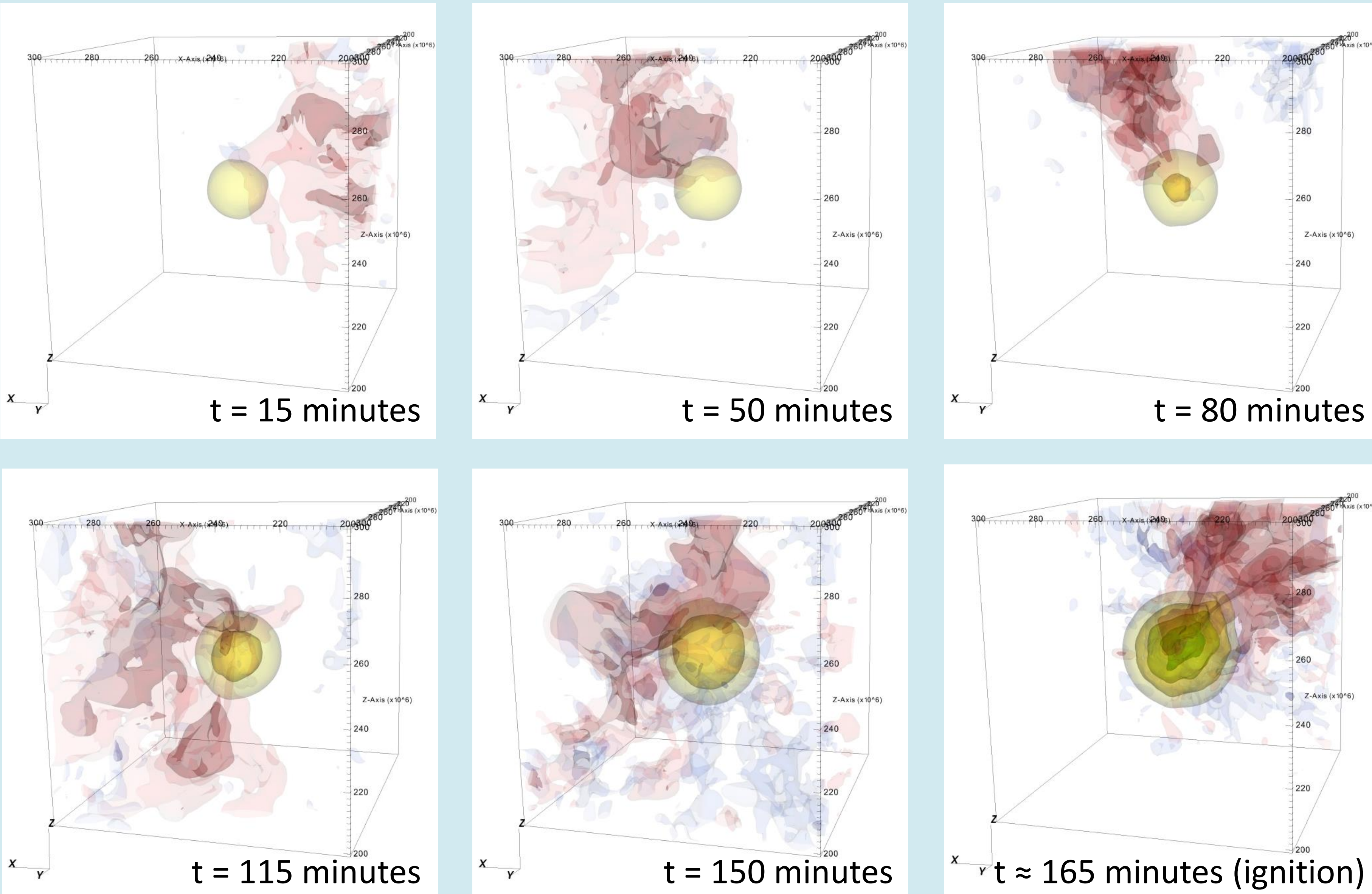
White Dwarf Convection: Long-Time Behavior

