LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

UCRL-CONF-234136

Codes to Model Stars in the Three Dimensions: Virtual Obersvatories

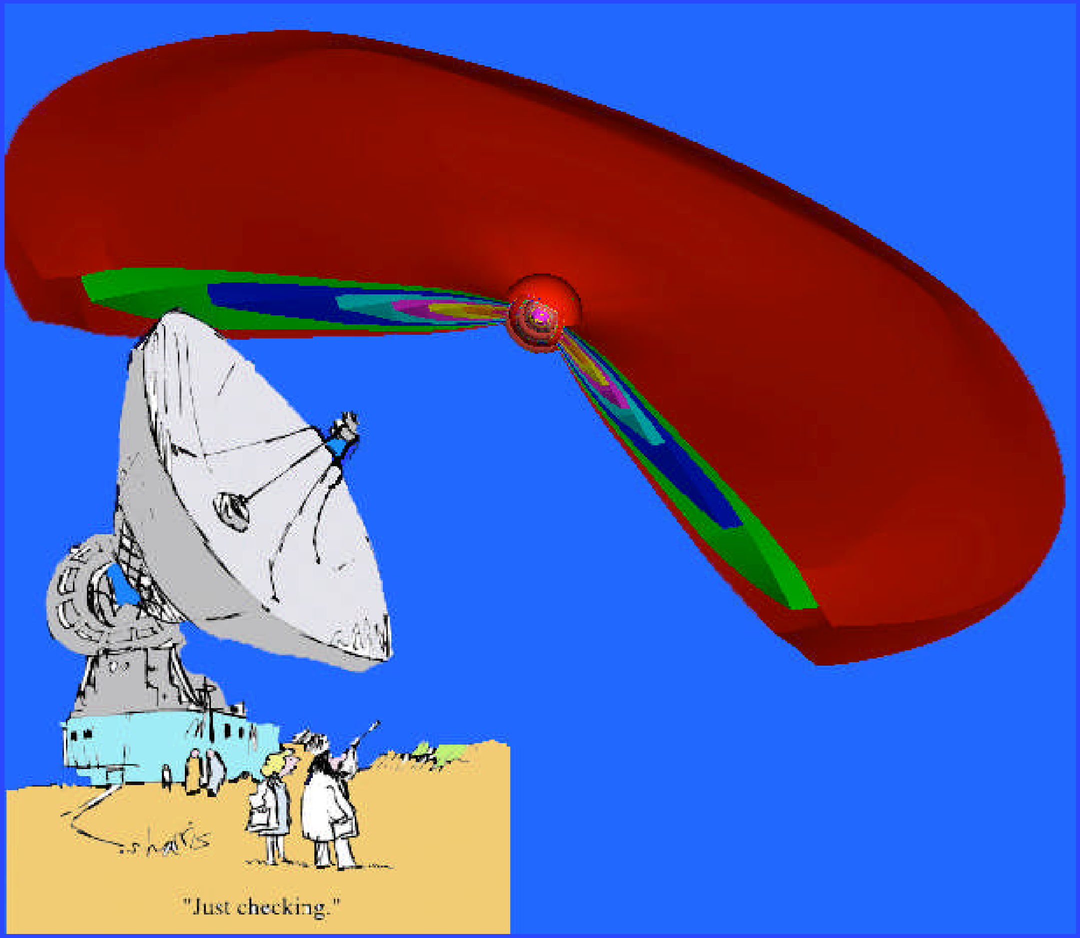
D. S. Dearborn

August 30, 2007

21st Centry Stellar Evolution
Cefalu, Italy
August 29, 2007 through September 2, 2007

Disclaimer

Codes to Model Stars in Three Dimensions:



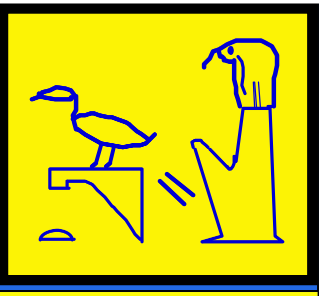
Virtual Observatories

D S P Dearborn
Lawrence Livermore National Laboratory.

UCRL-PRES-xxxxxxx
This work was performed under the auspices of the U.S. Department of Energy by the University of California,
Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

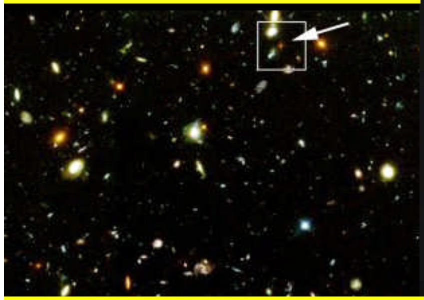
Stars Provide a Laboratory and a Metric

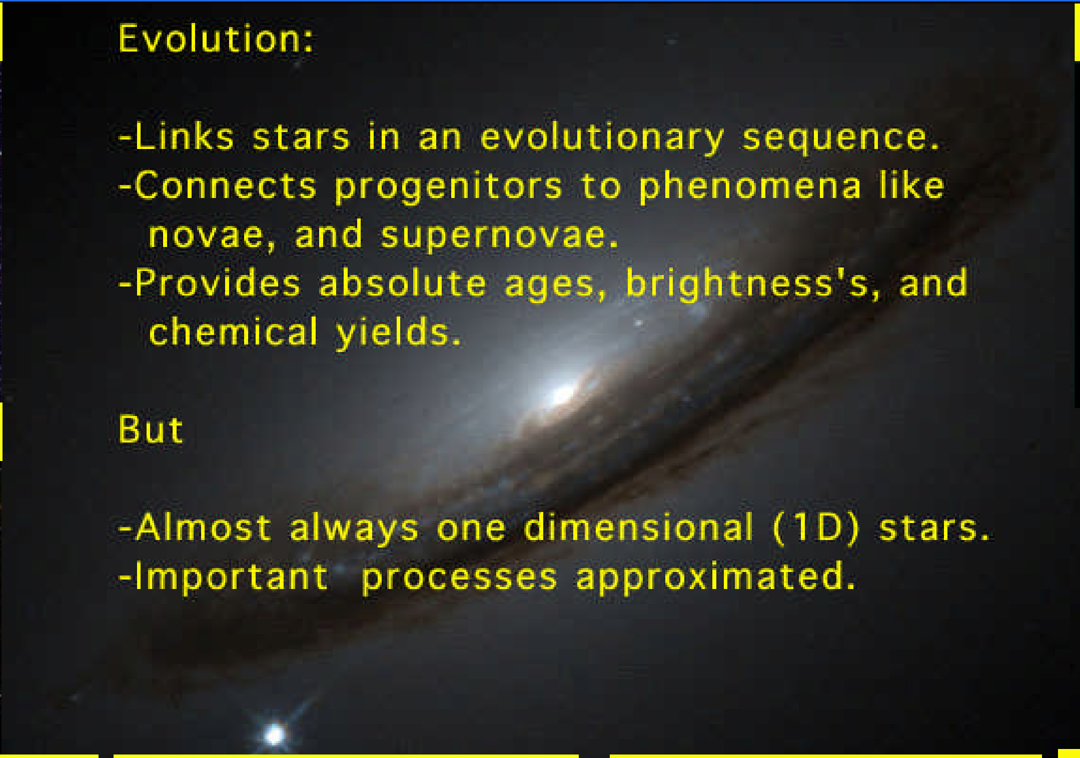
for exploration of the universe.



Age

Distance





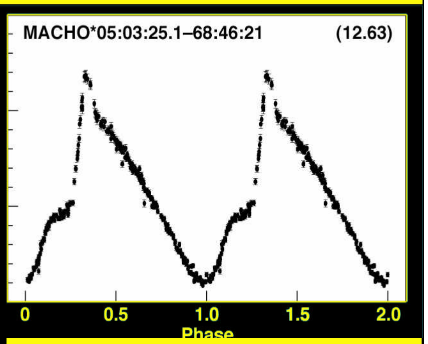
Evolution:

- -Links stars in an evolutionary sequence.
- -Connects progenitors to phenomena like novae, and supernovae.
- -Provides absolute ages, brightness's, and chemical yields.

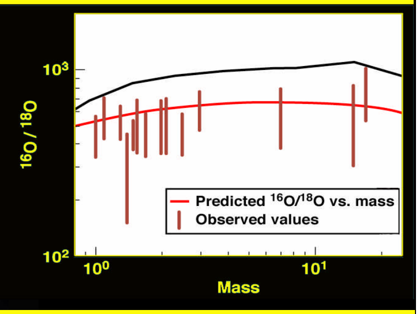
But

- -Almost always one dimensional (1D) stars.
- -Important processes approximated.

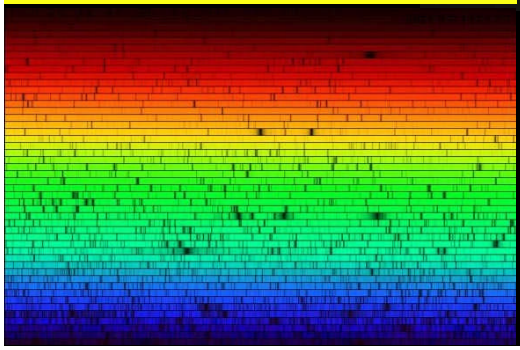
Opacities



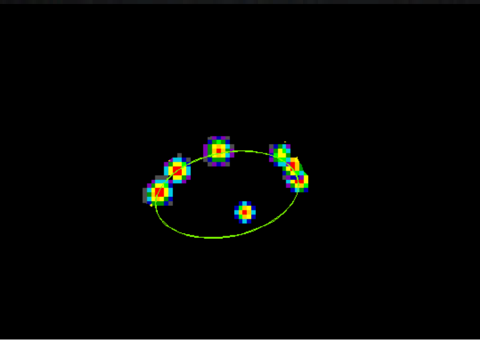
Nuclear Cross Section



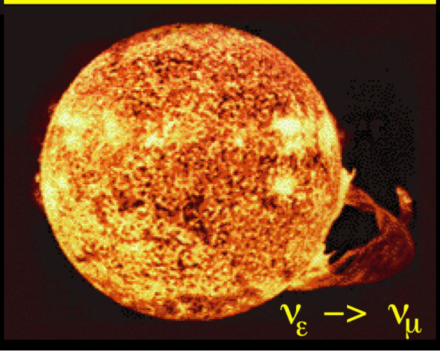
Composition



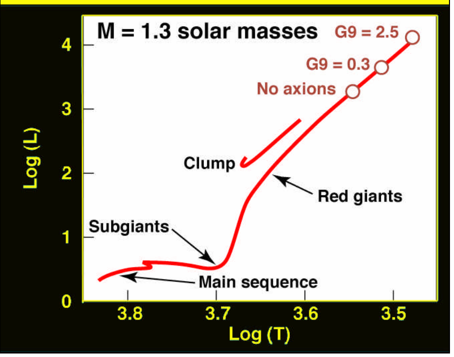
Mass



Neutrino Laboratory



Axion Properties



Evolution

The life cycle of stars.

Successes:

Links stars in an evolutionary sequence.

Connects progenitor stars to phenomena like novae, and supernovae.

Provides absolute ages, brightness's, and chemical yields.

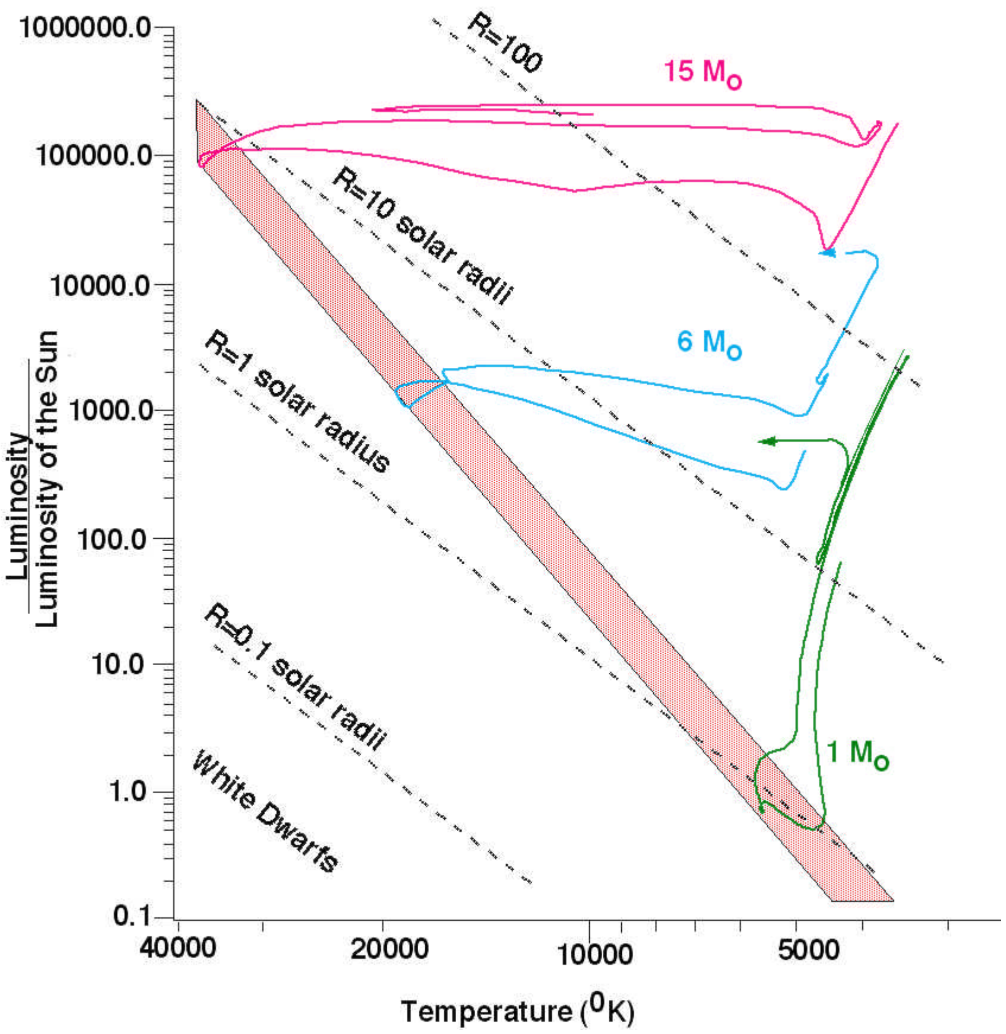
Constrains nuclear and atomic cross sections, exotic particle (axion, ν, …) masses, …..

