Low Mach Number Models in Computational Astrophysics

John Bell
Center for Computational Sciences and Engineering
Lawrence Berkeley National Laboratory

University of Tsukuba
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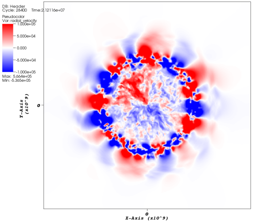
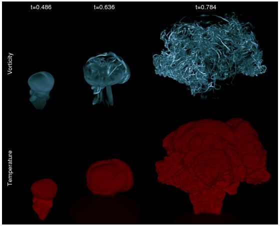
Collaborators: A. S. Almgren, A. J. Aspden, A. J. Nonaka,
S. E. Woosley, M. A. Zingale

Introduction

One thinks of astrophysical problems as dramatic, explosive events but a wide range of phenomena are characterized by low Mach number convective flows

- Convection leading up to ignition of a standard Chandrasekar SNIa
- Convection in some sub-Chandra SNIa scenarios
- Type 1 XRB
- Convection in main sequence stars
- Nuclear flame microphysics





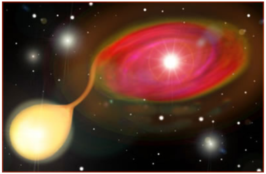
Type Ia Supernovae (SNe Ia)

- Largest thermonuclear explosions in the universe
- Brightness rivals that of host galaxy, L 10^{43} erg / s
- Definition: no H line in the spectrum, Si II line at 6150A.

SNe Ia: Theory

Suppose we want to study Type Ia supernovae ...

One of the models of a SN Ia progenitor is a carbon/oxygen white dwarf in a binary pair.

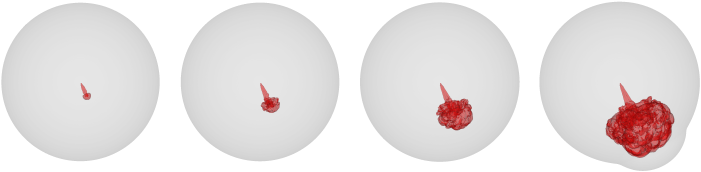


A carbon-oxygen white dwarf accretes mass from a binary companion ($\approx$ 10 million years to reach Chandrasekhar limit)

- Over a period of centuries, carbon burning near the core drives convection and temperature slowly increases.
- Over the last few hours, (low Mach number!) convection becomes more vigorous as the heat release intensifies and convection can no longer carry away the heat.
- Eventually, the star ignites, and finally explodes within seconds.

SNe Ia: Modeling

Traditional modeling approaches focus on the last few seconds.



Initial conditions:

- Radial profile from 1d stellar evolution code
- Assumptions about when & where of ignition "hot spots"

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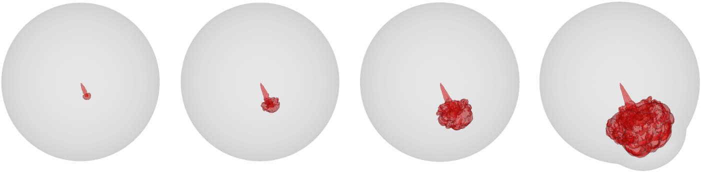

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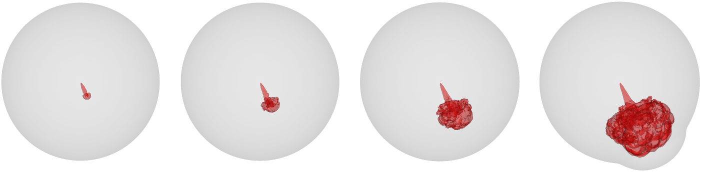

Initial conditions:

- Radial profile from 1d stellar evolution code
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But... the simulated explosions are very sensitive to the initial conditions.

$\Rightarrow$ We need to know more about how SNe Ia ignite.