- Maximum temperature and Mach number vs. time



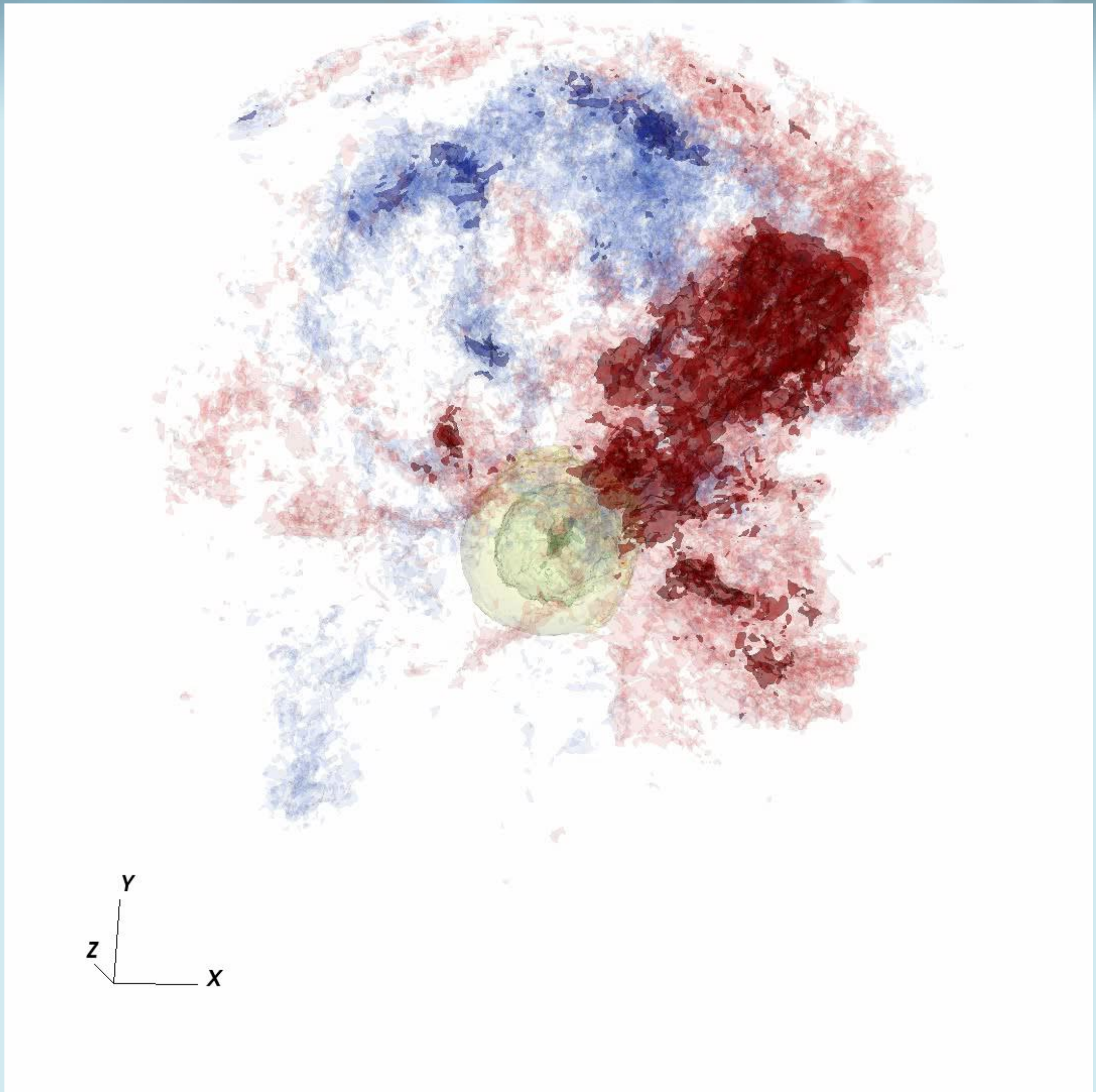


- Red / Blue = outward / inward radial velocity
- Yellow / Green = contours of increasing burning rate



