Low Mach Number Models in Computational Astrophysics

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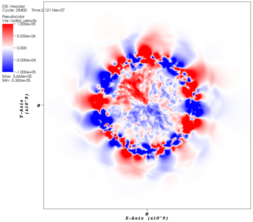
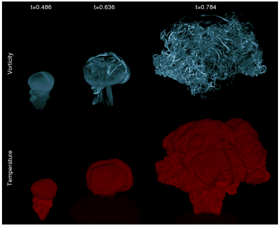
Introduction

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





Outline

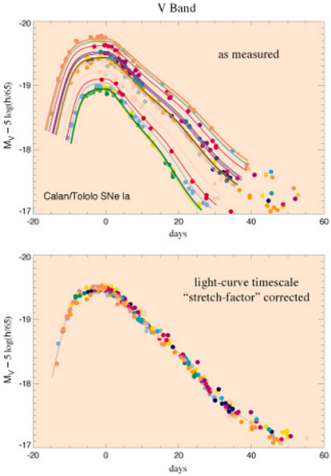
- Type Ia Supernovae
- Standard approach
- Low Mach Number Approach
- Numerical Issues
- Results

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.

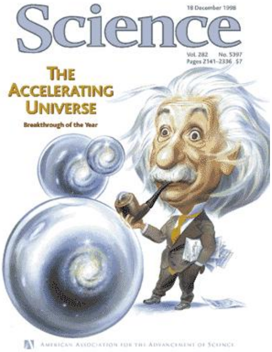
Light Curves

- Key observable for SNe Ia is the light curve (brightness vs time).
- Light curves from different SNe Ia have similar shape, except for brighter ≈ broader.
- With a single “time stretch” factor we can map all these curves onto a single curve.



1998 Science Breakthrough of the Year

(Supernova Cosmology Project and High-z Supernova Search Team)

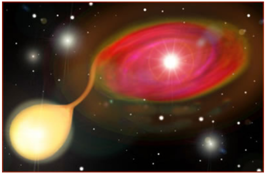


- By observing the duration of distant SNe Ia one could determine their absolute magnitude (standard candles).
- absolute vs. apparent brightness $\rightarrow$ distance
- distance vs. redshift $\rightarrow$ Hubble diagram.

This led to the discovery that the rate at which the Universe is expanding is increasing.

SNe Ia: Theory

The best model for SNe Ia is the thermonuclear explosion of a carbon/oxygen white dwarf.

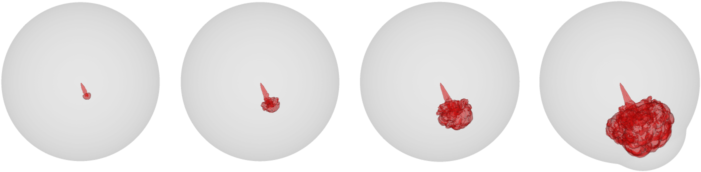


A carbon-oxygen white dwarf accretes mass from a binary companion ($\approx$ 10 million years to reach Chandrasekhar limit)

- Over a period of centuries, carbon burning near the core drives convection and temperature slowly increases.
- Over the last few hours, 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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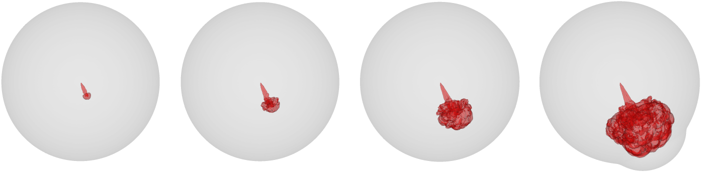

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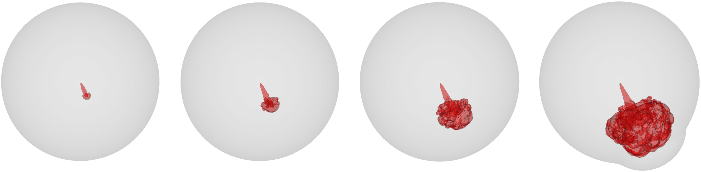

