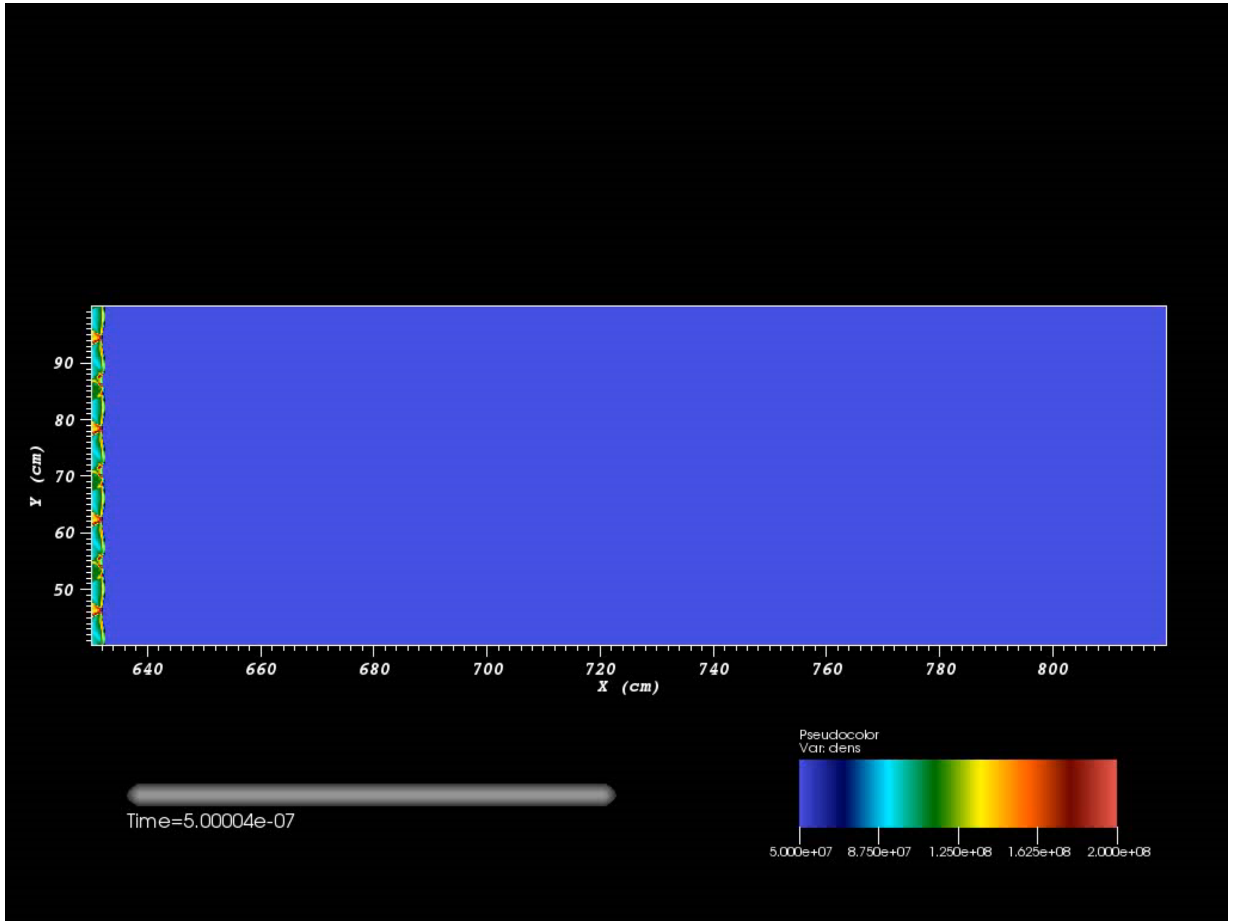
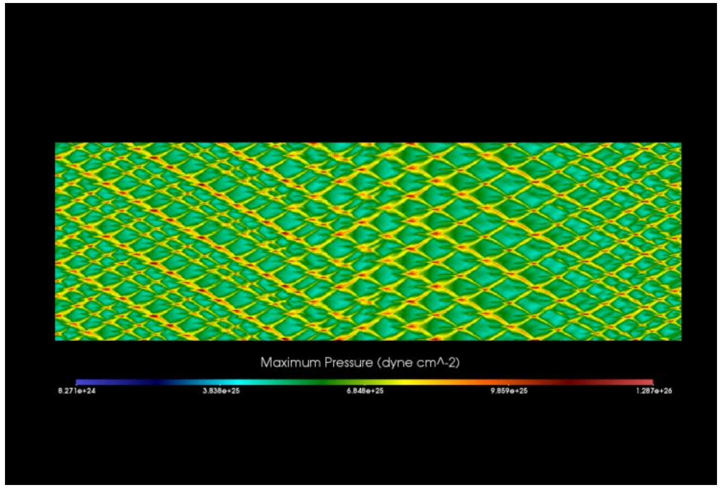
On Numerical Considerations for Modeling Reactive Astrophysical Shocks



Thomas L. Papatheodore - P599 Particle Physics, Astrophysics and Cosmology Seminar - February 19, 2014