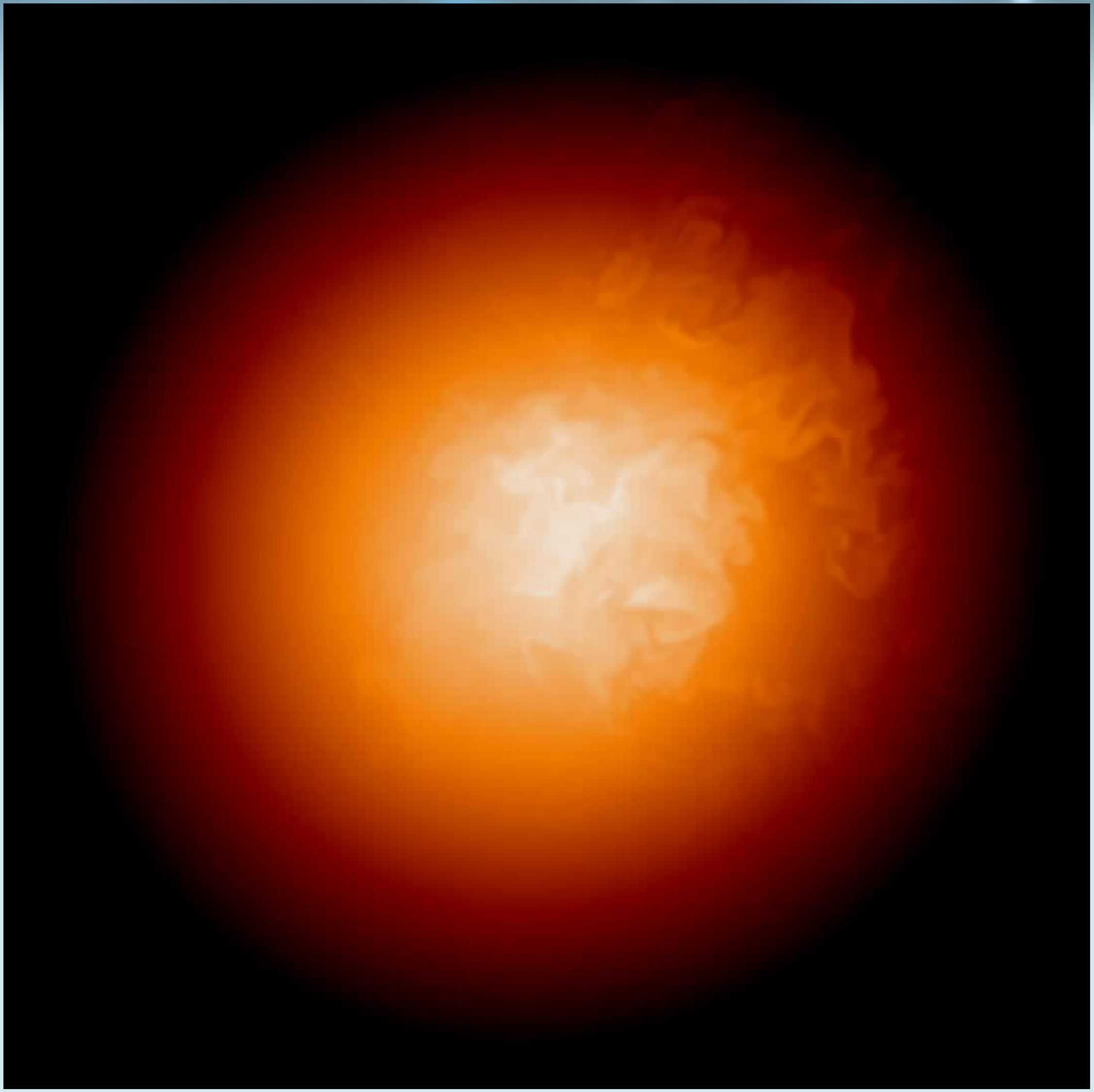
White Dwarf Convection: Ignition

- Convective flow pattern a few minutes preceding ignition
  - Inner 1000 km^3 of star
  - Effective 2304^3 resolution (2.2km) with 3 total levels of refinement
  - Red / Blue = outward / inward radial velocity
  - Yellow / Green = contours of increasing burning rate