Initial conditions:

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

⇒ 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:

$$
\begin{aligned}
\rho_t + \nabla \cdot \rho U &= 0 \\
(\rho U)_t + \nabla \cdot (\rho U U + p) &= -\rho g \mathbf{e}_r \\
(\rho E)_t + \nabla \cdot (\rho U E + U p) &= \nabla \cdot \kappa \nabla T - \rho g (U \cdot \mathbf{e}_r) + \rho H \\
(\rho X_m)_t + \nabla \cdot \rho U X_m &= \rho \dot{\omega}_m
\end{aligned}
$$

ρ	density	e	internal energy
U	flow velocity	X_m	mass fractions
p	pressure	$\dot{\omega}_m$	X_m production rate
T	temperature	$\vec{g}$	force of gravity
$E = e + U^2/2$	total energy	$H = \sum_m \rho q_m \dot{\omega}_m$	heating

Modeling cont'd

Timmes equation of state provides:

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

$$\begin{aligned} e_{ele} &= \text{fermi} \\ e_{rad} &= aT^4/\rho \\ e_{ion} &= \tfrac{3kT}{2m_p} \textstyle\sum_m X_k/A_m \end{aligned} \qquad \begin{aligned} p_{ele} &= \text{fermi} \\ p_{rad} &= aT^4/3 \\ p_{ion} &= \tfrac{\rho kT}{m_p} \textstyle\sum_m X_k/A_m \end{aligned}$$

Standard approach: explicit integration of compressible equations with AMR

- Hillebrandt, Niemeyer et al. at MPI, Garching
- Oran et al. at NRL
- Rossner, Kokhlov, Plewa, et al. at U. Chicago
- Woosley, CCSE

SNe Ia: Ignition

Compressible models work well for modeling the explosion of the star but to capture ignition . . .

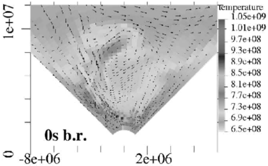
- Need to simulate 2 hours (not 2 seconds)
- Mach number is very low before ignition
- Issues with maintaining hydrostatic balance

Convection leading up to ignition is basically infeasible with standard explicit compressible codes

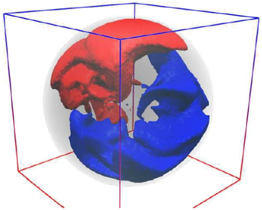
Model needs to include a number of effects

- Background stratification
- Nonideal equation of state
- Reactions and heat release
- Overall expansion of the star

Prior art



Hoflich and Stein (2002) modeled a 2-d wedge with an implicit code. Found compression near center suggesting a central ignition



Kuhlen et al. (2006) modeled a convectively unstable region with center cut out using an anelastic model. They observed a characteristic dipole feature suggesting off-center ignition

No previous calculations have modeled the entire star

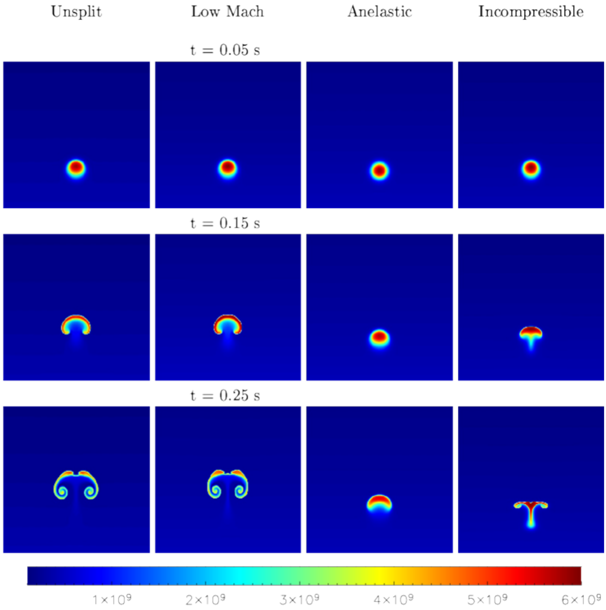
A hierarchy of possible models

We want to eliminate acoustic waves (so we don't have to track them) but make as few assumptions as possible about the magnitude of density and temperature variations.