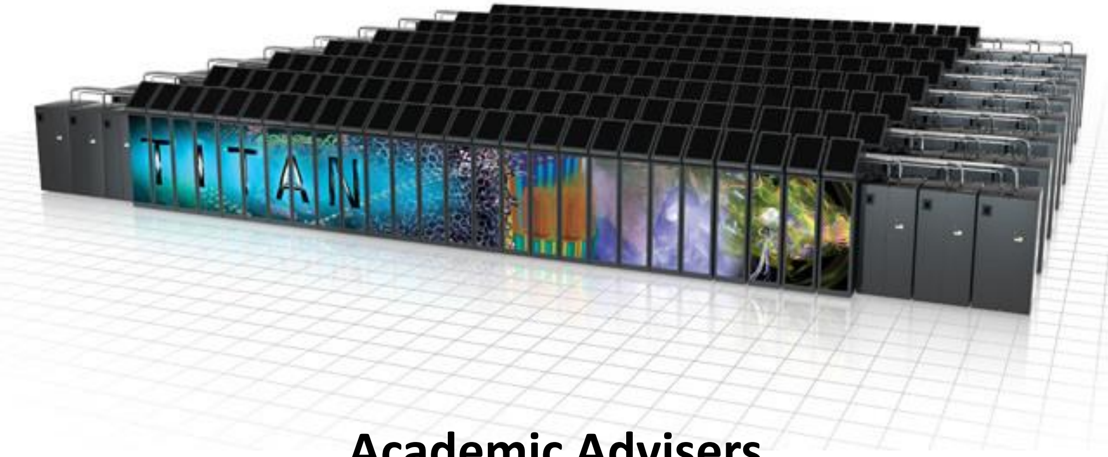
My Research

Simulate propagation of detonation fronts through Type Ia SNe progenitor environments.



Specifically, how do the details of propagation change with nuclear network size?

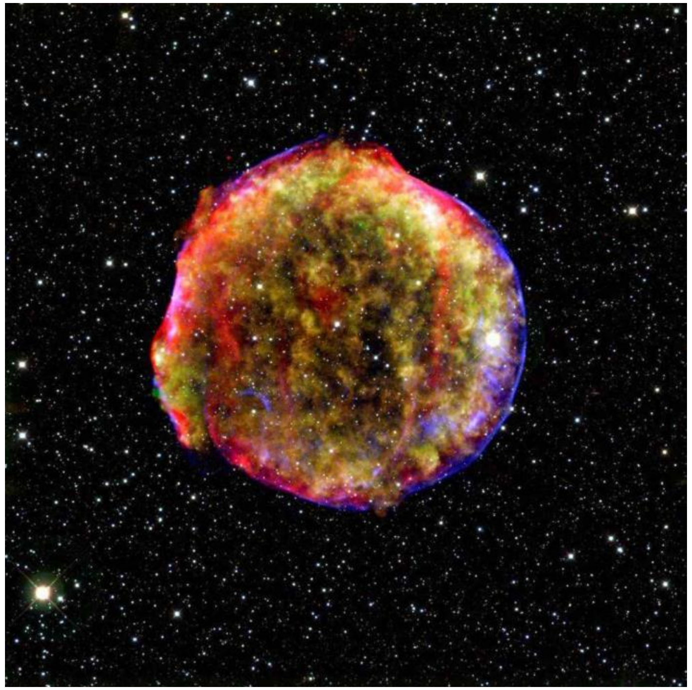
FLASH Code
FLASH Center – University of Chicago



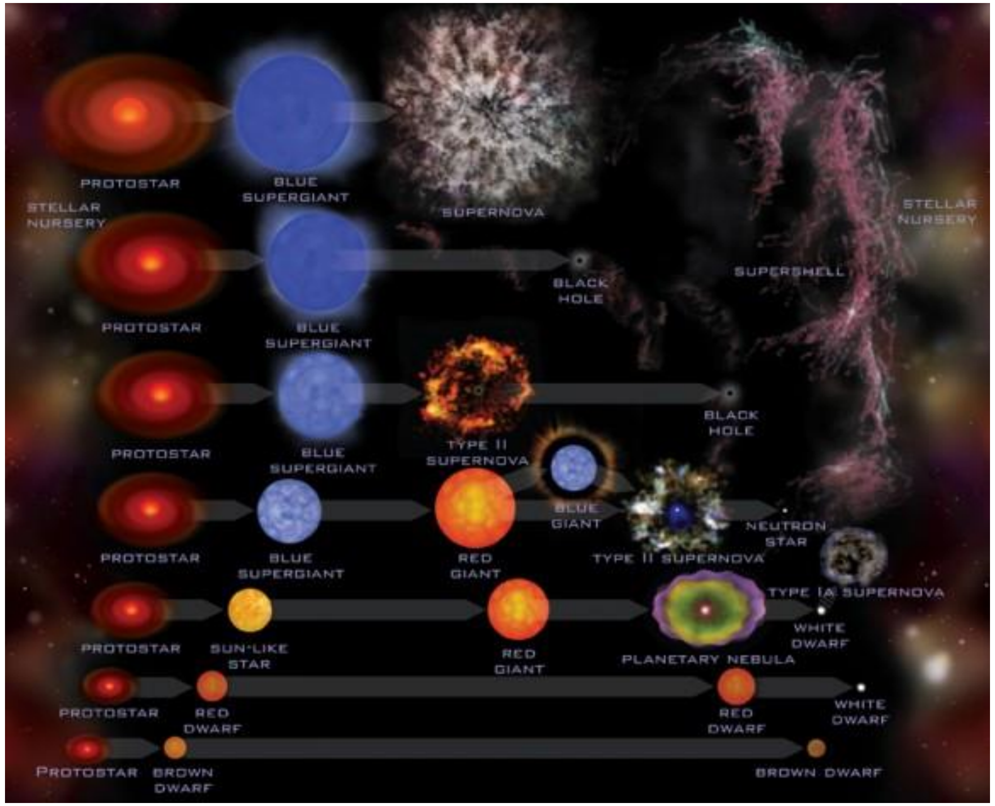
Academic Advisers

Background : Type Ia SNe

Widely believed to be thermonuclear explosion of C/O white dwarf in binary stellar system.