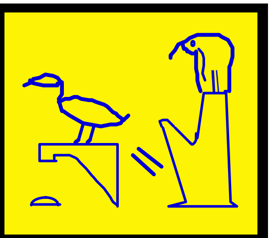
View of extreme physical states (degeneracy, neutron fluids, strong gravitational fields).

Limitations:

Almost always one dimensional (1D) stars.

Important energy transport processes that can only be approximated in 1D.





Why 3-D?
Reducing the art in the State of the Art.

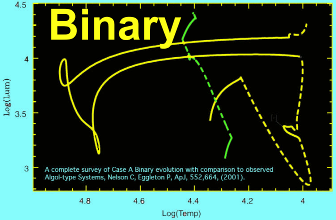
3-D Systems:

Disk Accretion

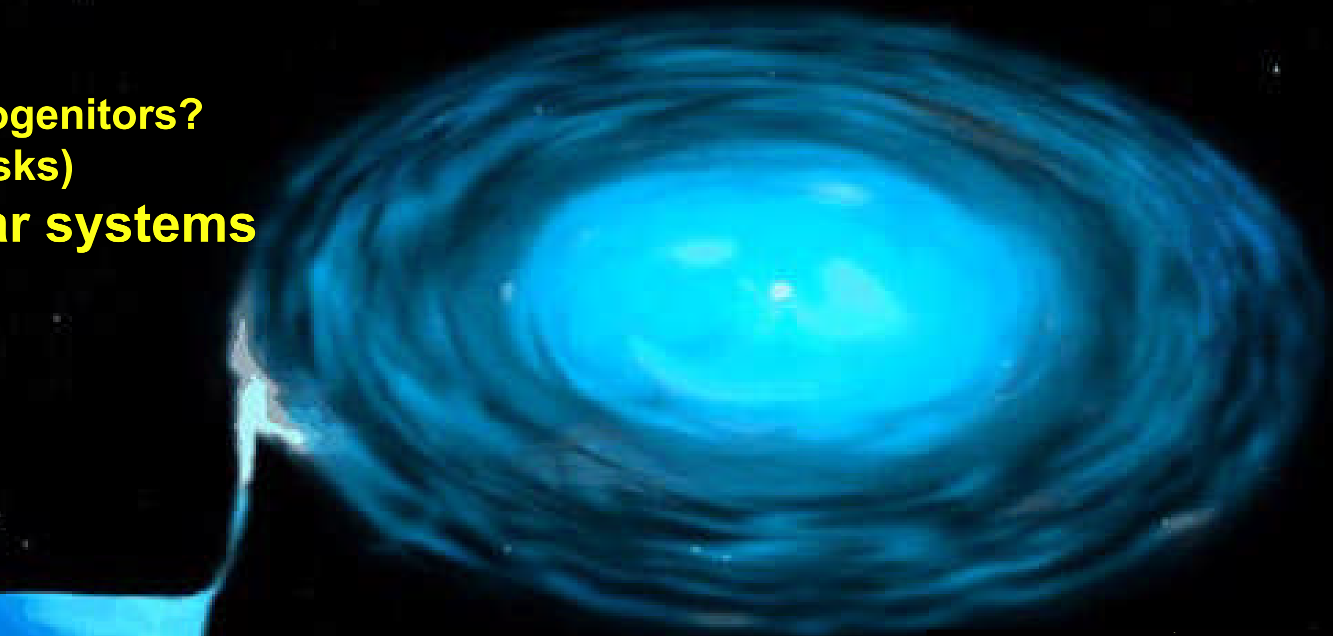
- Type 1a SN progenitors?
- Novae (with disks)

Distorted stellar systems

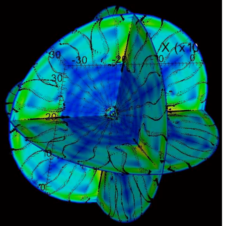
- Rotation
- Binary



A complete survey of Case A Binary evolution with comparison to observed Algol-type Systems, Nelson C, Eggleton P, ApJ, 552,664, (2001).

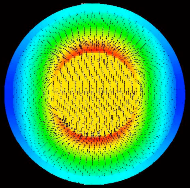


Artful 3-D processes in 1-D codes include:

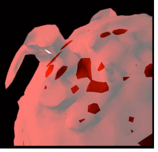


Convection:

- Overshoot
- Time dependence

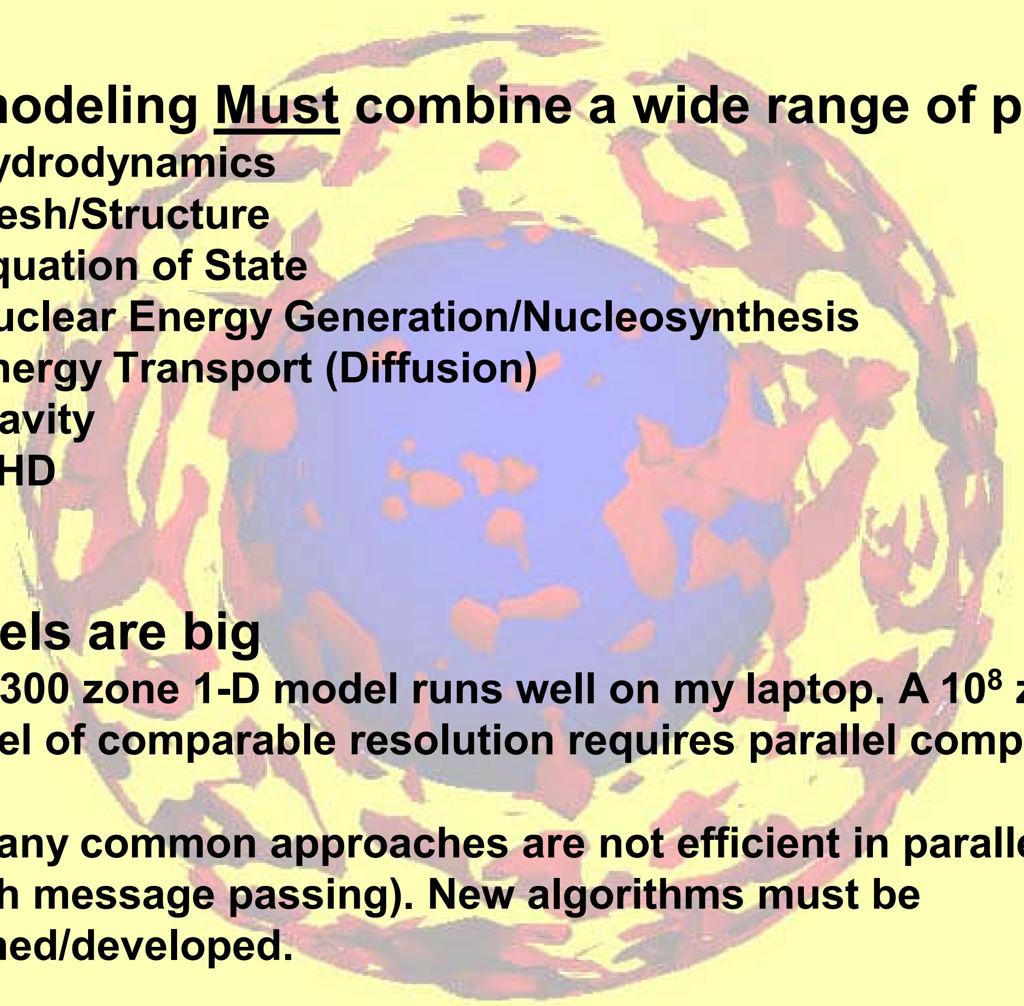


B-fields



Rotation

Building a 3-D Code
Choices.



Stellar modeling Must combine a wide range of physics:

- a) Hydrodynamics
- b) Mesh/Structure
- c) Equation of State
- d) Nuclear Energy Generation/Nucleosynthesis
- e) Energy Transport (Diffusion)
- f) Gravity
- g) MHD
- h) ?

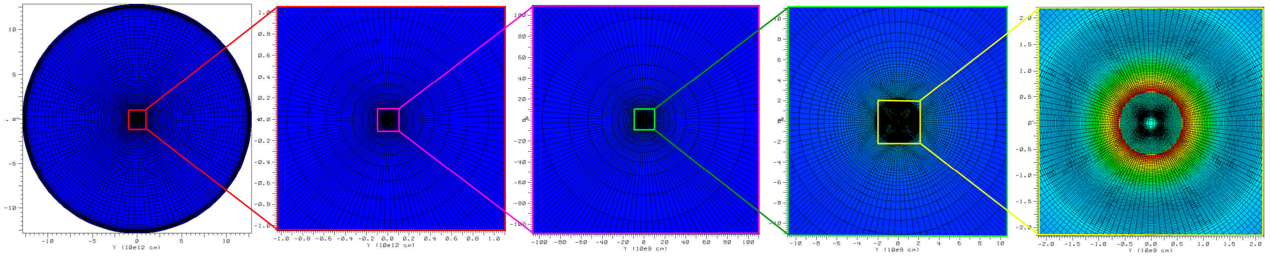
3-D models are big

a) A 300 zone 1-D model runs well on my laptop. A 10^8 zone 3-D model of comparable resolution requires parallel computing.

b) Many common approaches are not efficient in parallel (too much message passing). New algorithms must be learned/developed.

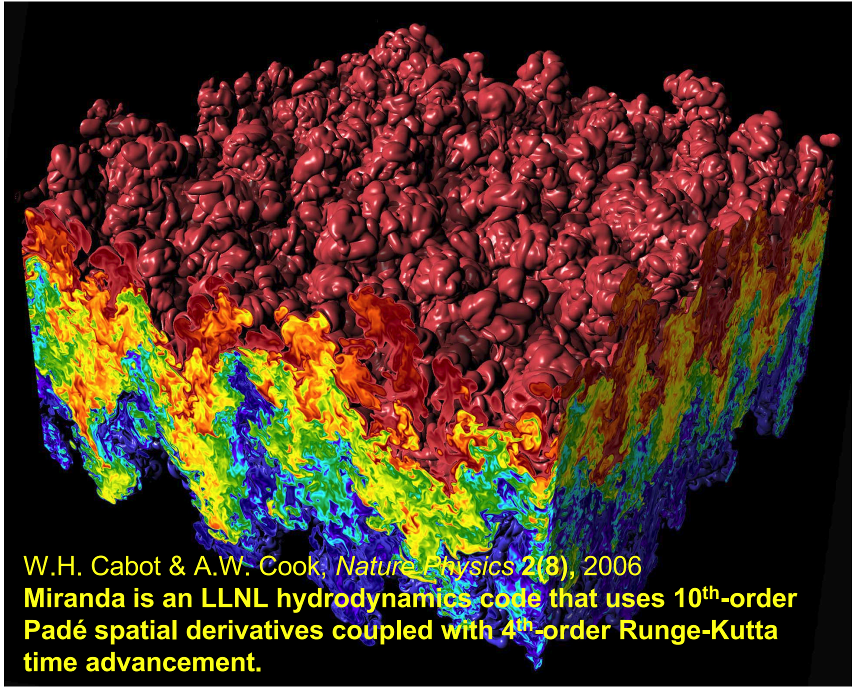
Choices
What is Modeled?

An entire star?
Reduces resolution and
increases fewer run time.



A small segment of a star

A detailed simulation on a 3072^3 grid of the asymptotic growth a Rayleigh-Taylor & Rictmyer Meshkov instability, for Type 1a flame propagation.