Possible models for convective motion:

- Boussinesq: simplest model - allows heating-induced buoyancy in a constant density background (constant p_0, ρ_0, T_0)
- Variable-ρ incompressible: finite amplitude density variation but incompressible
- Anelastic: allows small variations in temperature and density from a stratified background state $(p_0(r), \rho_0(r), T_0(r))$
- Low Mach number : large variations in temperature and density in a time-varying stratified background state $(p_0(r), \rho_0(r), T_0(r))$

Buoyant bubble rise



Low Mach Number Approach

Asymptotic expansion in the Mach number, $M = |U|/c$, leads to a decomposition of the pressure into thermodynamic and dynamic components:

$$p(\mathbf{x}, t) = p_0(r, t) + \pi(\mathbf{x}, t)$$

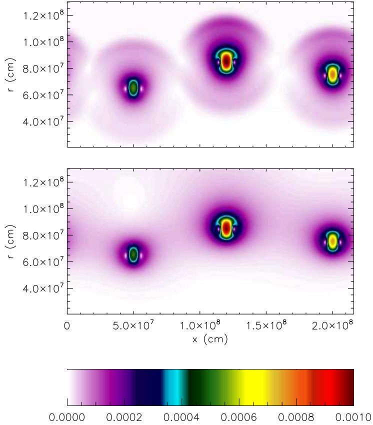
where $\pi / p_0 = O(M^2)$.

- p_0 affects only the thermodynamics; π affects only the local dynamics,
- 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.

Instantaneous Equilibration

Mach number in compressible (top) vs low Mach number (bottom) simulation

- Features of bubble itself are identical
- Size of difference in M is 10^{-4}, so pressure difference is $O(10^{-8})$



Low Mach Number Model

$$\begin{aligned}
\frac{\partial(\rho X_k)}{\partial t} &= -\nabla\cdot(U\rho X_k) + \rho\dot{\omega}_k \ , \\
\frac{\partial(\rho h)}{\partial t} &= -\nabla\cdot(U\rho h) + \frac{Dp_0}{Dt} - \sum_k \rho q_k \dot{\omega}_k + \rho H_{\rm ext} \ , \\
\frac{\partial U}{\partial t} &= -U\cdot\nabla U - \frac{1}{\rho}\nabla\pi - \frac{(\rho-\rho_0)}{\rho} g\mathbf{e}_r \ , \\
\nabla\cdot(\beta_0 U) &= \beta_0\left(S - \frac{1}{\overline{\Gamma} p_0}\frac{\partial p_0}{\partial t}\right)
\end{aligned}$$

where

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

Cannot assume fixed background for net large-scale heating. We need evolution equations for p_0, ρ_0, etc.

Use average heating to evolve base state. Remaining dynamics evolves perturbations

$$\frac{\partial p_0}{\partial t} = -w_0\frac{\partial p_0}{\partial r} \quad \text{where} \quad \mathrm{w}_0(\mathrm{r},\mathrm{t}) = \int_{\mathrm{r}_0}^{\mathrm{r}} \overline{\mathrm{S}}(\mathrm{r}',\mathrm{t})\ \mathrm{dr}'$$

Self gravity introduces additional complexity

Projection method

Incompressible Navier Stokes equations

$$U_t + U \cdot \nabla U + \nabla p = \mu \Delta U$$

$$\nabla \cdot U = 0$$

Projection method

Advection step

$$\frac{U^* - U^n}{\Delta t} + U \cdot \nabla U = {}^1\!/\!_2 \mu \Delta (U^* + U_n) - \pi^{n-{}^1\!/\!_2}$$