MPIA/NASA/Calar Alto Observatory



Stellar evolution: chandra.Harvard.edu

WD: C/O, electron degeneracy, $\rho \sim 10^7 - 10^9$ g cm^{-3}

SNe Ia Observations

Among most energetic events in universe

→ known to outshine their host galaxies

→ useful as distance indicators

SN 1994d

Differentiated by strong Si lines and an absence of hydrogen near maximum light.

The **light curves** are remarkably homogeneous

→ rise to max light in ~20 days

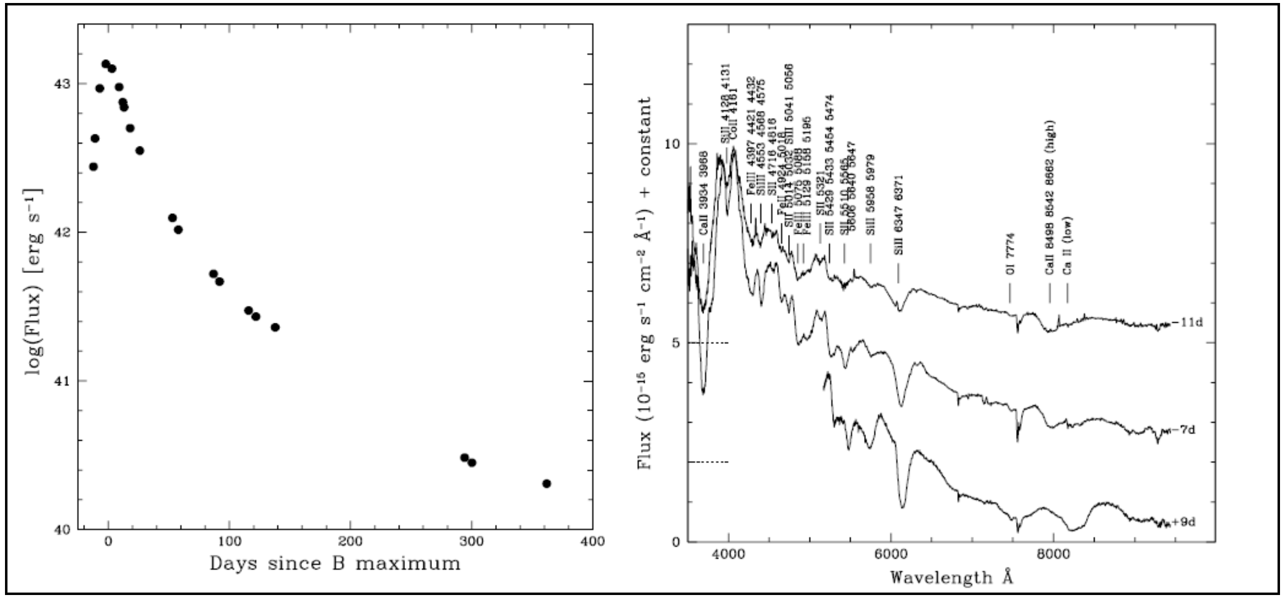
→ followed by a steep decline

→ exponential decay

Powered by the decay of

$^{56}Ni \rightarrow {}^{56}Co \rightarrow {}^{56}Fe$

The **spectra** show large amounts of ^{56}Ni and other iron-group nuclei as well as intermediate-mass elements (IMEs) such as Ne, Mg, Si, S, and Ca in the outer layers.