Modeling of Type Ia Supernovae

Typically, numerical simulations of SNe Ia have used the compressible Navier-Stokes equations with reactions:

$$
\begin{aligned}
\frac{\partial(\rho X_k)}{\partial t} + \nabla \cdot (\rho U X_k) &= \rho \dot{\omega}_k \\
\frac{\partial(\rho U)}{\partial t} + \nabla \cdot (\rho U U + p) &= -\rho g \mathbf{e}_r \\
\frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\rho U E + U p) &= -\rho g (U \cdot \mathbf{e}_r) + \rho \sum_k q_k \dot{\omega}_k
\end{aligned}
$$

ρ	density	e	internal energy
U	velocity	X_k	mass fractions
p	pressure	$\dot{\omega}_k$	X_k production rate
$E = e + U^2/2$	total energy	$\vec{g}$	gravity

with Timmes equation of state:

$$p(\rho, T, X_k) = p_{ele} + p_{rad} + p_{ion}$$

where

$$p_{ele} = \mathrm{fermi},\ \ p_{rad} = aT^4/3,\ \ p_{ion} = \frac{\rho k T}{m_p} \sum_m X_k / A_m$$

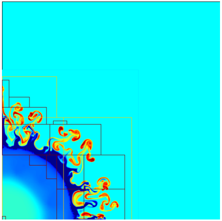
Compressible Formulation

Time-explicit methods for hyperbolic conservation laws with source terms:

$$\mathbf{U}_t + \nabla \cdot \mathbf{F} = \mathbf{S}$$

have the advantages that they are

- easy to program
- easy to parallelize – great weak scaling to 200K cores
- straightforward with AMR (synchronization is explicit as well)



But the time step is the problem – to capture ignition we need to simulate 2 hours, not 2 seconds.

Low Mach Number Approach

We want to develop a model based on separation of scales between fluid motion and acoustic wave propagation.

One approach is based on asymptotic expansion in the Mach number, $M = |U|/c$, which leads to a decomposition of the pressure into thermodynamic and dynamic components:

$$p(\mathbf{x}, t) = p_0(r, t) + p'(\mathbf{x}, t)$$

where $p'/p_0 = O(M^2)$.

- p_0 replaces p in the thermodynamics; p' appears only in the momentum equation,
- Physically: acoustic equilibration is instantaneous; sound waves are “filtered” out
- Mathematically: resulting equation set is no longer strictly hyperbolic; a constraint equation is added to the evolution equations
- Computationally: time step is dictated by fluid velocity, not sound speed.

Criteria for a New Model

We want to eliminate acoustic waves (so they don't limit the time step) but make as few additional limiting assumptions as possible.

New model, in addition to allowing a larger Δt, needs to incorporate

- Buoyancy
- Large variation from background state (or the star will never ignite!)
- Background stratification
- Nonideal equation of state (i.e. not constant γ)
- Reactions and heat release
- Overall expansion of the star

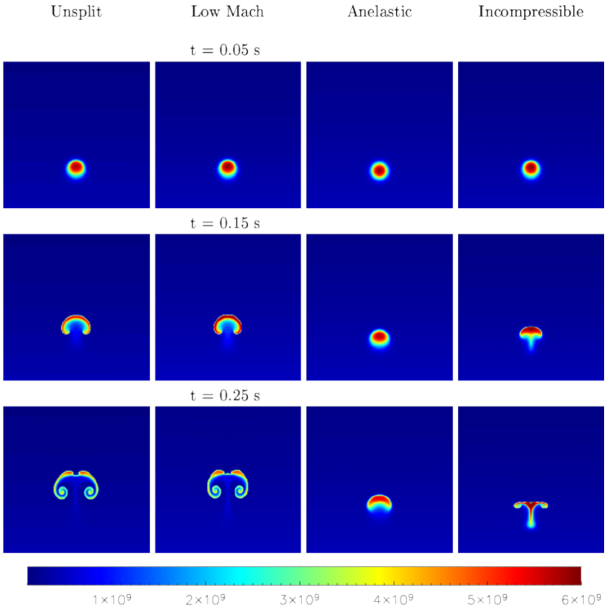
and, in the end, must have lower time-to-solution.