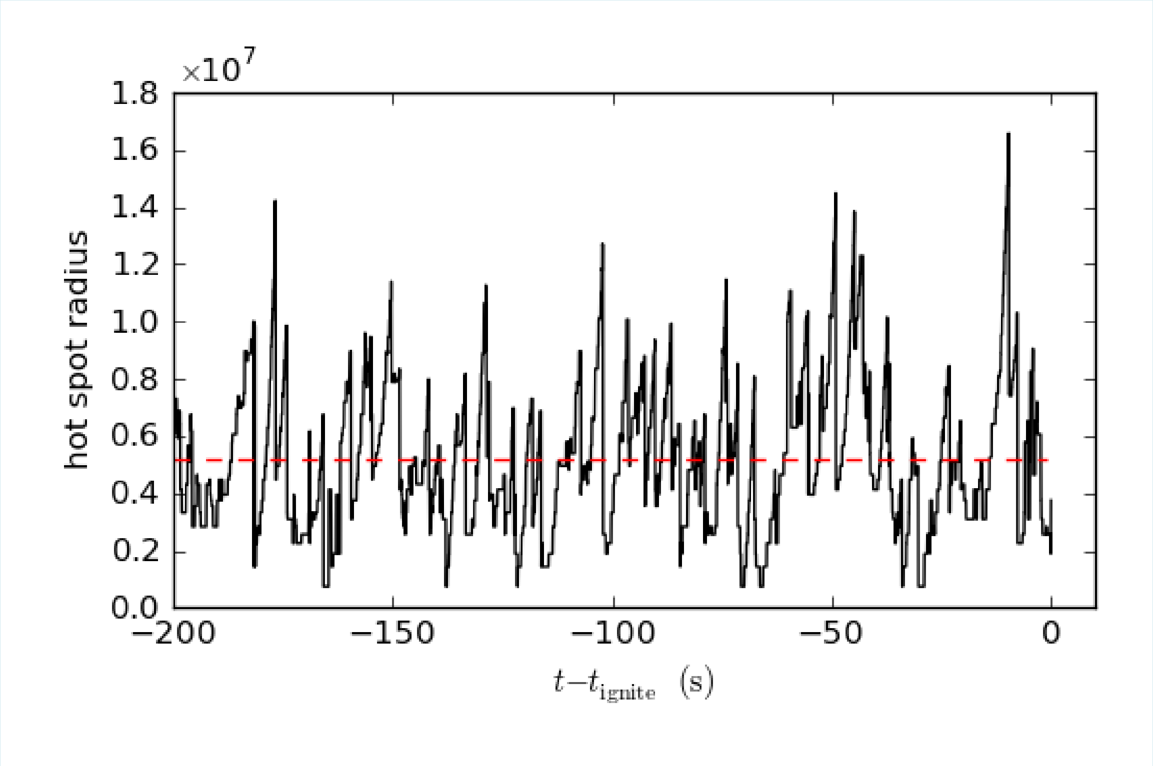
White Dwarf Convection: Ignition

- Same data from the previous simulation
- 2D slice of temperature profile a few minutes preceding ignition



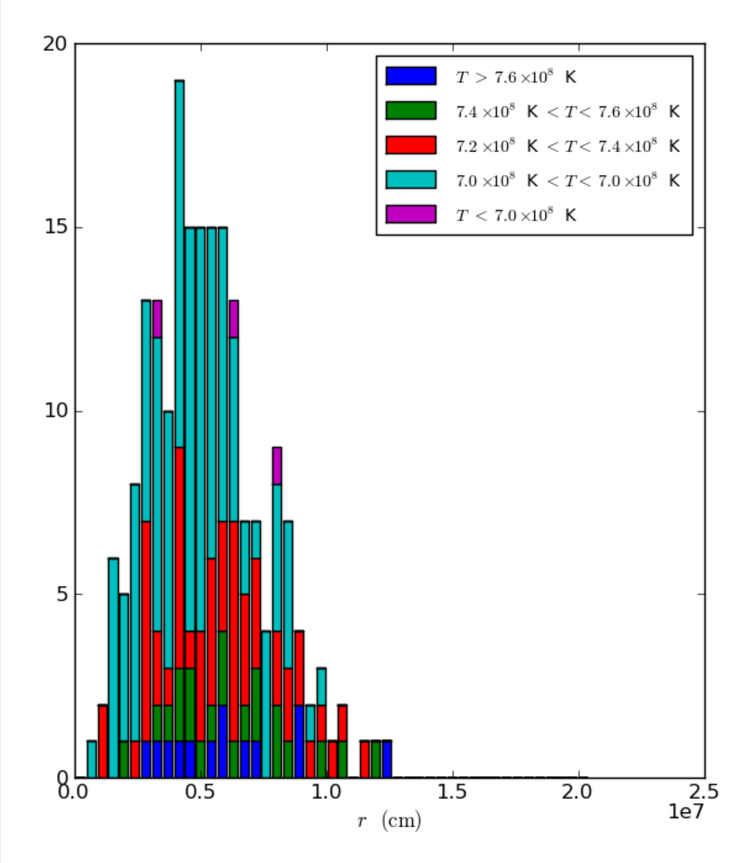
WD Convection: Ignition

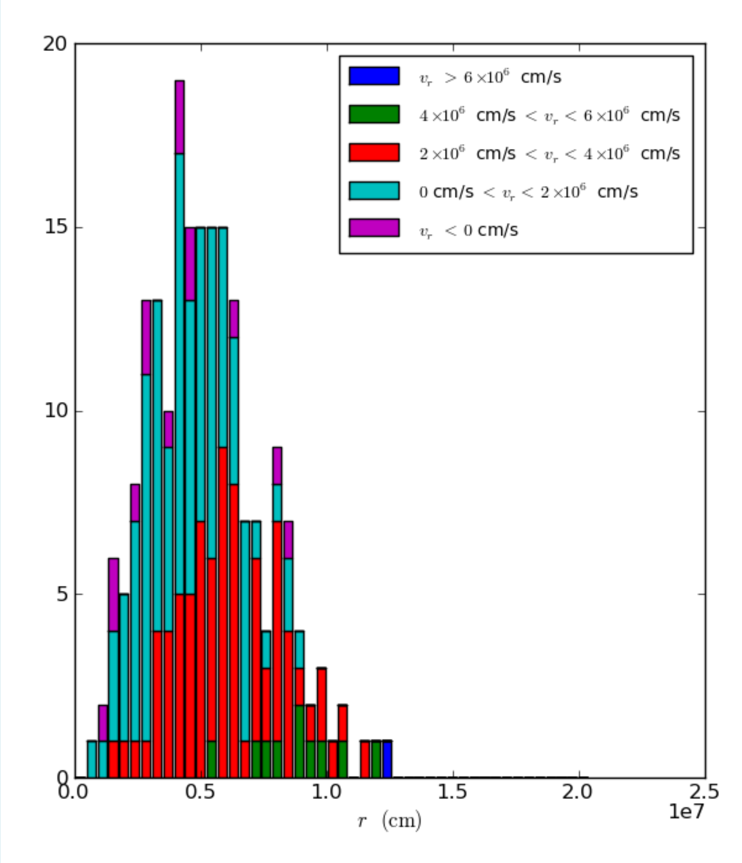
- Examining the radius of the hot spot over the last few minutes indicates ignition radius of 50-70 km off-center is favored.