G. C. Anupama et al.: Type Ia supernova 2003du

Background: SNe Ia explosion mechanisms

Single Degenerate Scenario

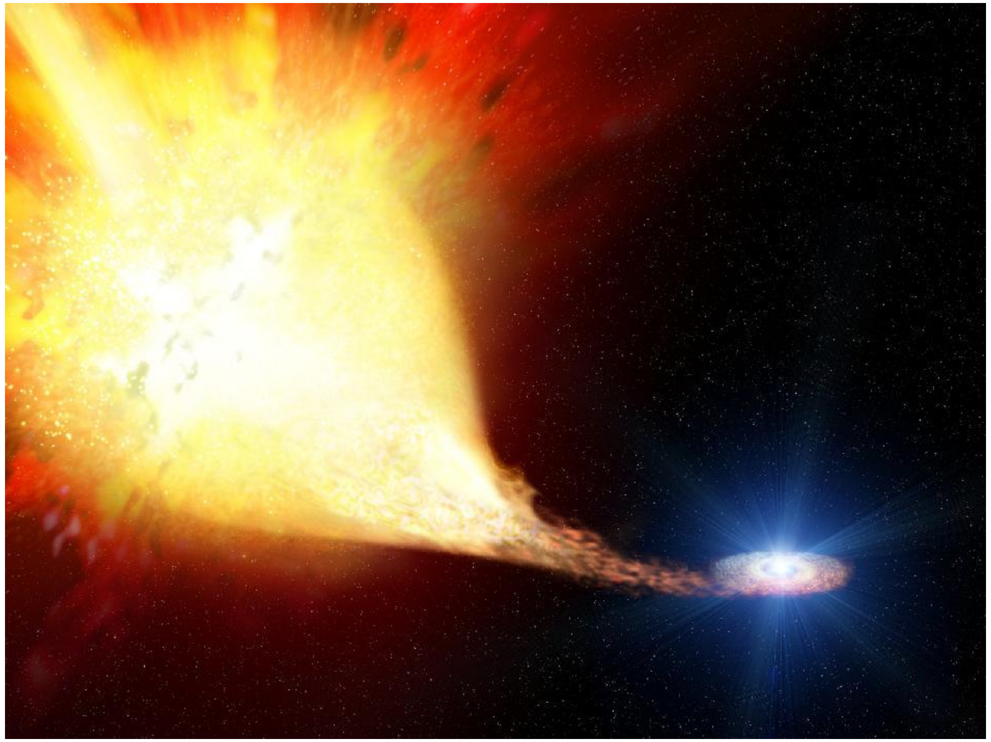


Image Credit: European Space Agency and Justyn R. Maund (University of Cambridge)

Double Degenerate Scenario

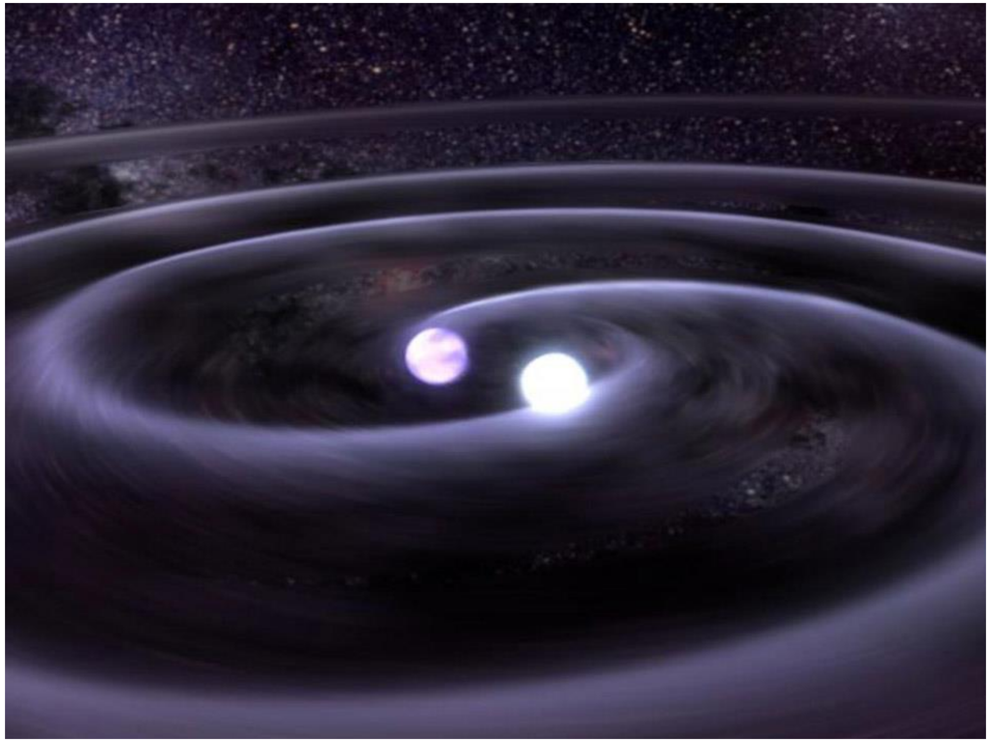


Image credit: NASA/Tod Strohmayer (GSFC)/Dana Berry (Chandra X-Ray Observatory)

Background: Single Degenerate Scenario (SD)

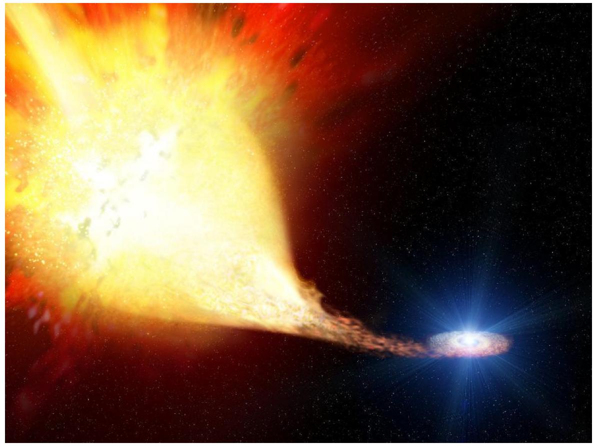


Image Credit: European Space Agency and Justyn R. Maund (University of Cambridge)

Most widely-studied version of this scenario

Accretion continues → C-burning triggered in the core of a near-Chandrasekhar-mass WD → but the exact details of the mechanism are unclear

- *Once thermonuclear runaway begins, does burning proceed as a deflagration or detonation?*

<u>Pure Detonations</u> (super-sonic propagation)

→ Shown to burn near-Ch-mass WDs completely to iron-peak elements (Arnett 1969)

In contrast to observations, traditionally eliminating this as suitable explanation

<u>Pure Deflagrations</u> (sub-sonic propagation)

→ Allows expansion to lower densities where IMEs observed in spectra can be created

→ Shown to produce enough energy to explode a star (Hillebrandt & Röpke 2005) but not enough ^{56}Ni to power observed light curves, except perhaps lowest energy events

→ Substantial mixing of elements in ejecta, in disagreement with observations.