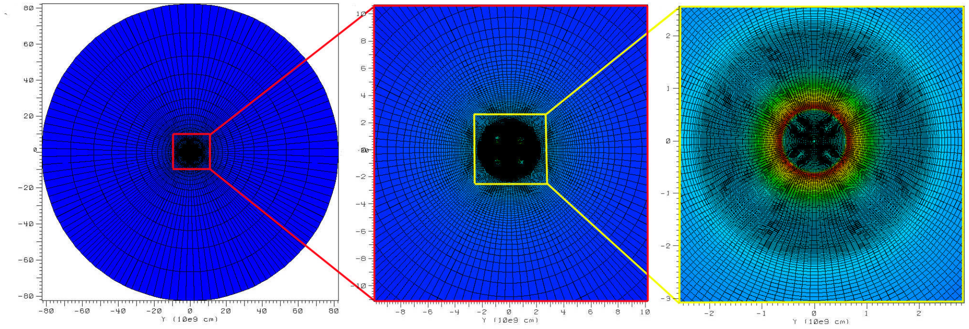


W.H. Cabot & A.W. Cook, *Nature Physics* **2(8)**, 2006

Miranda is an LLNL hydrodynamics code that uses 10th-order Padé spatial derivatives coupled with 4th-order Runge-Kutta time advancement.

A Portion of the star?
Boundary Conditions become critical.

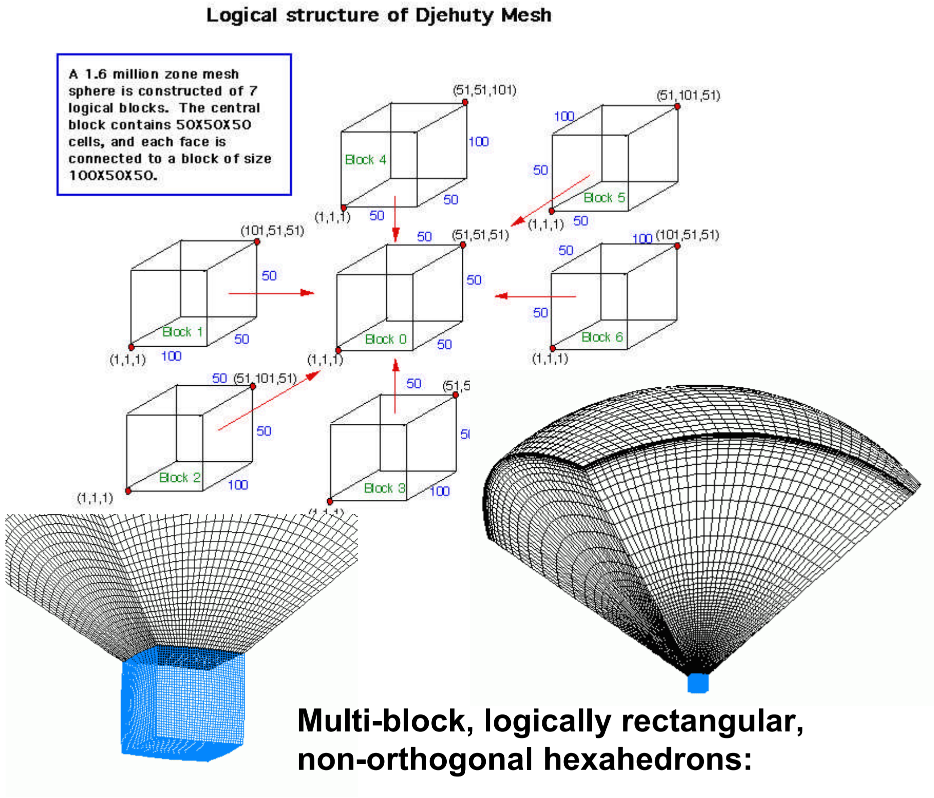
$$R_{boundary} \approx 30R_{core}$$



It depends on the question!

Choices
Mesh Geometry

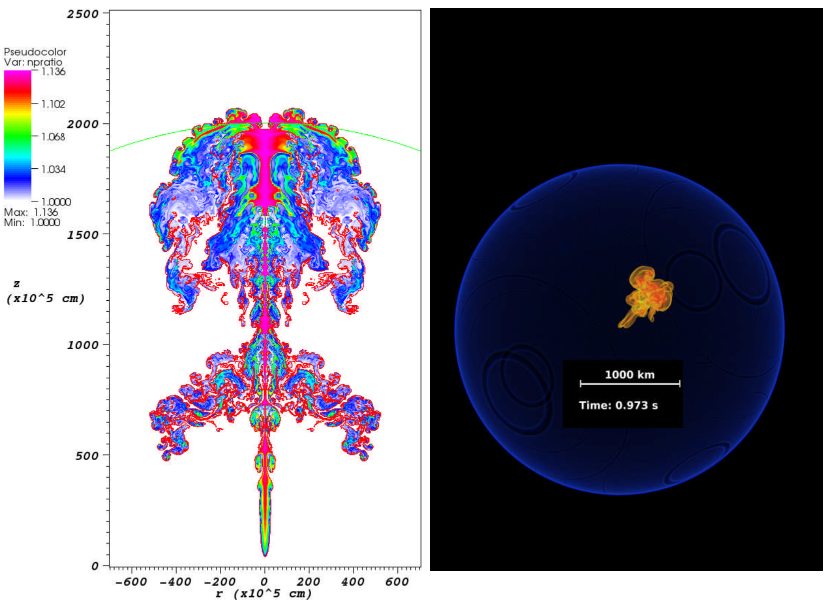
Spherical



A 1.6 million zone mesh sphere is constructed of 7 logical blocks. The central block contains 50X50X50 cells, and each face is connected to a block of size 100X50X50.

Multi-block, logically rectangular, non-orthogonal hexahedrons:

Rectangular



Three-Dimensional Simulations of the Deflagration Phase of the Gravitationally Confined Detonation Model of Type Ia Supernovae, by G C Jordan IV, R T Fisher, D M Townsley, A C Calder, C Graziani, S Asida, D Q Lamb, J W Truran (Submitted to ApJ letters).

Conformal zoning tracks curved moving interfaces with fewer zones. ALE (Arbitrary Lagrange Eulerian) eliminates mesh tangling.

Rectangular zoning easier to add physical processes like Diffusion or B fields, but diffusive when moving sharp interfaces. This was much improved by AMR (automatic mesh refinement).

Choices
Hydrodynamics

Lagrangian: ALE method with a predictor-corrector Lagrange-Remap formalism;

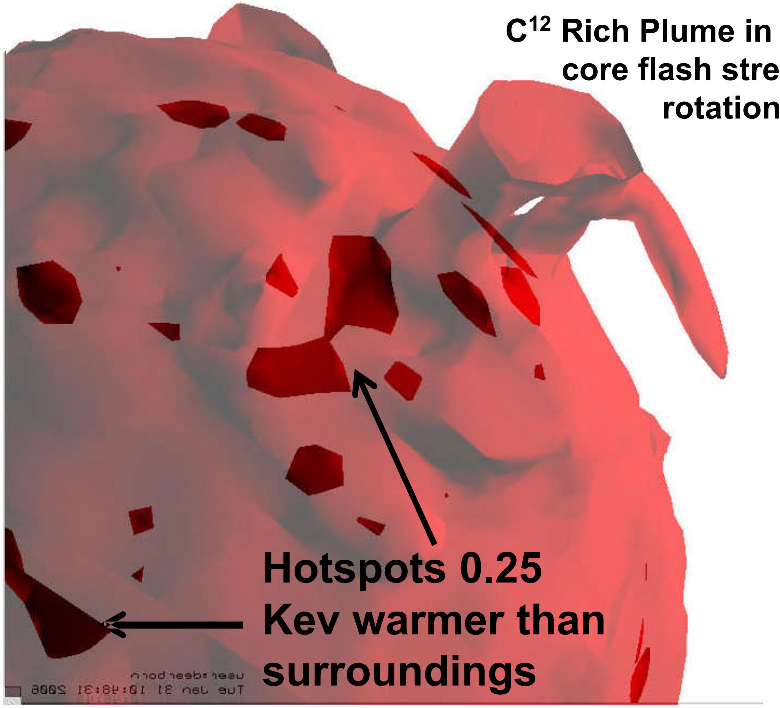
Second order accurate in time and space, but

$$\left.\begin{aligned} \dot{X}_{1/2} &= \dot{X} + \ddot{X}\,\delta t_{1/2} \\ X_{1/2} &= X + \dot{X}\,\delta t_{1/2} \end{aligned}\right\}$$

Reevaluate force and source terms.

$$\left\{\begin{aligned} \dot{X} &= \dot{X}_{1/2} + \ddot{X}\,\delta t \\ X &= X + 0.5\left(\dot{X}_{1/2} + \dot{X}\right)\delta t \end{aligned}\right.$$

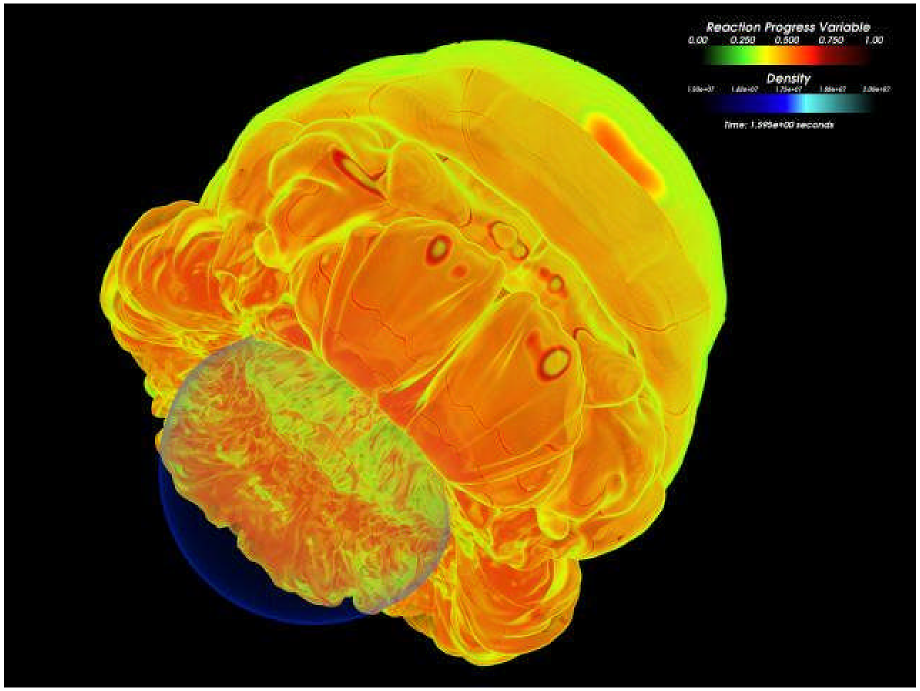
User is responsible for assigning adequate mesh.



C^{12} Rich Plume in a helium core flash stretched by rotational shear.

Hotspots 0.25 Kev warmer than surroundings

Eulerian: AMR with piecewise parabolic method (PPM)



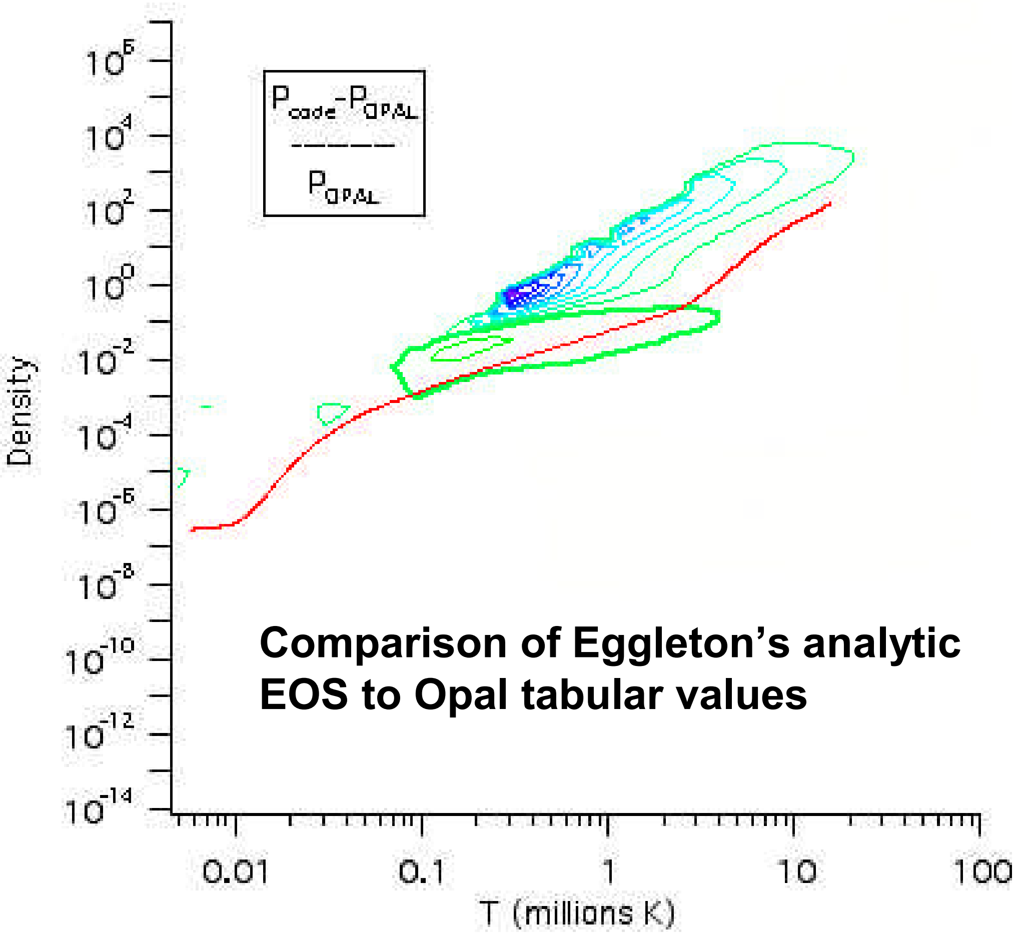
Three-Dimensional Simulations of the Deflagration Phase of the Gravitationally Confined Detonation Model of Type Ia Supernovae, by G C Jordan IV, R T Fisher, D M Townsley, A C Calder, C Graziani, S Asida, D Q Lamb, J W Truran (Submitted to ApJ letters).