White Dwarf Convection: Ignition

- Histograms of ignition conditions over the final 200 seconds
  - (Left) Temperature and location of peak hot spot
  - (Right) Radial velocity and location of peak hot spot





White Dwarf Convection Summary

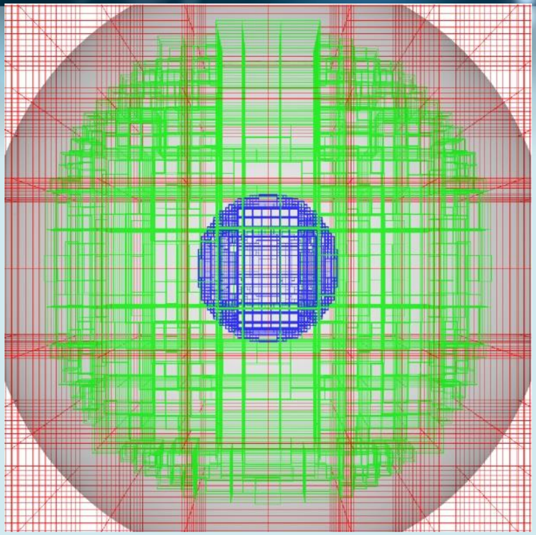
- We have performed the most detailed full-star calculations ever of convection up to the point of ignition in Type Ia supernovae
  - Low Mach number formulation
  - Adaptive mesh refinement
  - Performing science at 10K-20K cores, scaling to 100K cores
- Main scientific conclusions:
  - Likely ignition radius of 50-70km
  - Single ignition point strongly favored
  - Characterization of full state of the star, including the background velocity field

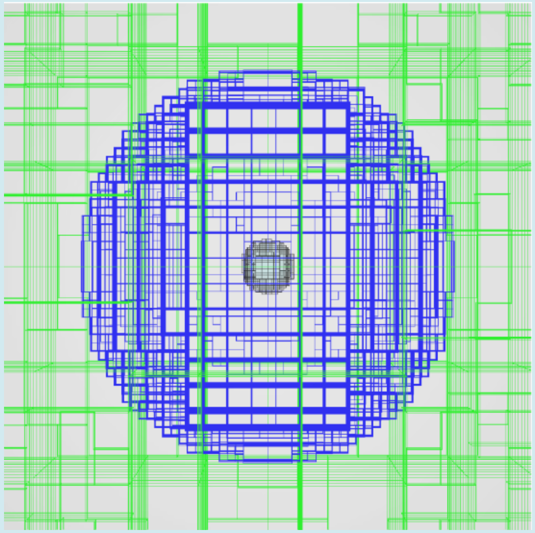
Compressible Simulations with CASTRO

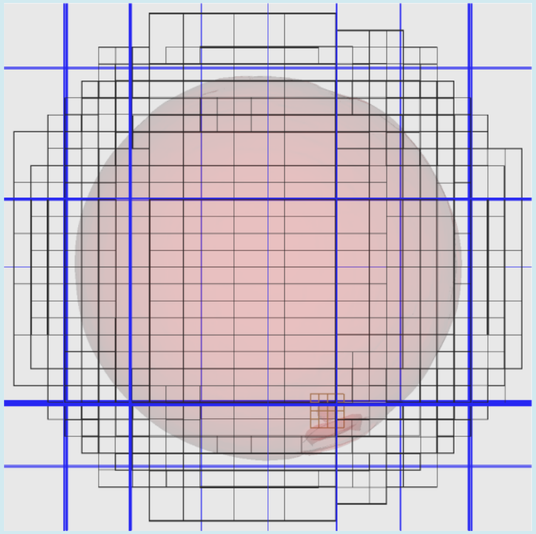
- Once the first flames have ignited, the Mach number becomes O(1), and the assumptions we used to derive the low Mach number equation set are no longer valid.
- We study post-ignition dynamics of early flames with CASTRO.
  - We can import the initial conditions directly from the MAESTRO simulation into the compressible code framework.