In contrast to observations.

Due to these contrary results, a widely-accepted mechanism for the SD channel is a deflagration that becomes a detonation at some point during the explosion.

Background: SD – Deflagration-Detonation Mechanism

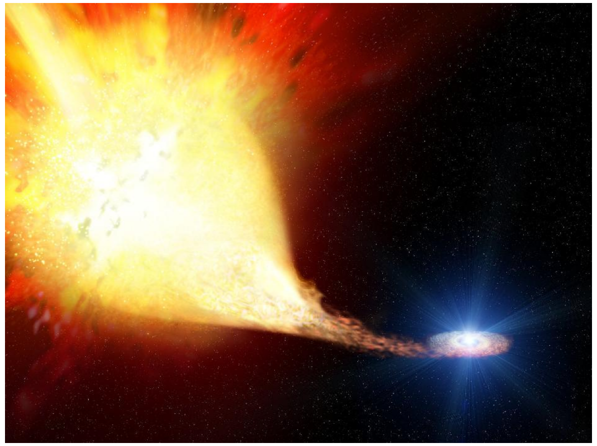


Image Credit: European Space Agency and Justyn R. Maund (University of Cambridge)

Main Variations

→ Delayed-Detonation (DDT; Khokhlov 1991)
→ Pulsating-Reverse-Detonation (PRD; Bravo & Garcia-Senz 2006)
→ Gravitationally-Confined-Detonation (GCD; Plewa et al. 2004)

A deflagration phase pre-expands the WD to lower density before a detonation occurs.

At sufficiently low density, O- and Si-burning times can become comparable with the sound-crossing time of the WD
→ leading to incomplete burning and resulting in the production of IMEs

Specifically, in Delayed-Detonation model, the critical density (ρ_c) at which the deflagration-to-detonation transition (DDT) occurs is an unknown parameter
→ manually tuned to match observations
→ previous studies suggest that $\rho_c \sim 10^7$ g cm^{-3} can produce results consistent with observations

Such parameterized models have been shown to reliably match light curves and elemental abundances (Kasen et al. 2009), but further investigation is needed to help establish a theoretical understanding.

Background: Double Degenerate Scenario (DD)

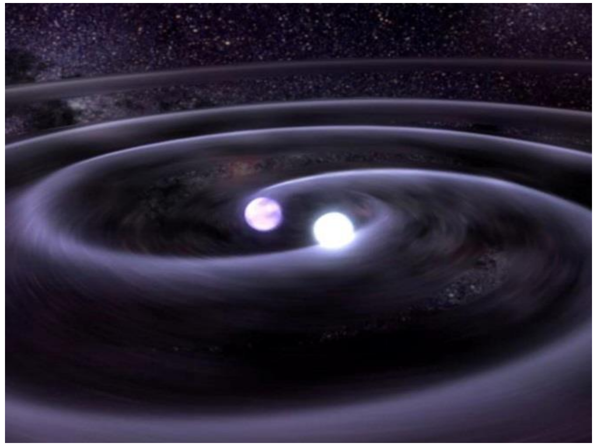


Image credit: NASA/Tod Strohmayer (GSFC)/Dana Berry (Chandra X-Ray Observatory)

A WD-WD binary pair spirals inward and eventually merges due to emission of gravitational waves, resulting in an explosion.

Until recently, DD scenario was considered by many to be unreasonable explanation for Sne Ia

→ such a merger was thought to result in accretion-induced collapse to a neutron star (Nomoto & Kondo 1991)

However, modern simulations (Pakmor et al. 2010, 2011, 2012) show explosions can occur if detonation is ignited <u>during</u> the merger process

→ these explosions are consistent with sub-luminous and normal classes of SNe Ia observations

The DD scenario has also received increasing support in recent literature due to merger rates consistent with SNe Ia rates (Wang & Zhanwen 2012), as well as a natural explanation for the lack of hydrogen in the spectra.

Background: SNe Ia explosion mechanisms

Based on energetics arguments, near-Chandrasekhar-mass progenitors have dominated Type Ia literature

However recent studies (Fink et al. 2010; Sim et al. 2010; van Kerkwijk et al. 2010; Pakmor 2012) indicate that sub-Chandrasekhar-mass systems might also be capable of explaining observations.

→ *Sub-Ch events may be described by the SD and/or DD scenarios*

SD: double-detonation mechanism (Nomoto 1982a,b; Woosley & Weaver 1994)

→ helium layer accumulates on the surface of a sub-Chandrasekhar-mass WD via accretion from a binary companion

→ detonation may occur in helium layer

→ drives shock waves into the core, inducing a subsequent carbon detonation at either

→ the helium-carbon interface (edge lit) or

→ the center of the WD (core compression)

DD: violent merger of a WD-WD system

→ merger (mass ratio near unity) can lead to a condensed object with mass less than Chandrasekhar-mass

→ detonates in envelope comprised of the remaining secondary WD material (Pakmor et al 2010, 2012)

Low density environments common in sub-Ch-mass WDs readily allows for production of IMEs, eliminating the need for pre-expansion phase.

As we shall see, simulating nuclear burning fronts under such low-density conditions requires caution, especially when complicated by multi-dimensional effects

In short, although there are competing hypotheses as to the progenitor system(s) of SN Ia, almost all viable options involve a detonation at some point during the explosion

Background: Detonation Theory (1D)

CJ-Theory: developed by Chapman (1899) and Jouguet (1905) at the turn of the twentieth century.