Mesh automatically resolves defined structures.
(Dynamic Load Balancing, Zone removal)

Choices

Physics- EOS

For purely hydrodynamic problems, a complex Equation of State (EOS) can be a significant time cost.



Comparison of Eggleton's analytic EOS to Opal tabular values

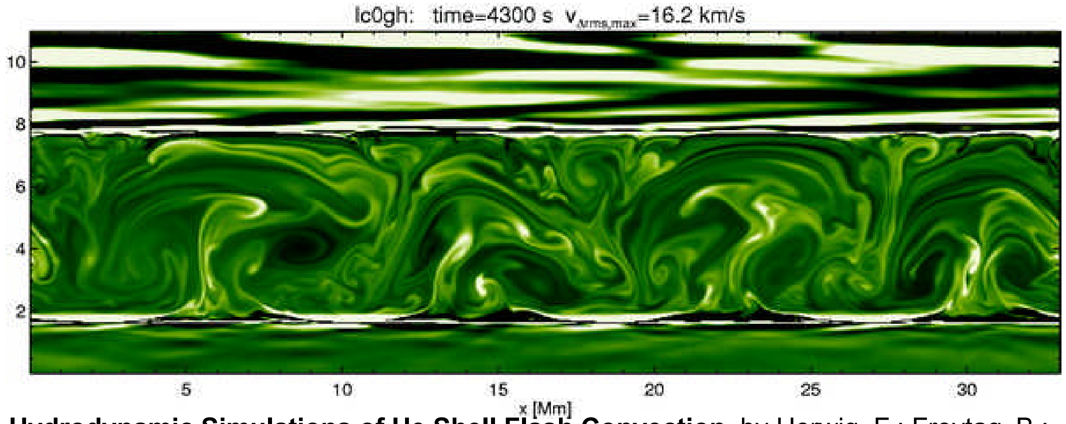
Gamma laws: very fast, but miss important physics.

Opal Tables: excellent for sun, but miss T-ρ regions for many stars.

Analytic EOS: Continuous derivatives, and better than 1% accuracy for the the whole evolution of stars between 0.7 to 50.0 solar masses. Models as low as 0.5 solar masses can be computed, with differences of only about 2% in their envelopes.

Choices
Physics: Gravity

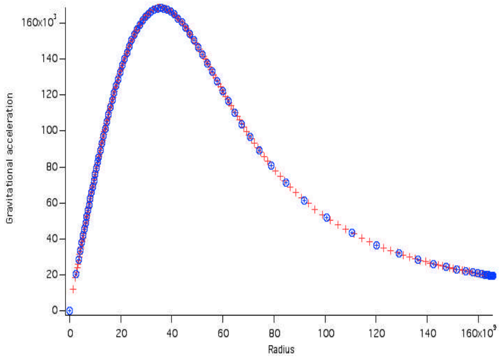
Constant

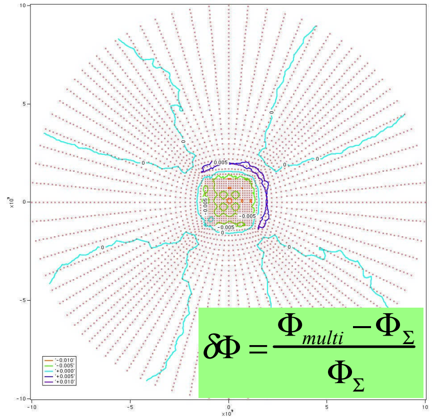


Hydrodynamic Simulations of He Shell Flash Convection, by Herwig, F.; Freytag, B.; Hueckstaedt, R. M.; Timmes, F. X., 2006 ApJ, Vol. 642, Issue 2, pp. 1057-1074 (Fig 8)

Gravity

Spherical **Multipole/Poisson Solver**





$$\delta\Phi = \frac{\Phi_{multi} - \Phi_{\Sigma}}{\Phi_{\Sigma}}$$

Constant:fast, but

the gravity here

should be 1/4th of

the gravity here.

Spherical: (integrate a mass radius relation) Fast and accurate for convection studies. Good for centrally condensed bodies (even a low mass disk system).

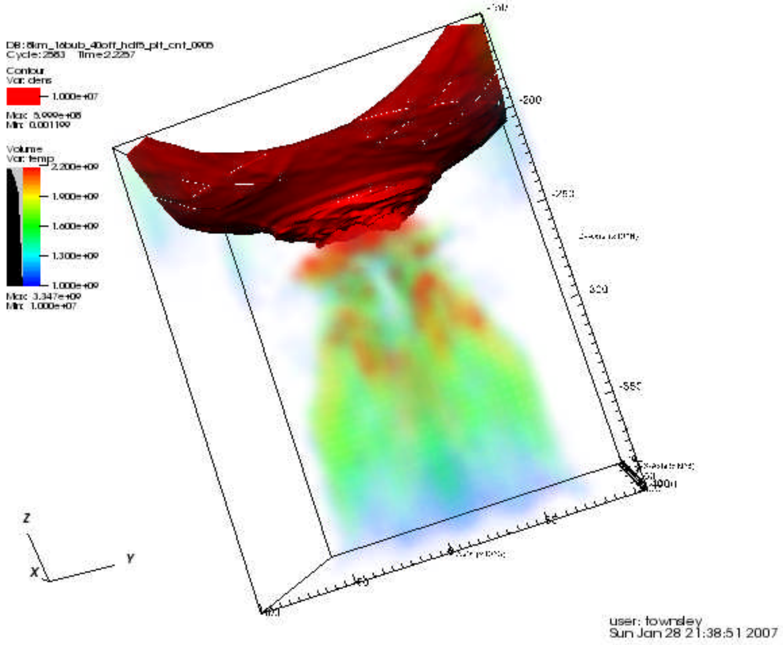
Multipole/Poisson: Essential for complex distributed systems (self gravitating disks, star forming regions, ...)

What Level of Approximation is acceptable?

Choices
Physics: Energy Production

Need 200-300 species to properly calculate the burning in a Type Ia supernovae, and a comparable number to do the full S-process in AGB stars.

Too much in 3D, so <u>must decide what features are important to capture</u>. Then develop a limited network to capture those features.



Three-Dimensional Simulations of the Deflagration Phase of the Gravitationally Confined Detonation Model of Type Ia Supernovae, by G C Jordan IV, R T Fisher, D M Townsley, A C Calder, C Graziani, S Asida, D Q Lamb, J W Truran (Submitted to ApJ letters).

Volume energy source matched to 1-D calculations,

or Nuclear Reaction Networks:

Small: ^{1}H, ^{3}He, ^{4}He, ^{12}C, ^{14}N, ^{16}O

More advanced stage: ^{1}H, ^{3}He, ^{4}He, ^{12}C, ^{13}C, ^{13}N, ^{14}N, ^{15}N, ^{15}O, ^{16}O, ^{17}O, ^{18}O, ^{17}F, ^{18}F, ^{19}F, ^{20}Ne, ^{22}Ne, ^{24}Mg, ^{28}Si, ^{32}S, ^{56}Ni

NSE following Timmes, Hoffman, and Woosley, 2000, ApJ, 129, 377-398

$$\frac{dY(^{4}He)}{dt} = -7Y(^{40}Ca)Y(^{4}He)\lambda_{\alpha\gamma}(^{40}Ca) + 7Y(^{44}Ti)\lambda_{\alpha\gamma}(^{44}Ti)$$

$$\frac{dY(^{28}Si)}{dt} = -Y(^{40}Ca)Y(^{4}He)\lambda_{\alpha\gamma}(^{40}Ca) + Y(^{44}Ti)\lambda_{\alpha\gamma}(^{44}Ti)$$

$$\frac{dY(^{56}Ni)}{dt} = +Y(^{40}Ca)Y(^{4}He)\lambda_{\alpha\gamma}(^{40}Ca) - Y(^{44}Ti)\lambda_{\alpha\gamma}(^{44}Ti)$$

Choices

Non-hydrodynamic energy transport (Diffusion IMC,?)

Flux Limited, 2T Diffusion (T_{rad} and T_{mat}), with Opal and Alexander Opacities, Hubbard-Lampe conduction.

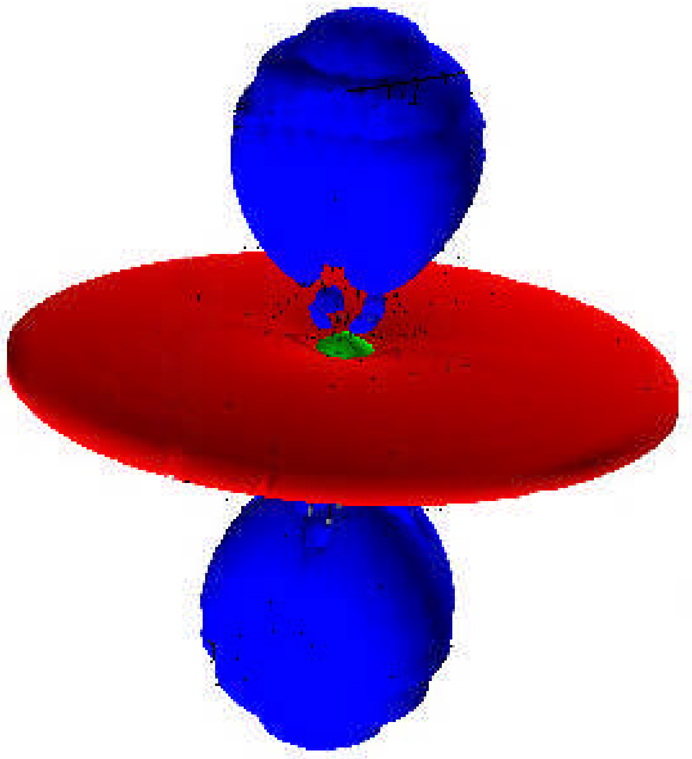
$$\rho C_v \frac{\partial T}{\partial t} = \nabla(D\nabla T) + \sigma\kappa_p \rho c(\varphi - T^4) + E_e$$

$$\sigma \frac{\partial \varphi}{\partial t} = \sigma\nabla(\kappa_r \nabla\phi) + \sigma\kappa_p \rho c(T^4 - \varphi) + E_\phi$$

Diffusion: requires efficient iterative solvers to operate in parallel computing environments.

Monte Carlo: easily implemented, and accurate in low optical depth regions. Challenging when mixed thin/thick regions (getting diffusion limit).

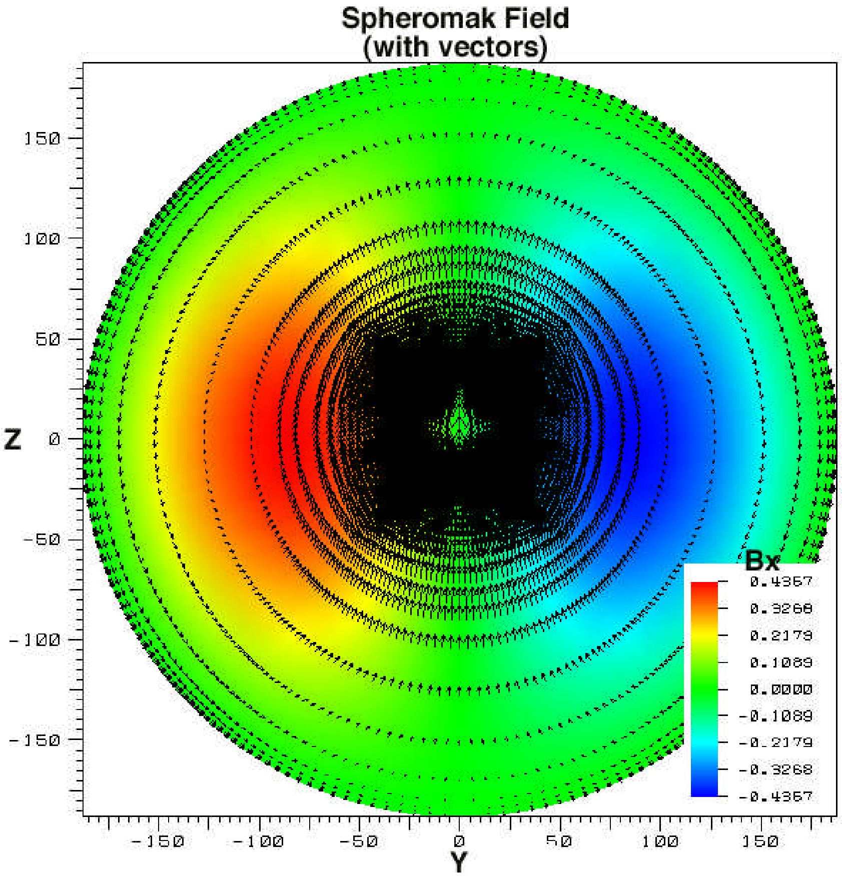
In start-up of a disk model, a low density region grows where $T_{mat} \neq T_{rad}$.