A hierarchy of possible models

- Incompressible $\nabla \cdot U = 0$
  - No compressibility effects
- Anelastic $\nabla \cdot (\rho_0 U) = 0$
  - Compressibility due to static stratified atmosphere
  - Only valid for small thermodynamic perturbations from a static hydrostatic (usually isentropic) background
- Low Mach number combustion $\nabla \cdot U = S$
  - Local compressibility due to heat release and diffusion
  - Large variation in density and temperature allowed
  - No stratification
- Pseudo-incompressible $\nabla \cdot (p_0^{1/\gamma} U) = S$
  - Compressibility due to both background stratification and heat release
  - Static background
  - Ideal gas EOS

None of these quite works.

Buoyant bubble rise



Low Mach Number Model

$$
\begin{aligned}
\frac{\partial(\rho X_k)}{\partial t} &= -\nabla \cdot (U\rho X_k) + \rho\dot{\omega}_k \ , \\
\frac{\partial(\rho h)}{\partial t} &= -\nabla \cdot (U\rho h) + \frac{Dp_0}{Dt} - \sum_k \rho q_k \dot{\omega}_k \ , \\
\frac{\partial U}{\partial t} &= -U \cdot \nabla U - \frac{\beta_0}{\rho}\nabla(\frac{p'}{\beta_0}) - \frac{(\rho - \rho_0)}{\rho} g\mathbf{e}_r \ , \\
\nabla \cdot (\beta_0 U) &= \beta_0 \left(S - \frac{1}{\bar{\Gamma} p_0}\frac{\partial p_0}{\partial t} \right)
\end{aligned}
$$

where, by differentiating the EOS, we can define

$$
S = -\sigma \sum_k \xi_k \dot{\omega}_k + \frac{1}{\rho p_\rho} \sum_k p_{X_k} \dot{\omega}_k
$$

Use average heating to evolve radial base state.

$$
\frac{\partial p_0}{\partial t} = -w_0 \frac{\partial p_0}{\partial r} \quad \text{where} \quad \mathrm{w_0(r,t)} = \int_{\mathrm{r_0}}^{\mathrm{r}} \overline{\mathrm{S}}(\mathrm{r}', \mathrm{t})\, \mathrm{dr}'
$$

Self-gravity introduces some additional complexity

But . . .

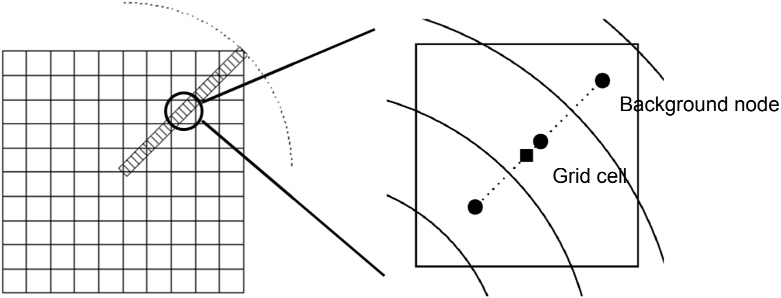
We want to simulate a full star on a Cartesian grid assuming a spherical background state

- Dynamics are driven by the perturbational density, which is much smaller than the background
- Thermodynamics are constrained by the background pressure
- Background state evolves slowly to represent expansion of the star

Need accurate two-way mapping between radial background state and full state

Background to grid mapping

For spherical problems, mapping from background state to the full state can be done using quadratic interpolation

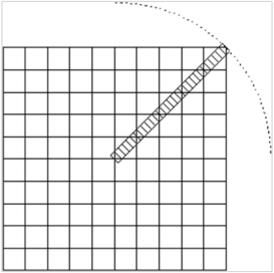


The background state grid spacing must be chosen to be smaller than the full state spacing