→ Models the detonation front as a sharp discontinuity between burned (ashes) and unburned (fuel) material.
→ Reactions occur instantaneously as the interface propagates into the fuel, leaving completely burned ashes behind it.
→ Given the energy released by burning fuel into ash, the detonation velocity and post-shock thermodynamic state can be obtained by this model, but it fails to describe the structure of the detonation.

ZND-Theory: Zel-dovich (1940), von Neumann (1942), and Döring (1943) expanded CJ-theory

→ Advance reactions according to their corresponding rates, thereby describing a finite reaction zone with an extended thermodynamic profile behind the discontinuous shock.

In such 1D models a burning length can be defined as the product of the detonation velocity and the total time to achieve a particular ash state.

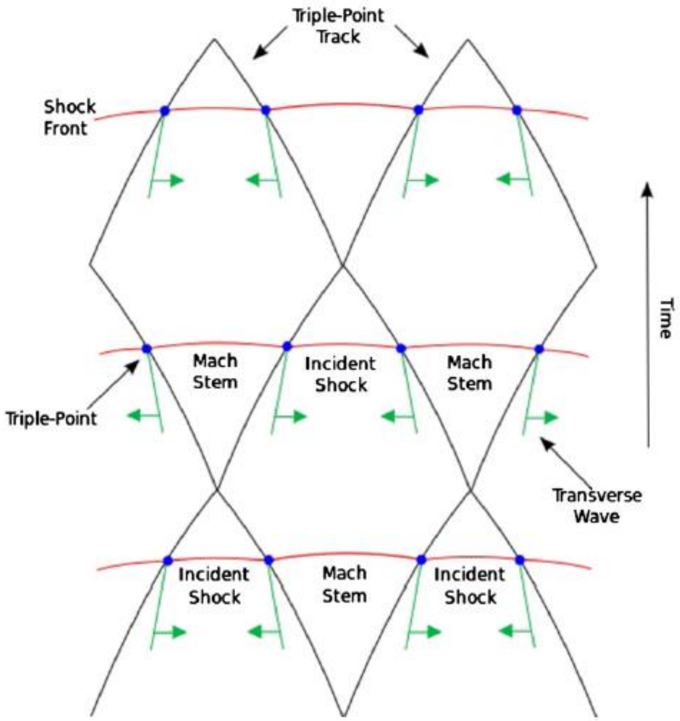
Background: Detonation Theory Applied (1D)

C/O fuel burns in roughly 3 stages: C-, O-, Si-burning

Khokhlov (1989) studied 1D detonations in Type Ia SNe

→ Calculated three distinct burning lengths corresponding to the burning time scales for C, O, and Si ($X_C << X_O << X_{Si}$).
→ Burning lengths increase with decreasing density
→ At sufficiently low density, burning lengths can become comparable to WD radius
- Incomplete burning can occur (IMEs)

Background: Detonation Theory (2D)



Despite many successes of 1D models, they do not agree with experimental results.

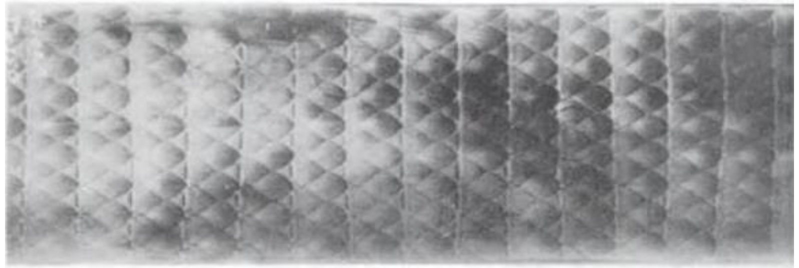
→ Real (i.e. multi-dimensional) detonations propagate at a slightly reduced speed and exhibit a complex cellular pattern within the reaction zone.

A physical burning front consists of alternating regions of Mach stems and incident shocks connected by transverse waves that extend back into the reaction zone.