Choice

When can you stop?

To Add New Physics or To Study Astrophysics


Spheromak Field
(with vectors)

Can impose various initial fields,

Added *J*X*B* to the Navier-Stokes equation

Included the induction equation in the Lagrangian form:

$$\frac{d}{dt}B\Big/\rho = \frac{1}{m}\int_s dS\cdot Bv + \frac{1}{m\mu_o}\int_s \frac{1}{\sigma}dS\times(\nabla\times B)$$

Have not developed a field conserving advection routine - more work.

Must find a balance between code development and astrophysics.

No Choice
Collaboration

Code must be:

Portable - machines evolve faster than codes.

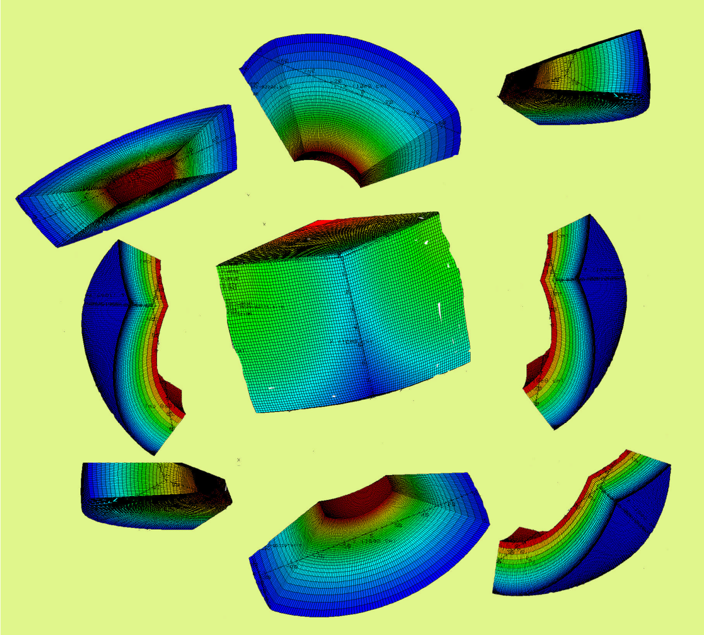
- **In past 7 years we have had to change machined 5 times**
- **Must test compilers, port libraries. (Flash-Excellent record)**

Efficient in parallel environment

- **Easy for non-interacting regions**
- **Not too bad for nearest neighbor processes**
- **Challenging for implicit- algorithm development**

<u>Requires collaboration</u>

- **Computer Scientists**
- **Applied mathematicians**
- **Astrophysicists**

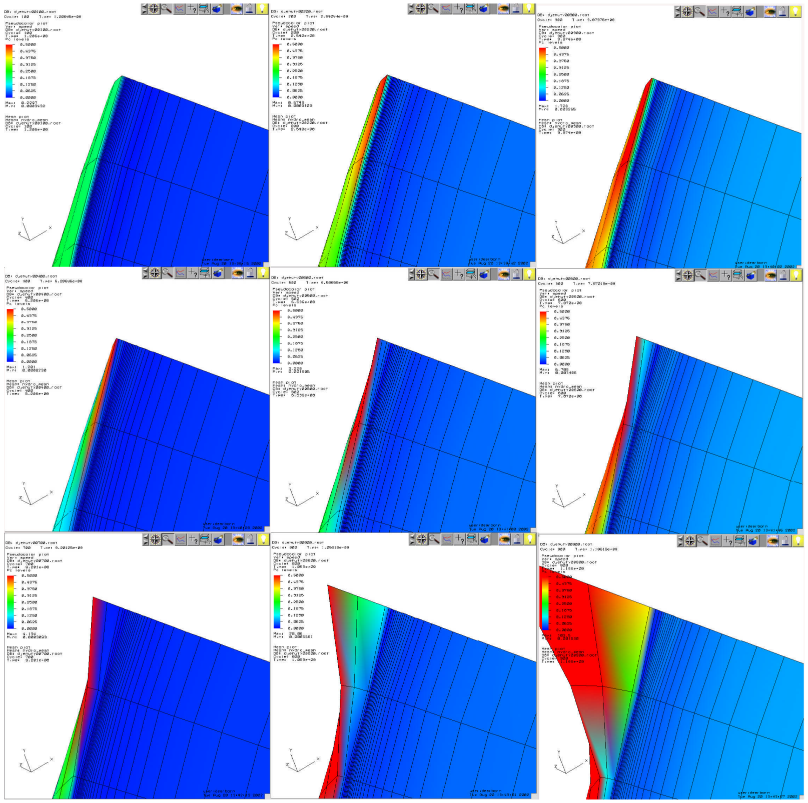


Djehuty Group includes:
David Dearborn (V div - Astrophysicist), **Peter Eggleton** (V div - Astrophysicist), **Don Dossa** (CASC - code architect), **Bob Palasek** (CAR, computer scientist), **Grant Bazan** (B div - code physicist), **Omar Hurricane** (A div - Magnetic fields), **Rob Cavallo** (B div - Physicist), **Kem Cook** (V div - astrophysicist),

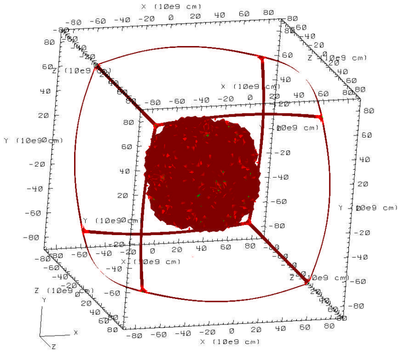
There are always Bugs:

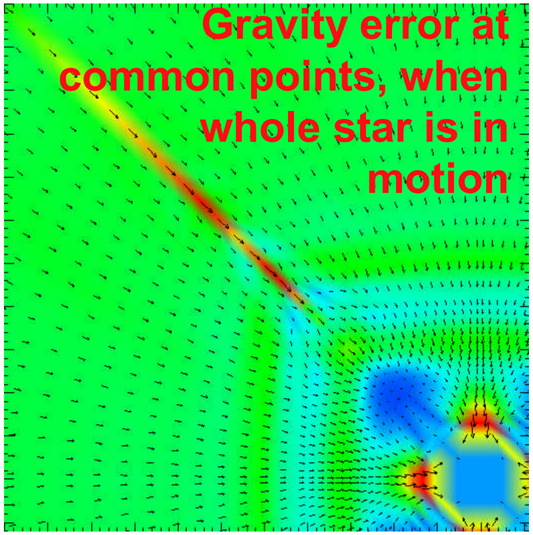
solved and unsolved.

Surface instability from inadequate boundary condition.



Artificial hydrodynamics at limited connectivity points in stable regions.

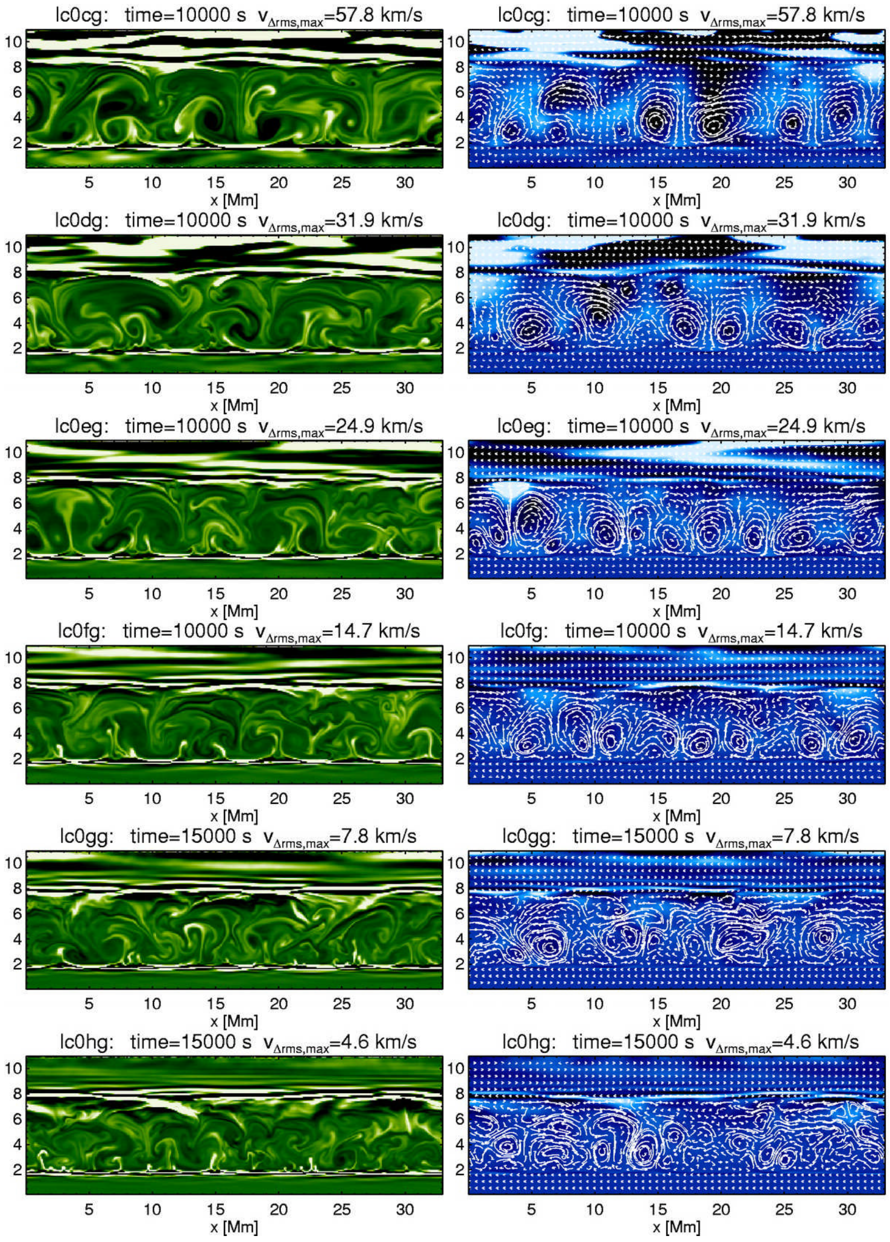




Gravity error at common points, when whole star is in motion

Bug Problem True of Most Codes (not just 3-D)

An Example
of choices.



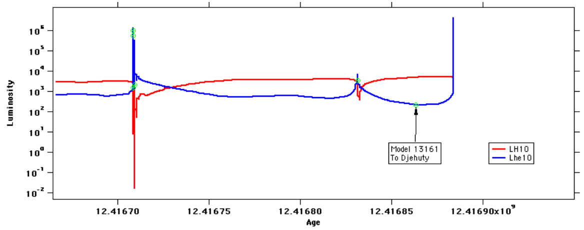
Hydrodynamic Simulations of He Shell Flash Convection,
by Herwig, F.; Freytag, B.; Hueckstaedt, R. M.; Timmes, F. X., 2006 ApJ, Vol. 642, Issue 2, pp. 1057-1074 (Fig 20)

Used Rage Code at LANL

- **2-D and 3-D simulations**
- **Plane parallel**
- **constant gravity**
- **Gamma Law EOS**
- **No diffusion/radiation transport**
- **Volume energy source**

Good initial analysis of G mode oscillations developed above the convective region.

Michelle Dolan, a Notre Dame graduate student is starting work on type of model.

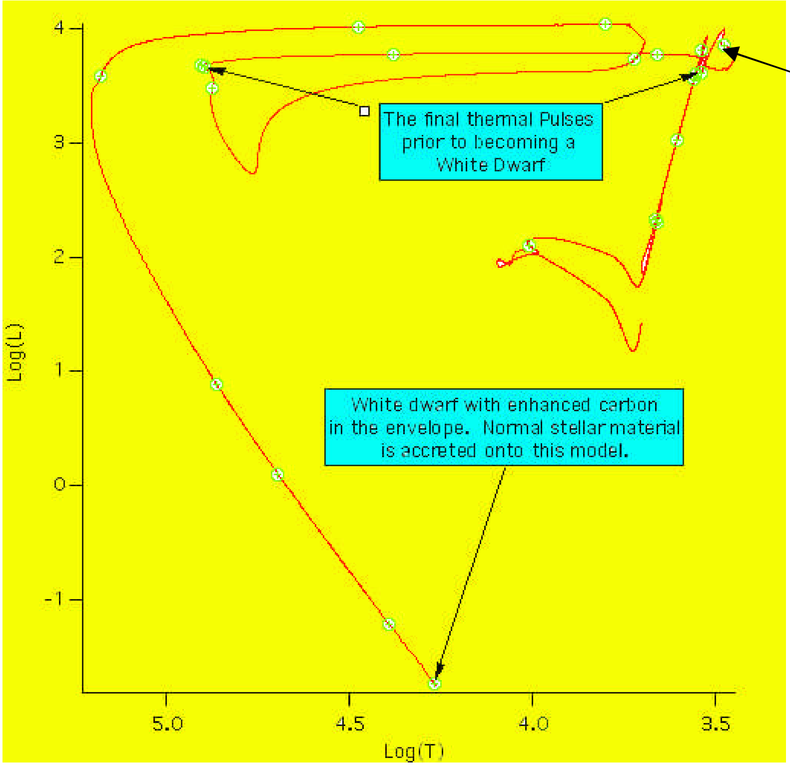


Initial Models

Not a problem for spherical stars.