Projection step to extract divergence-free component

$$U^{n+1} = \mathbf{P} U^*$$

Recasts system as initial value problem

$$U_t + \mathbf{P}(U \cdot \nabla U - \mu \Delta U) = 0$$

Generalized vector field decomposition

$$U^{n+1} + \frac{1}{\rho}\nabla\pi = U^*$$
$$\nabla \cdot \beta_0 U = S$$

Generalized vector field decomposition

$$U = U_d + \frac{1}{\rho}\nabla\pi$$

where

$$\nabla \cdot \beta_0 U_d = 0$$

Define an orthogonal projection

$$\mathbf{P}_{\beta_0,\rho}(U) = U_d$$

For inhomogeneity define

$$\nabla \cdot \beta_0 \nabla\xi = S$$
$$U^{n+1} = \mathbf{P}_{\beta_0,\rho}(U^* - \nabla\xi) + \nabla\xi$$

MAESTRO: Low Mach number method

Numerical approach based on generalized projection, 2nd order accurate
Fractional step scheme

- Advance velocity and thermodynamic variables
  - Advection
  - Diffusion
  - Reactions
- Project solution back onto constraint – single elliptic solve

Operator split approach to include nuclear burning:

- Reactions $\Rightarrow \Delta t/2$
- Advection – Diffusion $\Rightarrow \Delta t$
- Reactions $\Rightarrow \Delta t/2$

Also need to advance background state

But . . .

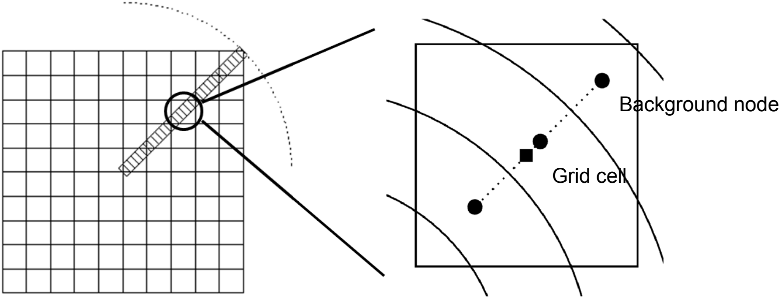
We want to simulate a full star on a Cartesian grid assuming a spherical background state

- 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

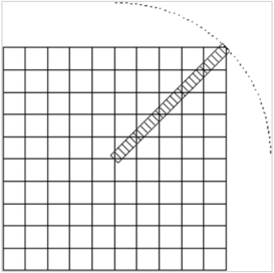


The background state grid spacing must be chosen to be smaller than the full state spacing

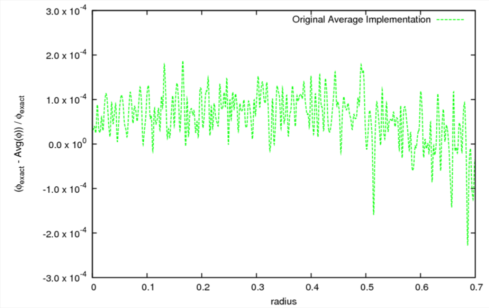
- $\Delta r = 1/5 \Delta x$ works well

Cartesian grid to background mapping

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



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



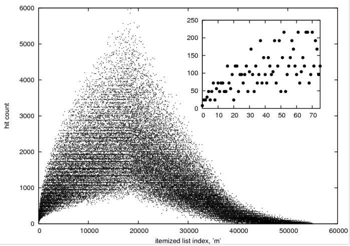
Cartesian grid to background mapping

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 $O(10^{-8})$



Block-structured AMR

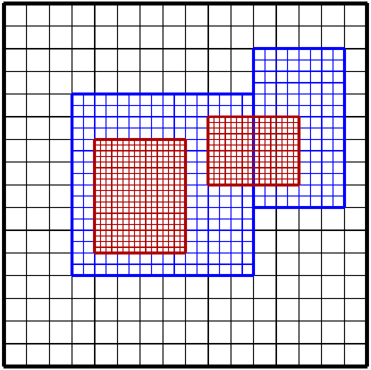
AMR – exploit varying resolution requirements in space and time