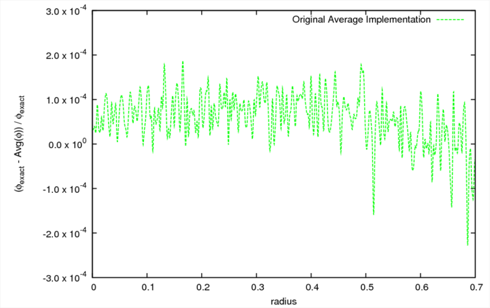
- $\Delta r = 1/5 \Delta x$ works well

Cartesian grid to background mapping

Mapping from the full state to the background state requires more care



Simple averages give reasonable errors but test show it isn't accurate enough

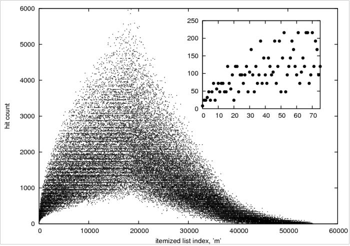


Cartesian grid to background mapping

Mapping form the full state to the background state requires more case

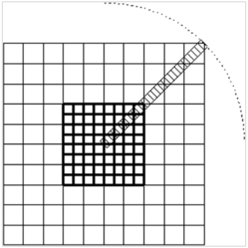
Observation: Every Cartesian cell center has radius of the form

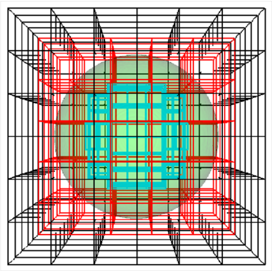
$$r_m = \Delta x \sqrt{0.75 + 2m}$$



- Create list of radii for all possible cell centers
- Collect average over these bins
- Interpolate from this list to background state array
- Gives relative errors that are $O(10^{-8})$

AMR issues for full-star modeling





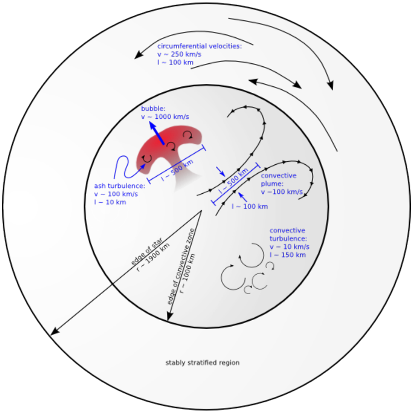
- Use single radial base state at finest level
- Separate lists for each level
- Interpolate levels separately then combine
- Preserves $O(10^{-8})$ accuracy

MAESTRO: Low Mach number method

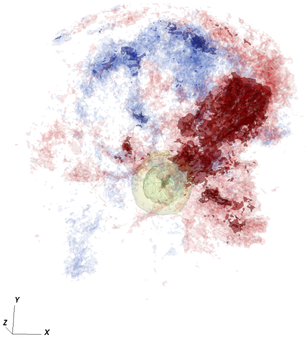
- Numerical approach based on generalized projection method
- 2nd-order accurate fractional step scheme
  - Advance velocity and thermodynamic variables – unsplit Godunov method
  - Project solution back onto constraint – involves solving an elliptic equation for the pressure perturbation (using multigrid)
- Strang splitting (or better coupling) for reaction terms – local implicit ODE integration
- Also need to advance background state
- Built in BoxLib, a reusable software framework for block-structured AMR application codes:
  - supports block-structured AMR
  - scales to 100000's of processors
  - linear solvers for solving elliptic and parabolic equations
  - hybrid MPI / OpenMP
  - modular EOS and reaction networks – "plug 'n play"

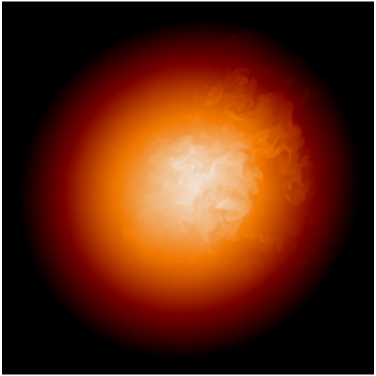
White Dwarf Convection

Using MAESTRO, we can simulate the flow before the star ignites.