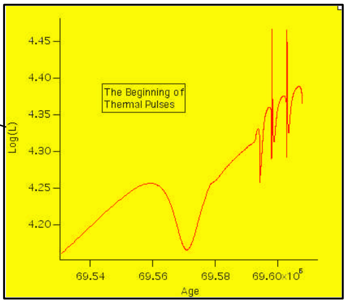
We generate 3-D spherical models from the output of a standard one dimensional stellar evolution code.

Evolution of a 4 solar mass star

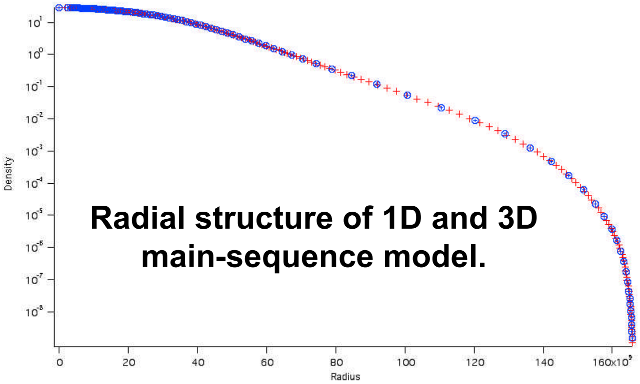


The final thermal Pulses prior to becoming a White Dwarf

White dwarf with enhanced carbon in the envelope. Normal stellar material is accreted onto this model.



The Beginning of Thermal Pulses



Radial structure of 1D and 3D main-sequence model.

-Any evolutionary stage.

-Djehuty uses the radial structure from 1D.

-1-D code:

Uses the same physics packages.

Can re-map to a 1D model with improved radial mass matching.

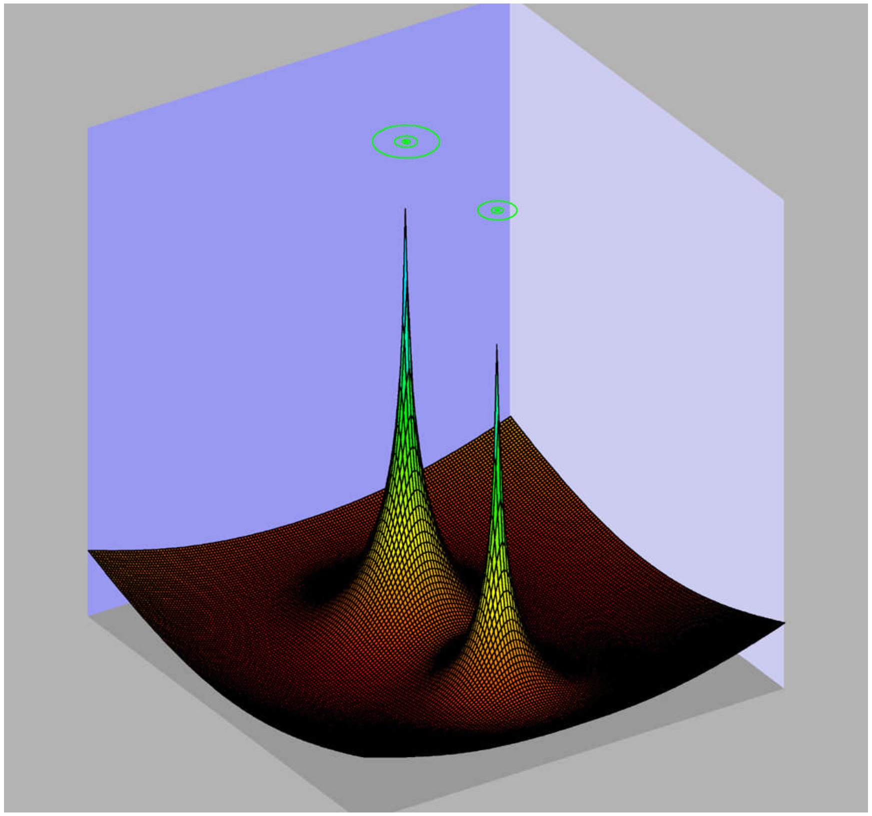
-Can read Arnett's models, will soon read Lattanzio's models.

What about Non-Spherical systems?

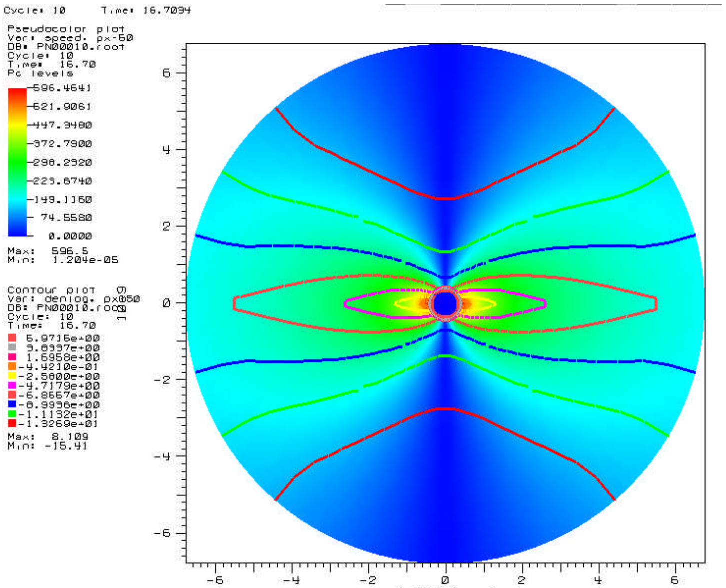
Pre-Nova/Supernova Disk Models

Good initial 3-D models (where none exist) are nontrivial.

Gravitational Potential of a 1.2 $M_\odot$ star orbiting with a 0.6 $M_\odot$ star



0.6 $M_\odot$ Non-Rotating White Dwarf
+
Alpha disk with keplerian rotation
+
Orbits system center of mass with a point mass.



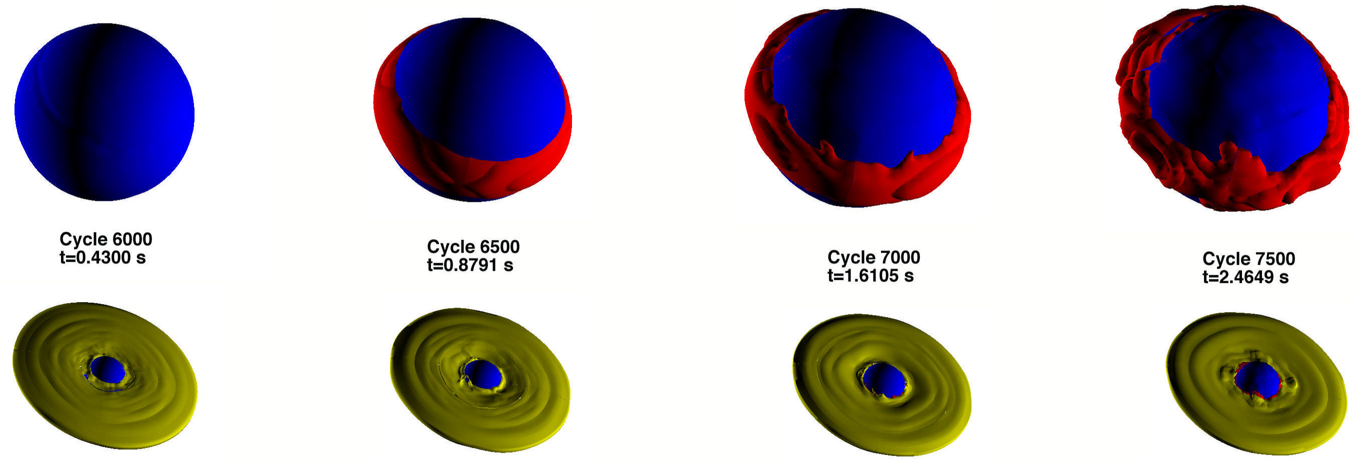
A color plot of speed with superimposed density contours.

Simply adding components from different models results in arbitrary discontinuities.

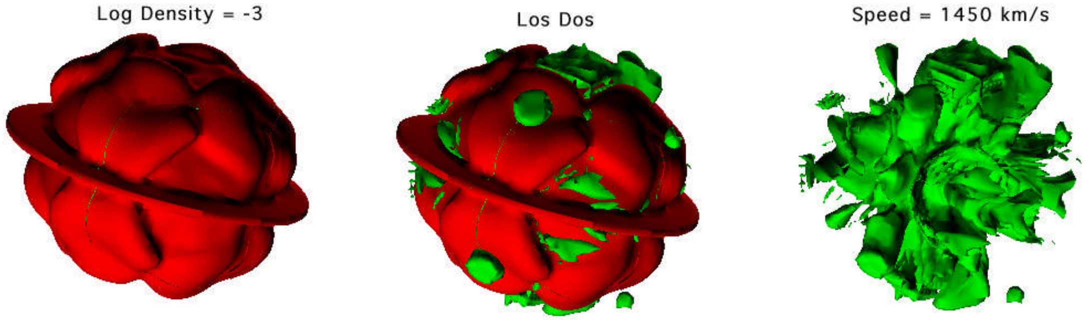
Arbitrary discontinuities - Arbitrary Results
Pre-Novae disk models

The arbitrary velocity discontinuity at the interface between the non-rotating White dwarf and the Keplerian disk led to hydrogen burning.

Hydrogen-Carbon mixing at the base of the disk leads to an erruption that peaks at 10^{12}Solar luminosities, 1.5 seconds into the calculation.



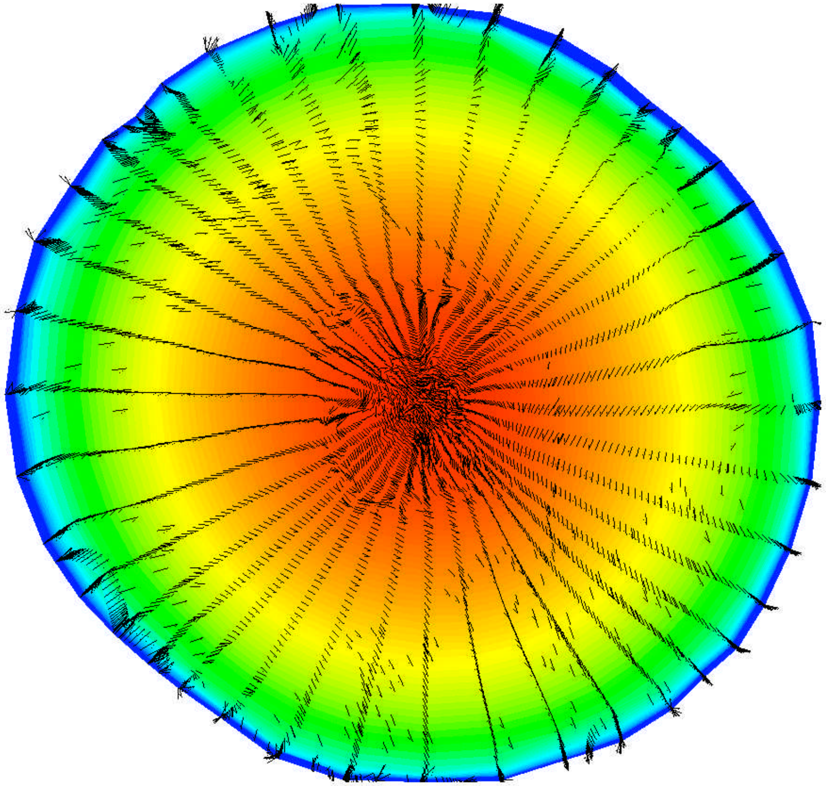
The Hydrogen burning region expands with velocities near 4000 km/s, disrupting inner disk.



Nova Looking, but not a nova

Too far from Spherical

Star in Binary Potential



QuickTime™ and a
Video decompressor
are needed to see this picture.

A quarter orbit before part of the star sloshes over the equipotential surface (better than the 3 hour attempt)

Convection

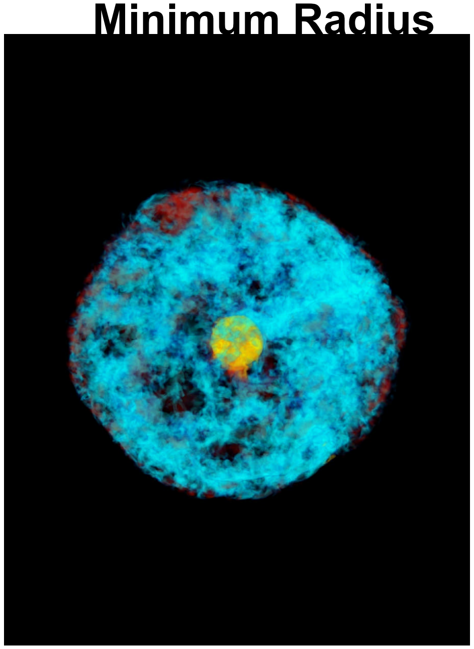
Red Giant Envelopes

3-D simulation of a red giant star by Porter, Anderson, and Woodward, University of Minnesota's Laboratory for Computational Science & Engineering.