Block-structured hierarchical grids

- Amortize irregular work

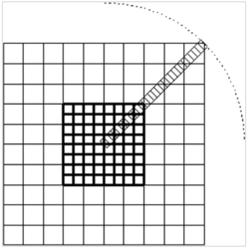
Each grid patch (2D or 3D)

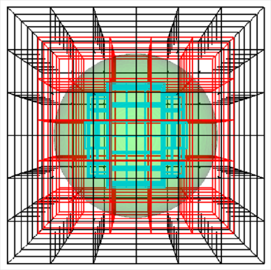
- Logically rectangular, structured
- Refined in space and (possibly) time by evenly dividing coarse grid cells
- Dynamically created/destroyed



2D adaptive grid hierarchy

AMR issues for full-star modeling



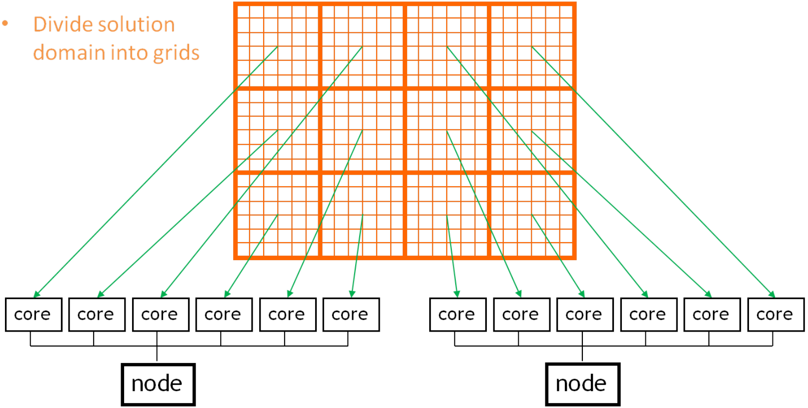


- Use single radial base state at finest level
- Separate lists for each level
- Interpolate levels separately then combine
- Preserves $O(10^{-8})$ accuracy

Parallelization

Pure MPI approach

- Divide solution domain into grids

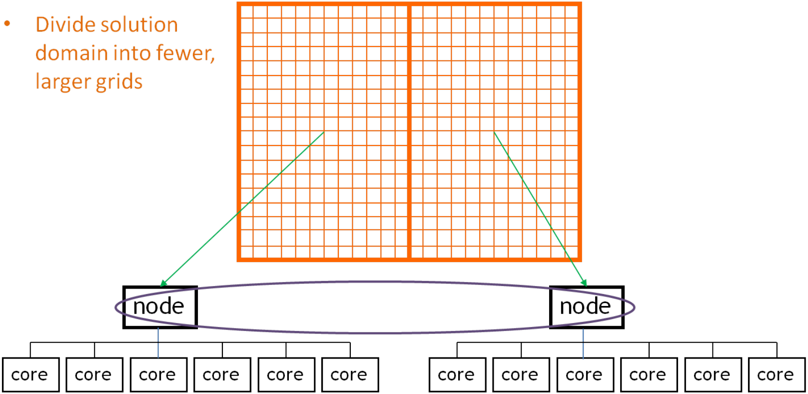


Each grid is assigned to a core

Cores communicate using MPI

Hybrid model for multicore architectures

- Divide solution domain into fewer, larger grids



Each grid is assigned to a node

OpenMP used to spawn threads so that cores within a node work on the grids simultaneously