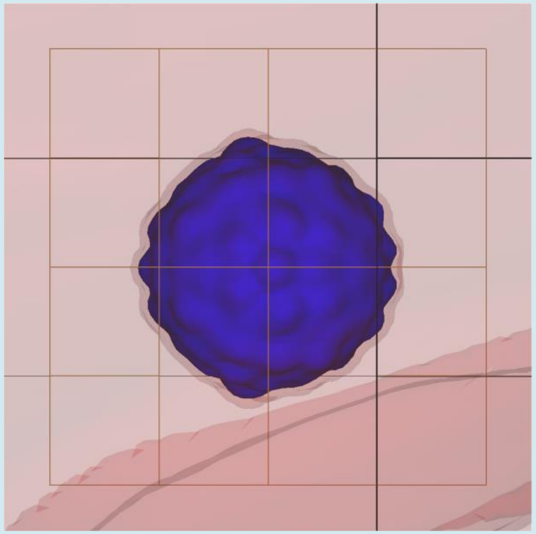
CASTRO Grid Configuration

- 5 levels of AMR
  - Divide 5000 [km] domain into 150 [m] zones
  - Effective $36,864^3$ zones would require 50 trillion grid points without AMR
  - With AMR we only use 1 billion zones









The Main Simulation

- We ran this simulation on 64,000 cores for 1 week.
  - Modeled first 0.5 seconds after ignition
- We included the background turbulent velocity field.
- We are interested in measuring properties of the spreading flame (size, rate of expansion) as well as the energy release and elemental production due to burning.

From Convection to Breakout:

porting results from MAESTRO to CASTRO

Malone, Nonaka, Almgren, Bell, Woosley, Zingale

Other Simulations

- We ran other simulations where we modified the ignition conditions and/or disabled the background velocity.

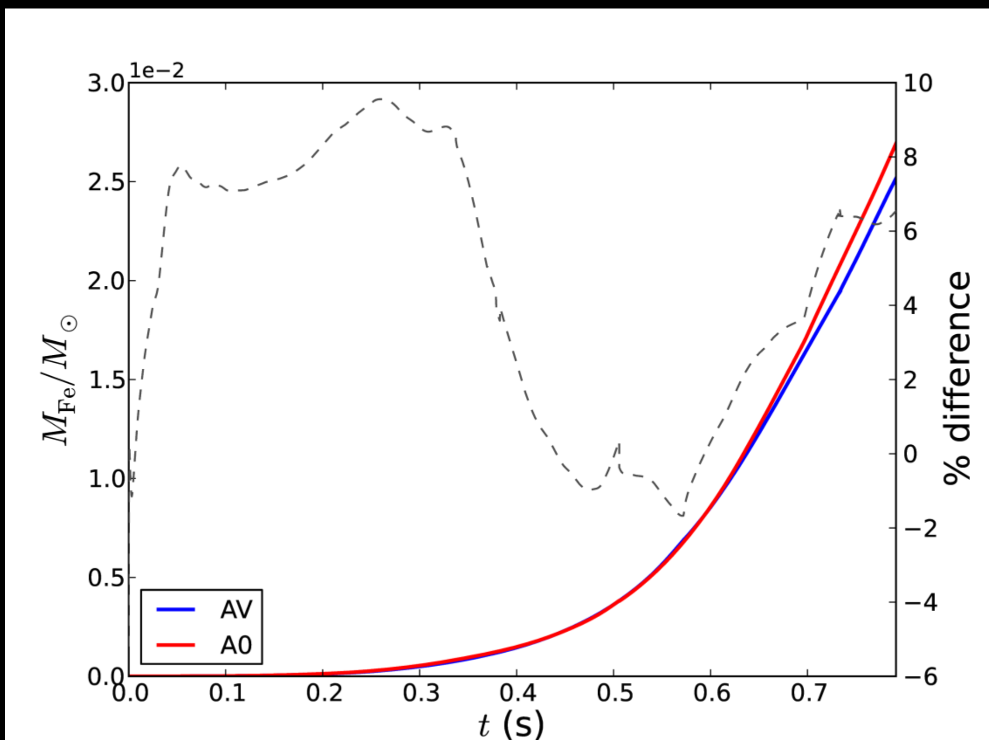
Simulation Name	Ignition Radius	Include Background Velocity?
AV	41km	Y
A0	41km	N
BV	10km	Y
B0	10km	N
CV	Center	Y
C0	Center	N

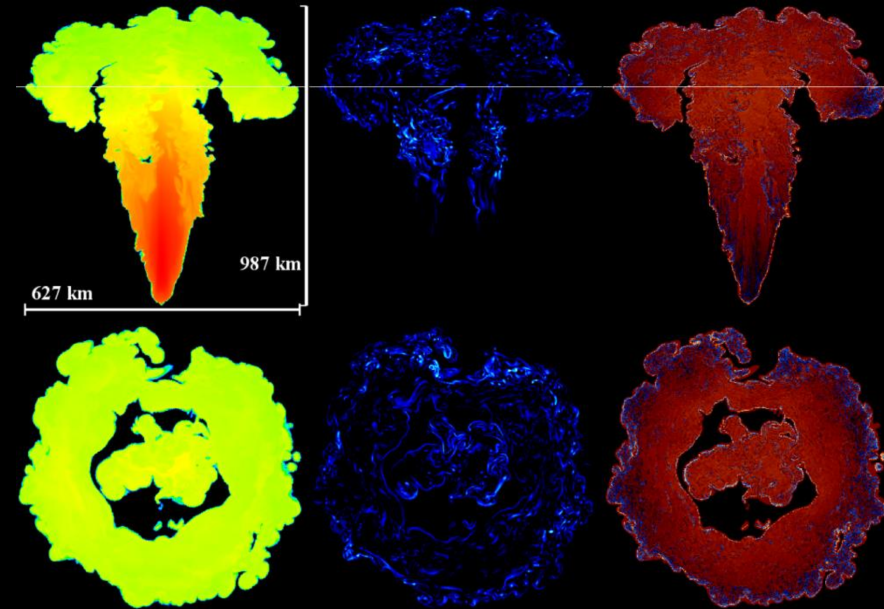
Comparison of simulations with different initial conditions