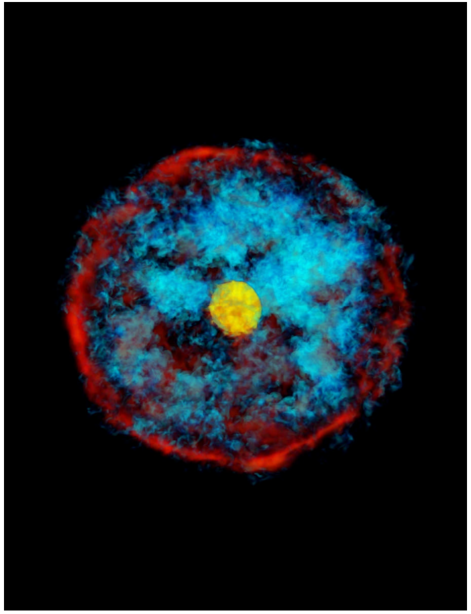
The deep convective envelope was dominated by a dipolar convection pattern.

They note hard to see how a mixing length comparable to a single pressure scale height in this envelope could characterize this global convection in any useful way.

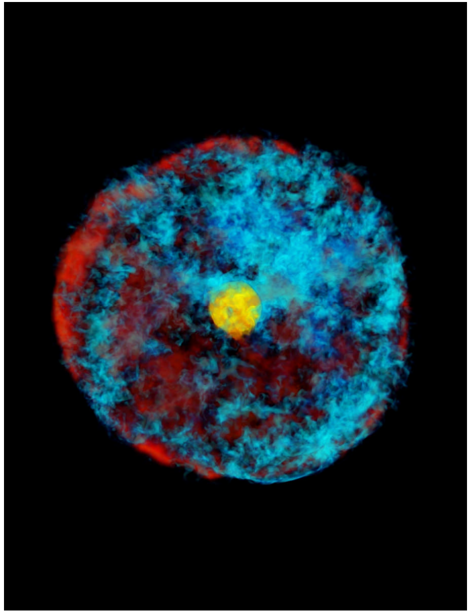
Minimum Radius



Middle Radius



Maximum Radius

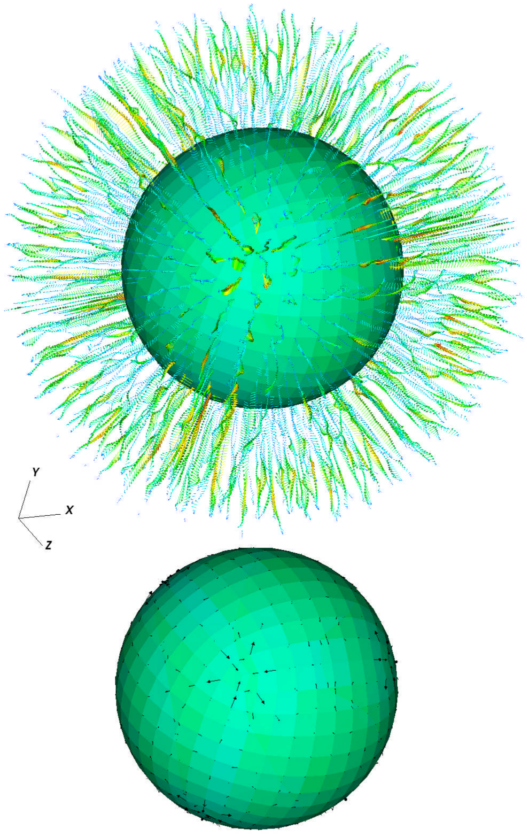


Flow pattern is most easily appreciated by viewing movie: http://www.lcse.umn.edu/research/RedGiant/

Convection
Red Dwarf Envelopes

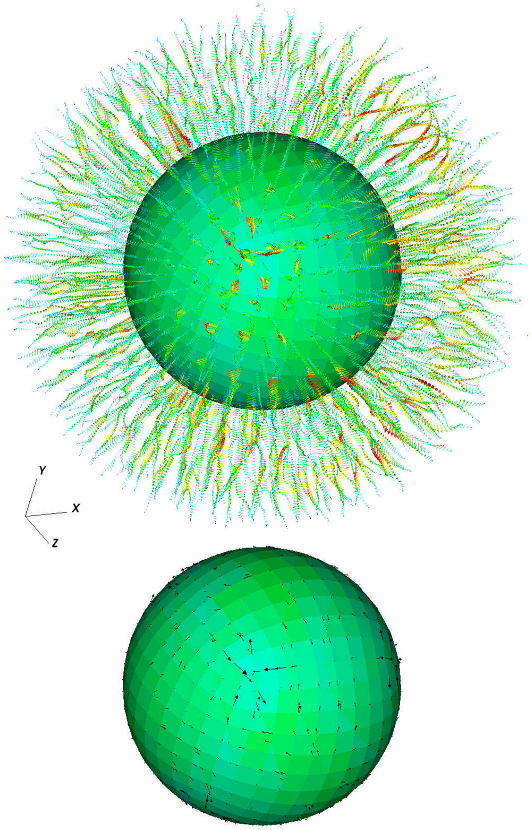
Initial motion shows an octapole (mesh related) pattern.

8.25 Hours
Into Calculation



QuickTime™ and a Video decompressor are needed to see this picture.

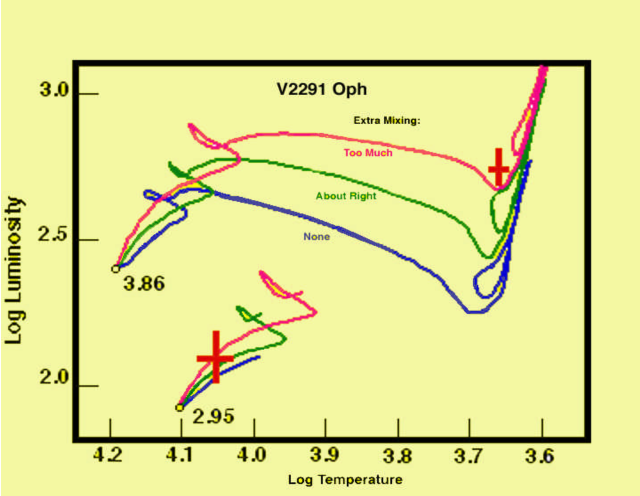
22.8 Hours
Into Calculation



That pattern is beginning to break up.

Convection and
Main Sequence Overshoot

Observational data requires larger convective cores!

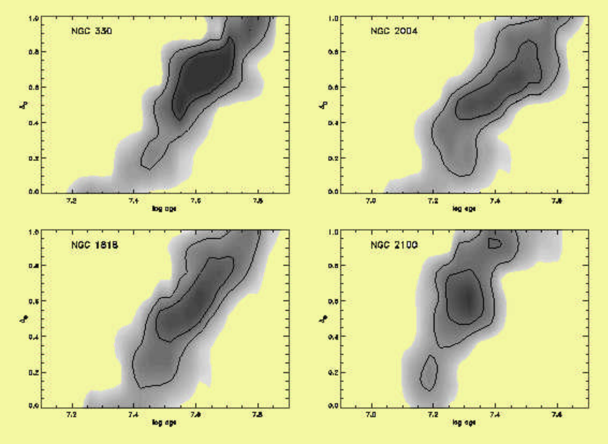


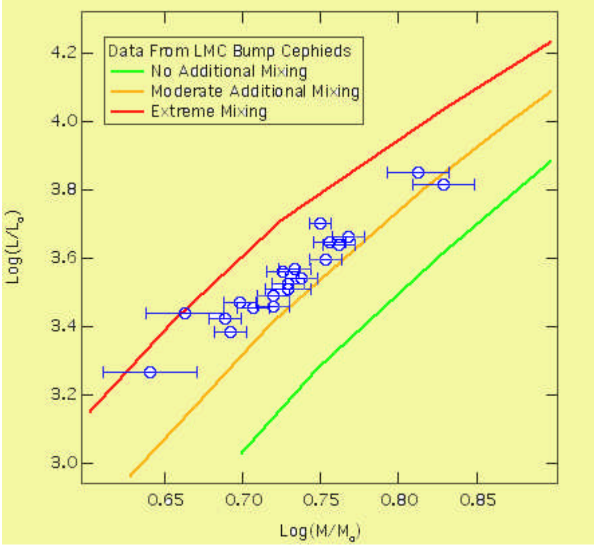
Binary Star Evolution

Iwamoto, N, Saio, H., 1999, ApJ, <u>521</u>, pp. 297-301

Main Sequence turn-off in clusters

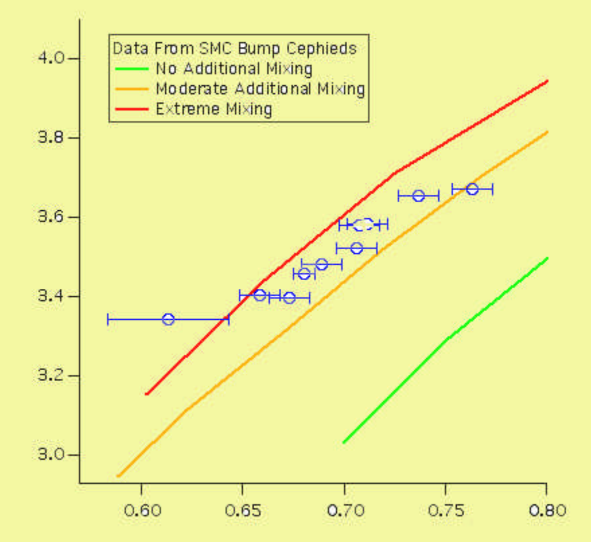
Keller, S C., E. K. Brebel, G. J. Miller, K. M. Yoss UBVI and H (alpha particle) Photometry of the h & Persei Cluster Astronomical Journal





Bump Cepheids in the LLNL Macho Data set.

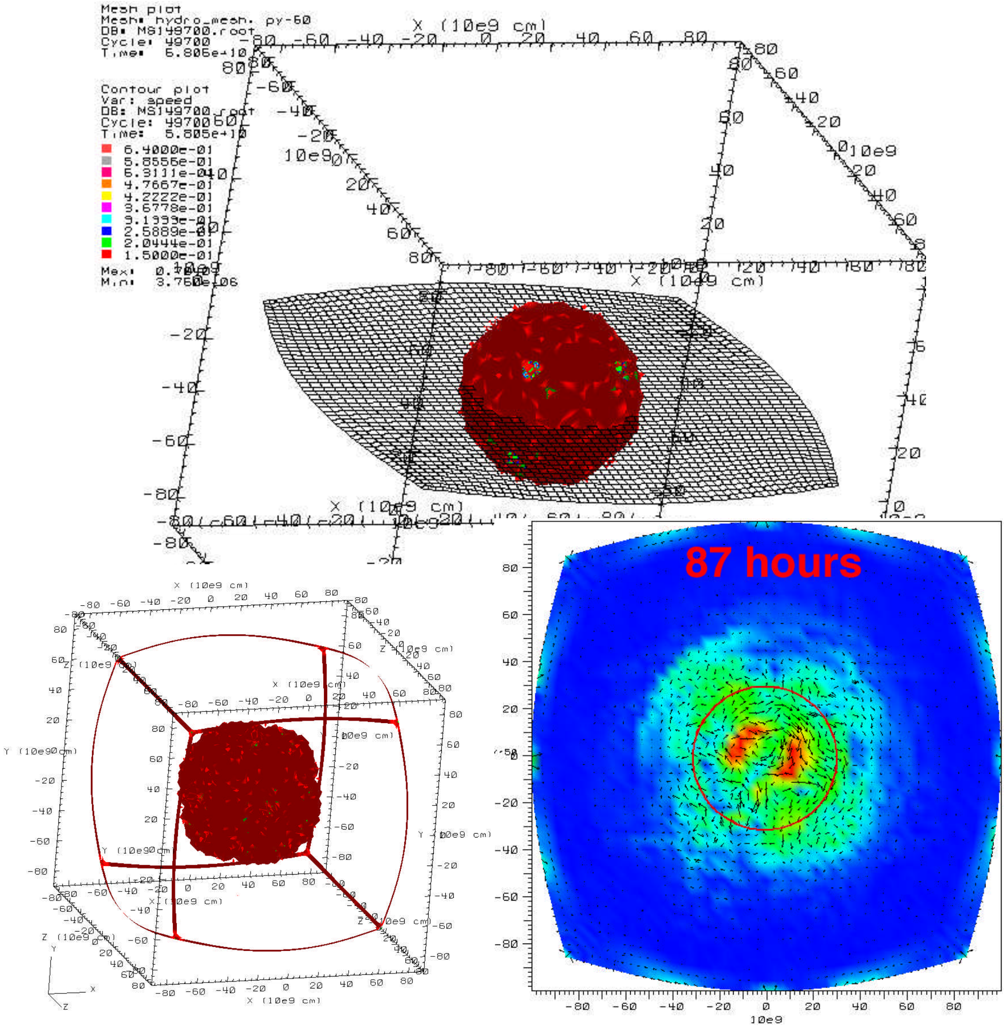
Keller, S C, P. R. Wood:Large Magellanic Cloud Bump Cepheids: Probing the Stellar Mass-Luminosity Relation UCRL-JC-148958 Astronomical Journal 2002