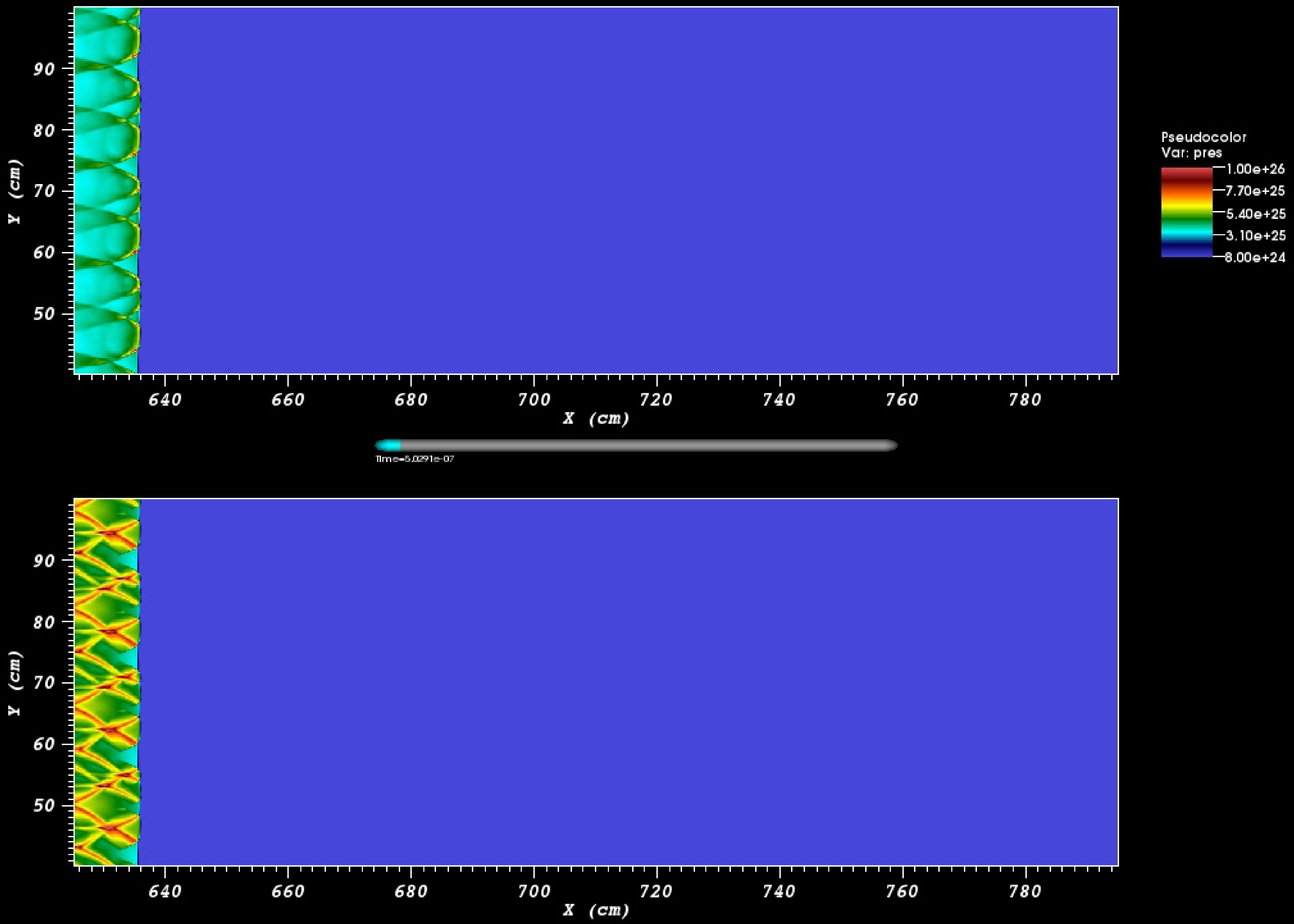
→ The points where these three structures meet are called triple-shock configurations, or triple-points.

- *It is the paths of these high-pressure points which trace out the characteristic cellular pattern.*

Cellular detonations were first observed in terrestrial gases by Denisov & Troshin (1959) and Voitsekhovskii et al. (1963).



The cellular pattern can be recorded experimentally as the triple-points etch their paths on the inside of soot covered “flame tubes” (Fickett & Davis 1979).


Pseudocolor
Var: pres
1.00e+26
7.70e+25
5.40e+25
3.10e+25
8.00e+24
Y (cm)
90
80
70
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X (cm)
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660
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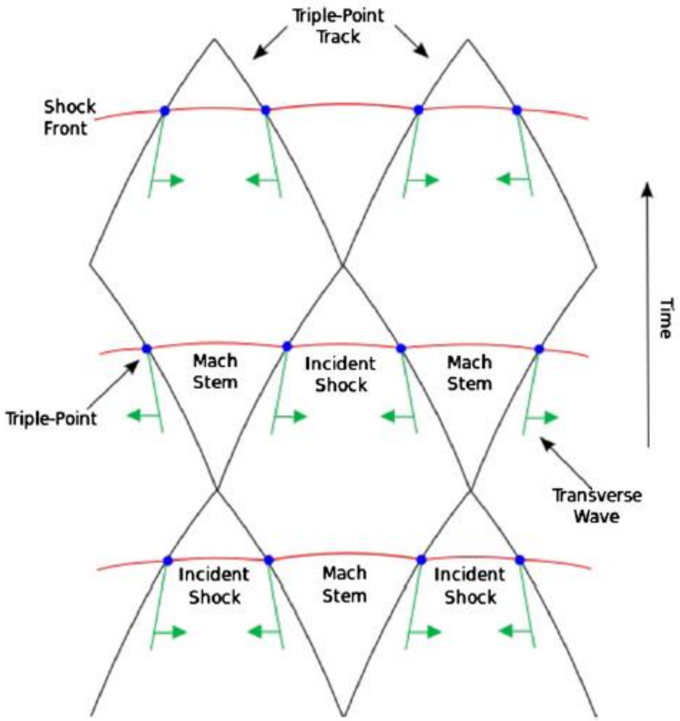
Background: Detonation Theory (2D)



Computational studies (Oran et al. 1998; Gamezo et al. 1999a) show that cellular burning can create low-pressure pockets of unreacted gas, the presence of which increases the length of the reaction zone compared to 1D results and can play an important role in detonations extinction.