AV Simulation
41km ignition point
Include background flow field

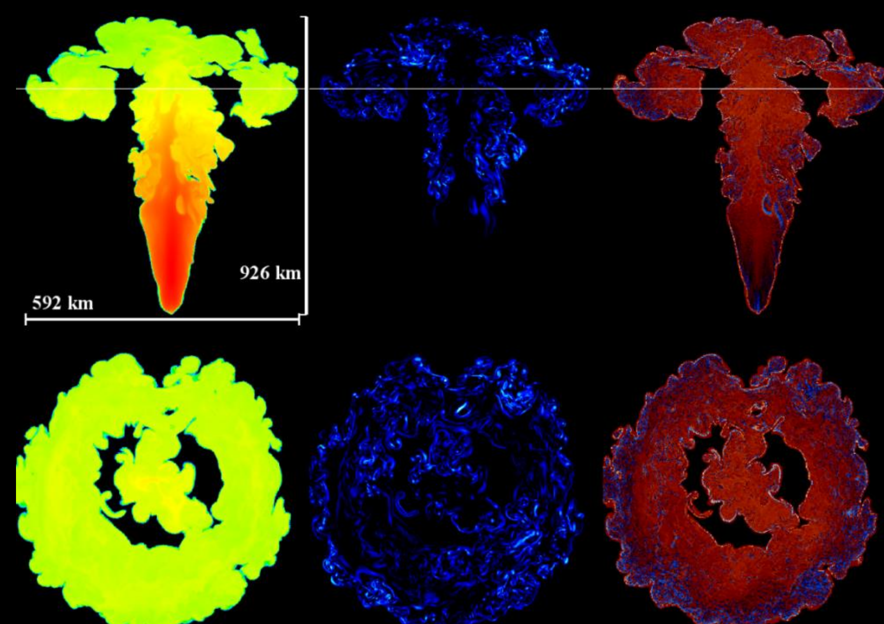
A0 Simulation
Same as above, but now
background flow field