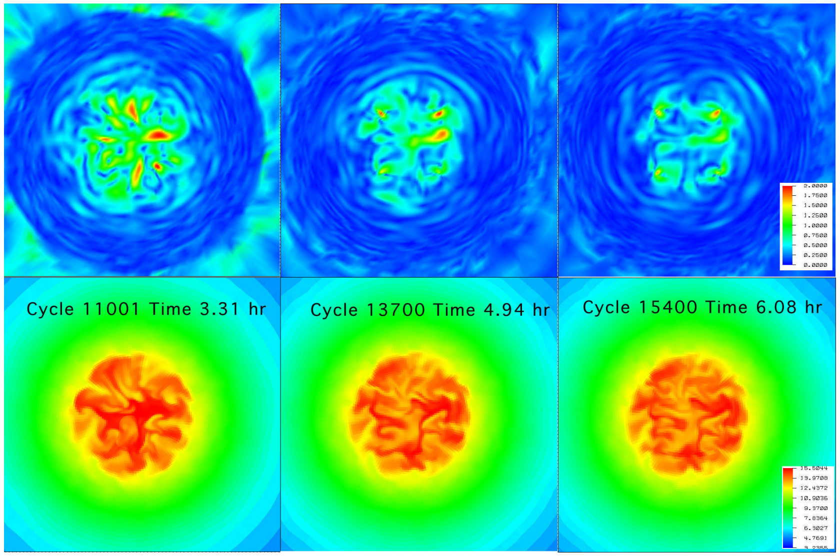
Overshoot
continued.

Continuing work by P P Eggleton studying the core of a 4 Mo Star

Static Start: convective region appears ≈ 30% larger than in the 1D model (in mass).



Seeded Convective Motion (avoid the start-up pulse)

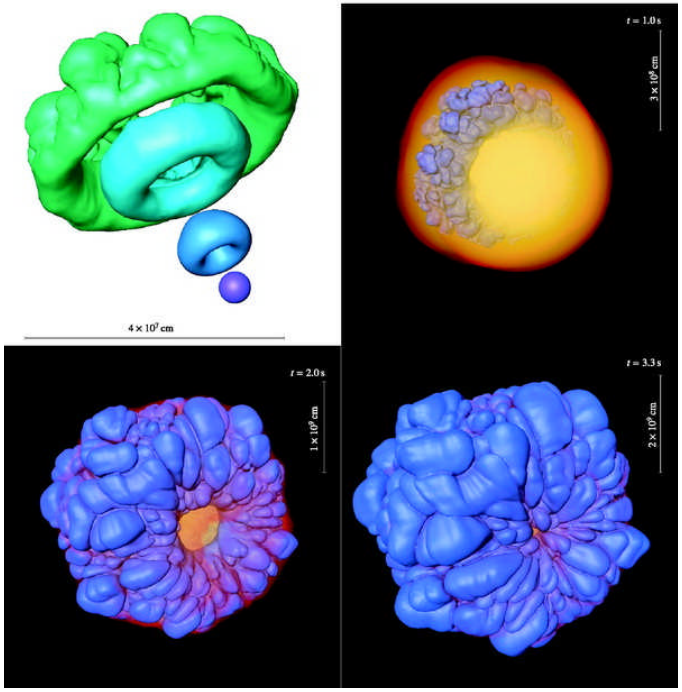


No Mixing Length

Additional Events with Energy > 10^{28} Megatons

Off-Center Ignition in Type Ia Supernovae. Initial Evolution and Implications for Delayed Detonation,

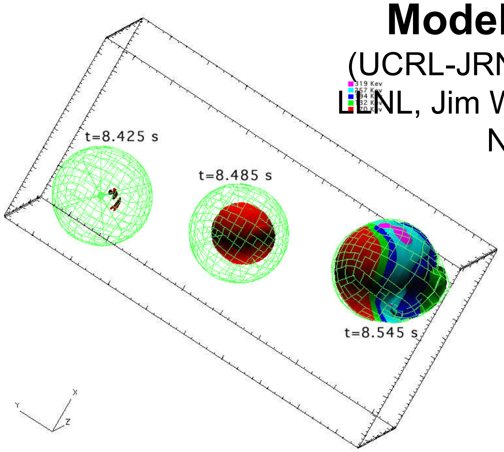
by F. K. Röpke ,1 S. E. Woosley , and W. Hillebrandt, ApJ, 660:1344-1356, 2007



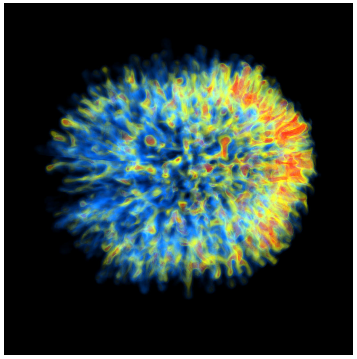
Code tailored to follow turbulent combustion in Type 1a SN, tracking the flame propagation (Reinecke et al., 1999) with sub-grid scale model for turbulence (Niemeyer & Hillebrandt, 1995; Schmidt, Niemeyer, Hillebrandt & Roepke, 2006). Hydrodynamics is based on the Prometheus implementation of PPM. Reinecke et al, 2002; Roepke & Hillebrandt, 2005; Roepke, Hillebrandt, Niemeyer & Woosley, 2006.

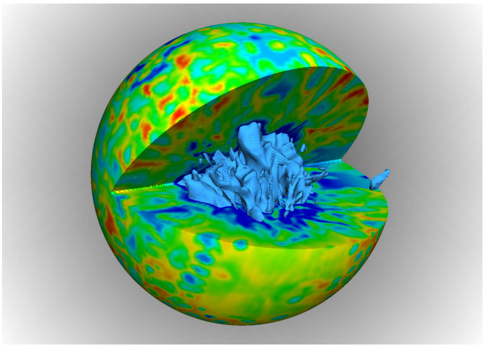
Relativistically-Compressed Exploding White-Dwarf Model for SGR-A East,

(UCRL-JRNL-208008, David Dearborn LLNL, Jim Wilson LLNL and G Mathews Notre Dame) - ApJ

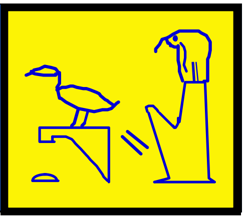


Grant Bazan (LLNL, B div) studied the Ni^{56} structure that develops in a Type II Supernova by sourcing the energy into a late stage massive star model, and tracking subsequent nucleosynthesis.





Conclusions



1) Everything is harder in 3D:
Volume/area conserving oscillations (Hourglassing) requires little(no) energy to grow to large amplitude.
in 1-D 0 modes
in 2-D 2 modes
in 3D 27 modes

2) Pretty pictures are easy. Understanding is difficult.

3) It is a facility: Codes can costs more than the computers. Require collaboration to develop, maintain, and use (code architects, physicists with specialty in input physics).

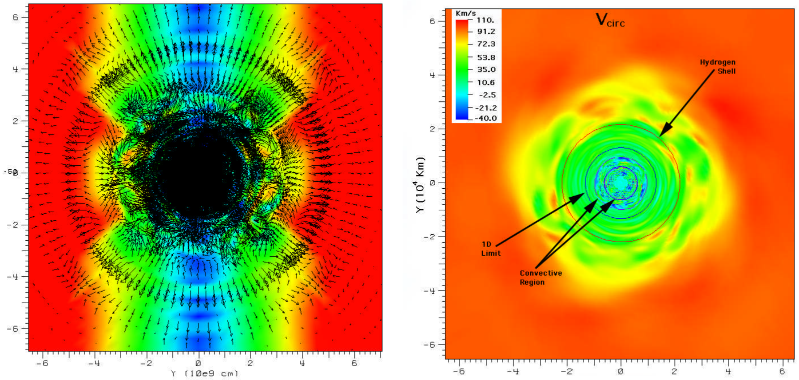
4) Postdoc's and students cannot afford the time learn a 200,000 line code as they could 2,000 line 1-D codes. They will be dependant on support to integrate their contribution into such codes.

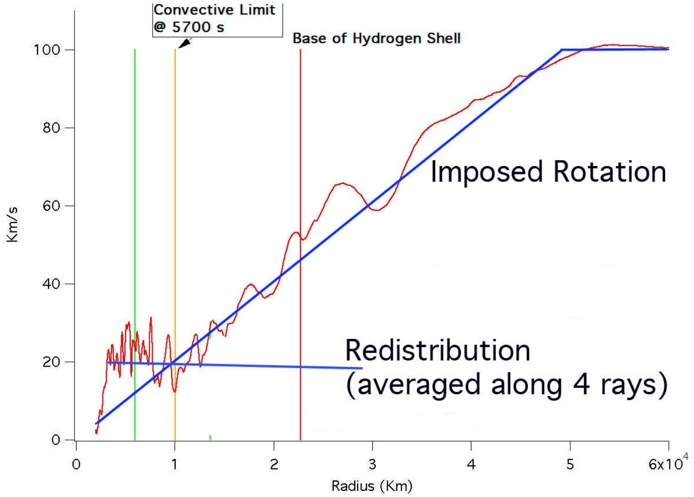
5) 3-D codes are still not model free, and there is much work to be done.

Valore per la Pena?
Penso si!

Speed Color Coded

Y-Z plane **X-Y plane**

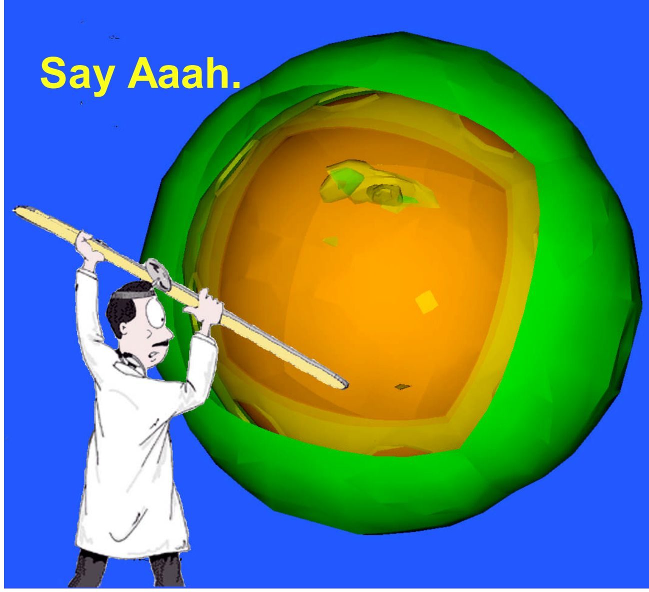


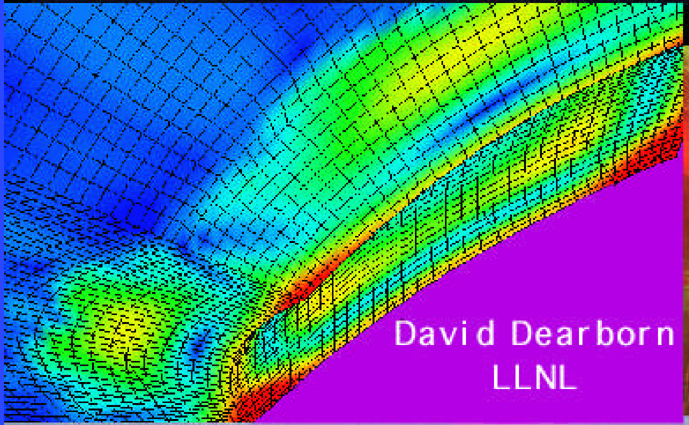


"Three Dimensional Simulations of Core Helium Flash – with Rotation", John Lattanzio, David Dearborn, Peter Eggleton, and Don Dossa, Proceedings of Science, International Symposium on Nuclear Astrophysics, Nuclei and the Cosmos, IX. In Press 2006, UCRL-Proc-228166.

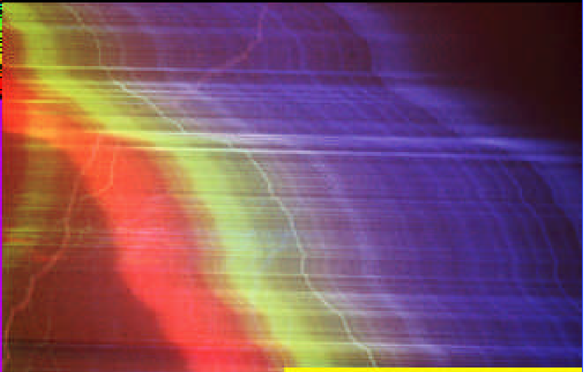
The End

QuickTime™ and a
Video decompressor
are needed to see this picture.





David Dearborn
LLNL



Djehuty

Simulating Stars
in Three Dimensions