White dwarf convection





Convective flow pattern on inner 1000 km of star

- Red / blue is outward / inward radial velocity
- Yellow / green shows burning rate

Two dimensional slices of temperature a few minutes before ignition

Distribution of ignition

What we would like to know the the distribution of the ignition site and the structure of the turbulence

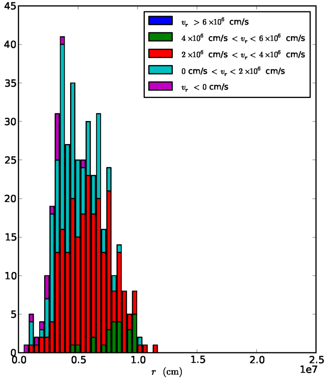
Monitor peak temperature and radius during simulation

Filter data

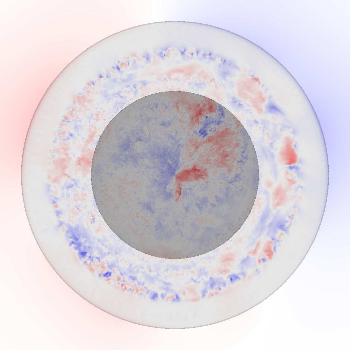
Bin data to form histogram

Assume that hot spot locations are “almost” ignitions

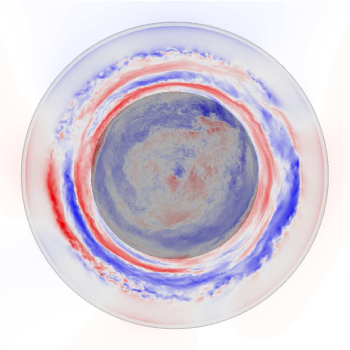
Detailed analysis of hot spots shows that likely ignition is a single isolated location



Structure of the velocity field



Radial velocity



Theta velocity

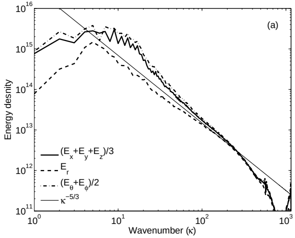
Characterization of the turbulence

What can we say about the structure of the turbulent flow

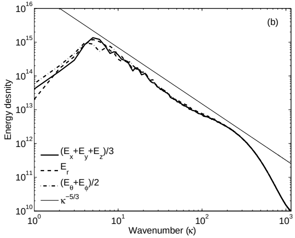
- Intensity and structure of turbulence impacts subsequent evolution
- Focus on core region
- Integral scale approximately 200 km
- Turbulent intensity approximately 16 km / sec.
- Turbulent intensity too small for spontaneous detonation

What happens next?

After brief initial transient, early stages of subsequent evolution dominated by turbulent entrainment in buoyant ash bubble, not turbulent flame propagation (generalization of Morton, Taylor, Turner analysis of buoyant plumes)



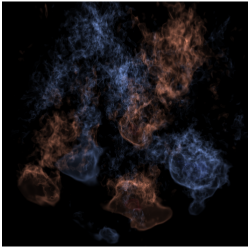
Turbulent energy spectra – full star

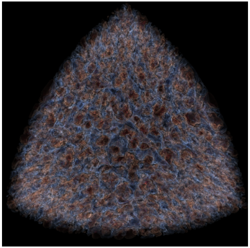


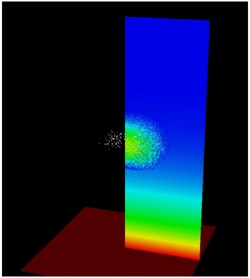
Turbulent energy spectra in the core

Where Do We Go From Here?

Oher applications:


X-ray burst


Sub-Chandra SN Ia


Cloud formation

Additional capability

- Stellar rotation
- Long wavelength acoustics
- Magnetic fields

We have a companion code, CASTRO, that does multigroup, flux-limited diffusion coupled with compressible hydrodynamics

Both codes are available from github