Nodes communicate using MPI

MPI versus Hybrid model

Advantages of hybrid model

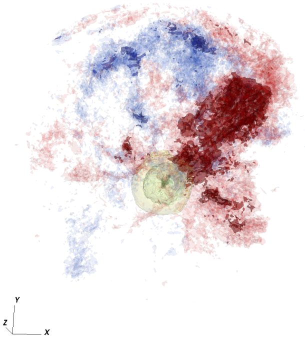
- Fewer MPI processes lead to reduced communication time
- Less memory for storing ghost cell information
- Reduced work from larger grids – surface to volume effect

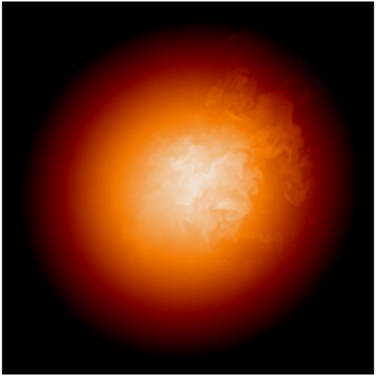
Disadvantages of hybrid model

- Spawning threads is expensive – makes performance worse for small core counts
- Can't hide parallelization from physics modules

With hybrid model, we have been able to scale MAESTRO to O(100K) processors

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

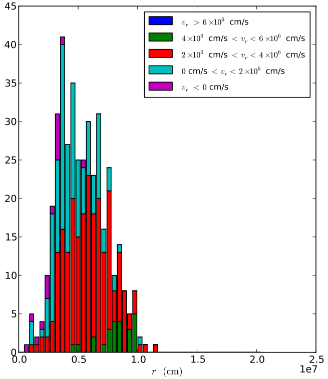
Monitor peak temperature and radius during simulation

Filter data

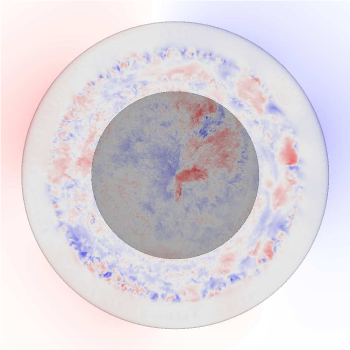
Bin data to form histogram

Assume that hot spot locations are "almost" ignitions

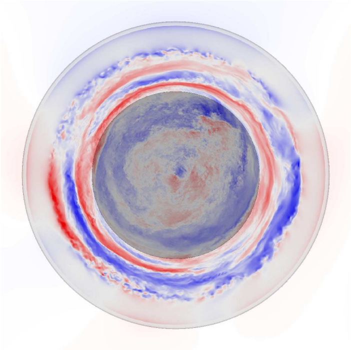
Detailed analysis of hot spots shows that likely ignition is a single isolated location



Structure of the velocity field



Radial velocity



Theta velocity

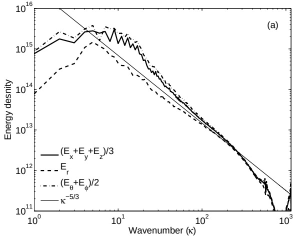
Characterization of the turbulence

What can we say about the structure of the turbulent flow

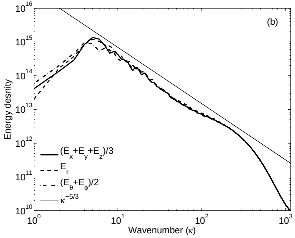
- Intensity and structure of turbulence impacts subsequent evolution
- Focus on core region
- Integral scale approximately 200 km
- Turbulent intensity approximately 16 km / sec.
- Turbulent intensity too small for spontaneous detonation

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

Summary

MAESTRO: Low Mach number model for convection in a white dwarf

- General equation of state
- Background stratification
- Reactions and heating
- Slow evolution of base state

Numerical issues

- Communication of radial base state and Cartesian representation of the star
- Base state evolution with expansion and self-gravity
- AMR issues

What's next?

- Map final state into CASTRO to model explosion data
  - Flame models and transition to detonation
- Map CASTRO results into SEDONA (Kasen) to compute light curve