Iron Production

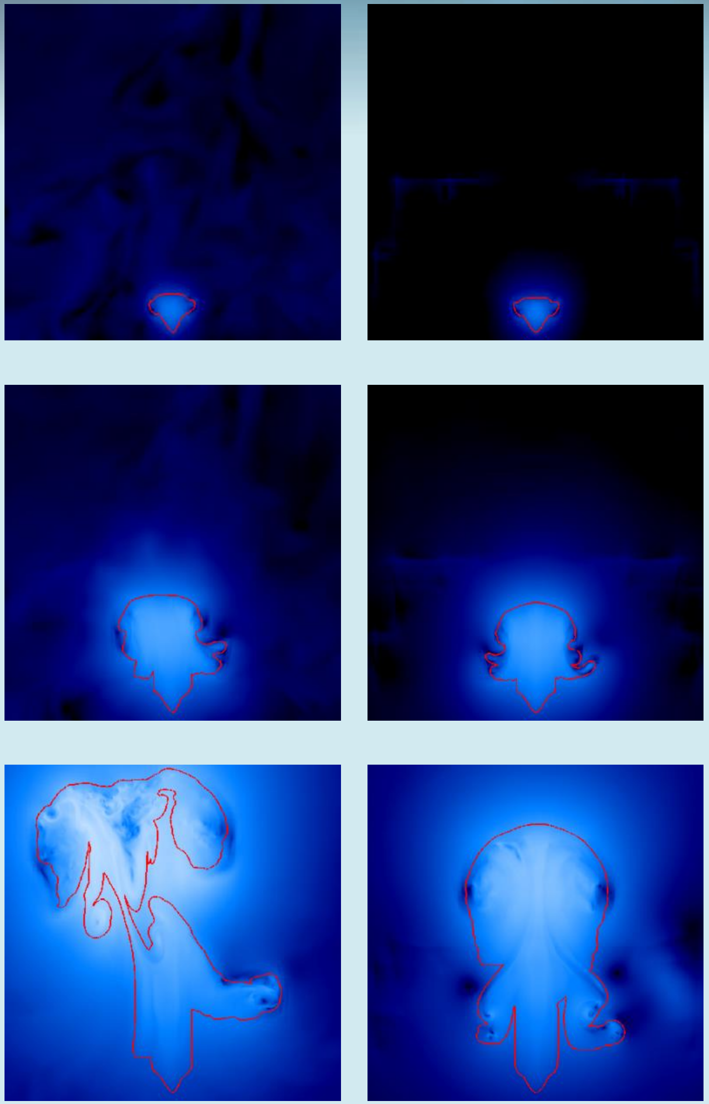




Temperature Vorticity Energy Release

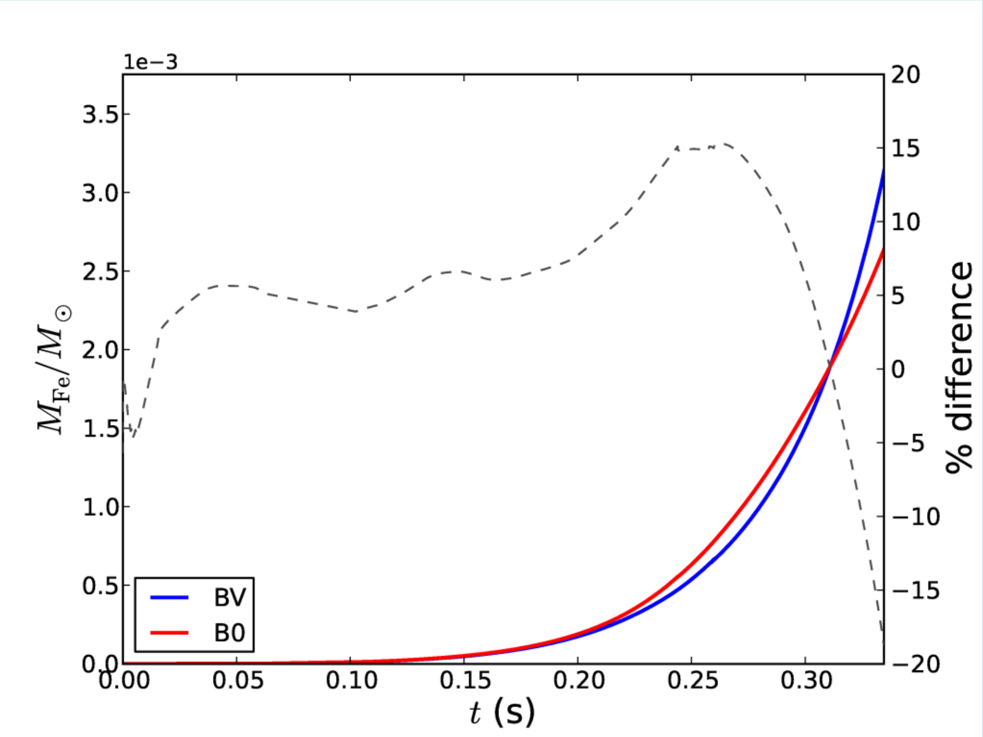


Effect of Velocity on Other Ignition Points



Comparing early flame evolution for artificial (10km) ignition with velocity field (left, “BV”) and without (right, “B0”).

Iron Production



Type Ia Supernova: Turbulent Combustion at the Grandest Scale

Deep inside a dying star in a galaxy far, far away, a carbon fusion flame ignites. Ignition may happen in the middle or displaced slightly to one side, but this simulation explores the consequences of central ignition. In a localized hot spot, represented here by a deformed sphere with an average radius of 100 km, carbon is assumed to have already fused to iron, producing hot ash (~ten billion K) with a density about 20% less than its surroundings. As the burning progresses, this hot buoyant ash rises up and interacts with cold fuel. Rayleigh-Taylor fingers give rise to shear and turbulence, which interacts with the flame, causing it to move faster. In about two seconds, the energy released blows the entire white dwarf star up, leaving nothing behind but a rapidly expanding cloud of radioactive nickel, iron, and other heavy elements. A Type Ia supernova is born.

Post Ignition Study Summary

- We have performed full-star simulations of early post ignition flame dynamics at unprecedented resolution
  - Compressible formulation
  - Adaptive mesh refinement
  - Performing science at 64K cores, scaling to 200K+ cores
- Main scientific conclusions:
  - Turbulent flow field has little effect on expected ignition conditions, but will have a stronger effect for more central ignition
  - Flame speeds prescribed by flame model have little effect since buoyant rise speeds dominate

Summary

- Recent advancements in mathematical modeling, numerical methods, and supercomputing allow us to gain new insight on complex phenomena such as Type Ia supernovae.

- In order to solve such problems, teams of interdisciplinary scientists, engineers, and mathematicians must closely work together.