Direct Numerical Simulations (DNS) of cellular detonations in Type Ia environments
→ Boisseau et al. (1996), Gamezo et al. (1999b), Timmes et al. (2000)

Analogous to terrestrial detonations
→ cellular burning created pockets of incompletely burned material, which altered their results relative to 1D calculations. They found

- increase in the length of the burning regions
- slight decrease in detonation velocity
- changes in the final composition

Background: Simulations of SNe Ia

Disparate length scales involved

flame thickness < 1 cm

radius of WD ~ 10^8 cm

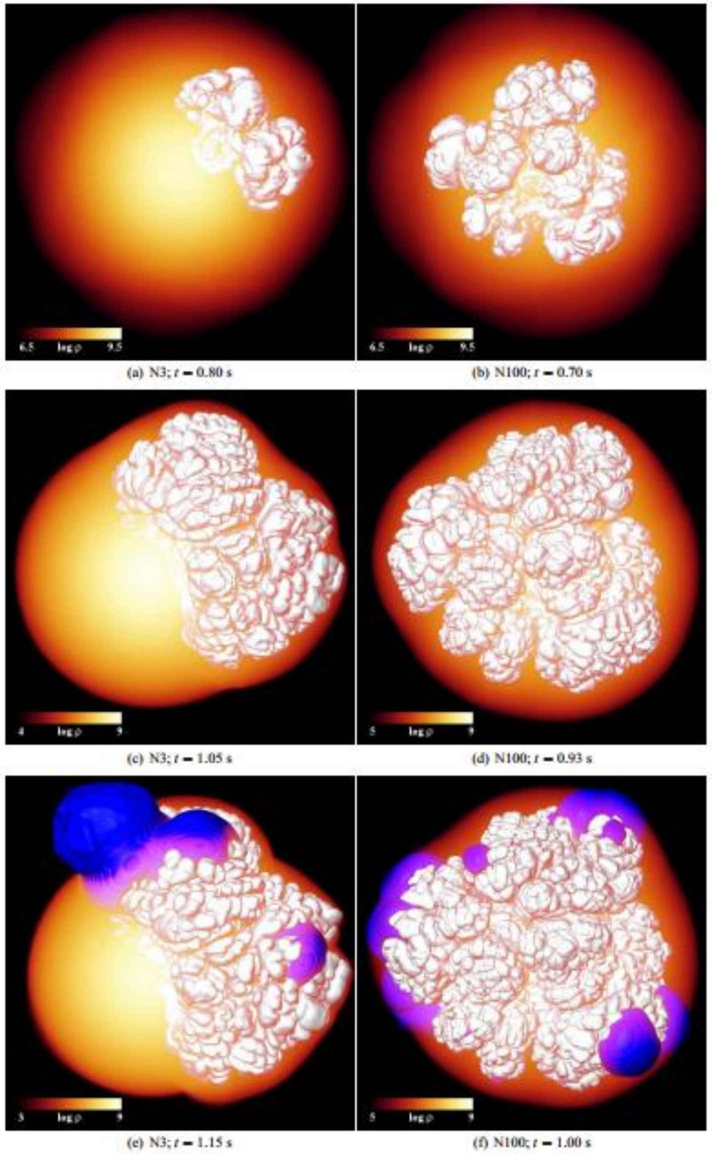
→ cannot resolve all length scales

Employ sub-grid approximations to burning

use DNS to inform sub-grid model

→ use sub-grid model in full-star simulations

Seitenzahl, I. R. et al. 2013, MNRAS, 429, 1156



Approximating Shock Structure

A physical shock is considered to be infinitesimally thin under such conditions, so fuel spends very little time within the shock itself as the detonation propagates.

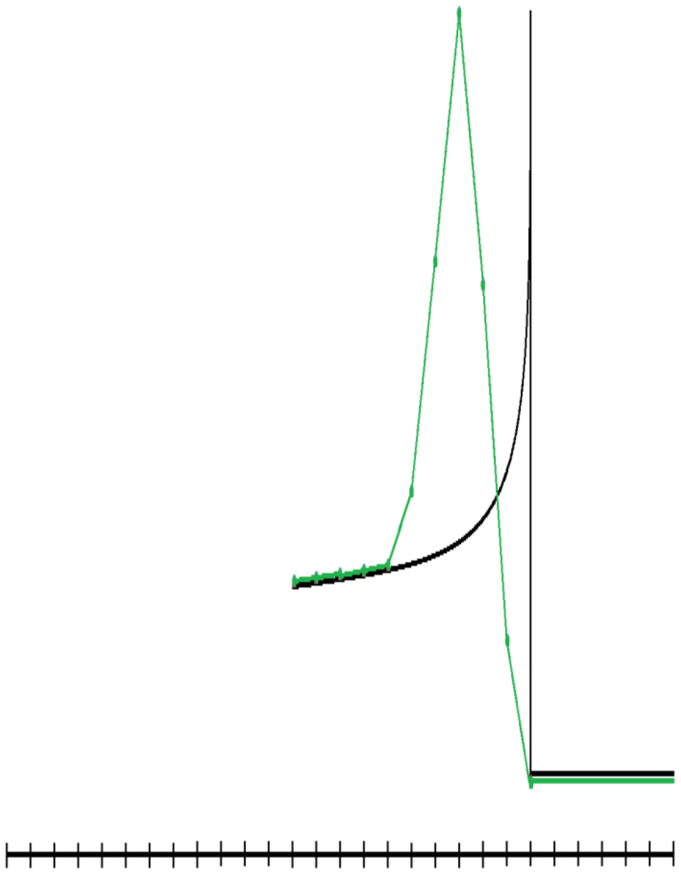
→ an insignificant amount of burning occurs naturally inside of a shock

The width of a numerical shock is constrained by the hydrodynamics scheme and spatial resolution employed.

→ Ex: an Eulerian PPM scheme typically artificially widens shock to ~2-4 computational zones

- on a sufficiently coarse grid an appreciable amount of burning may occur inside the shock

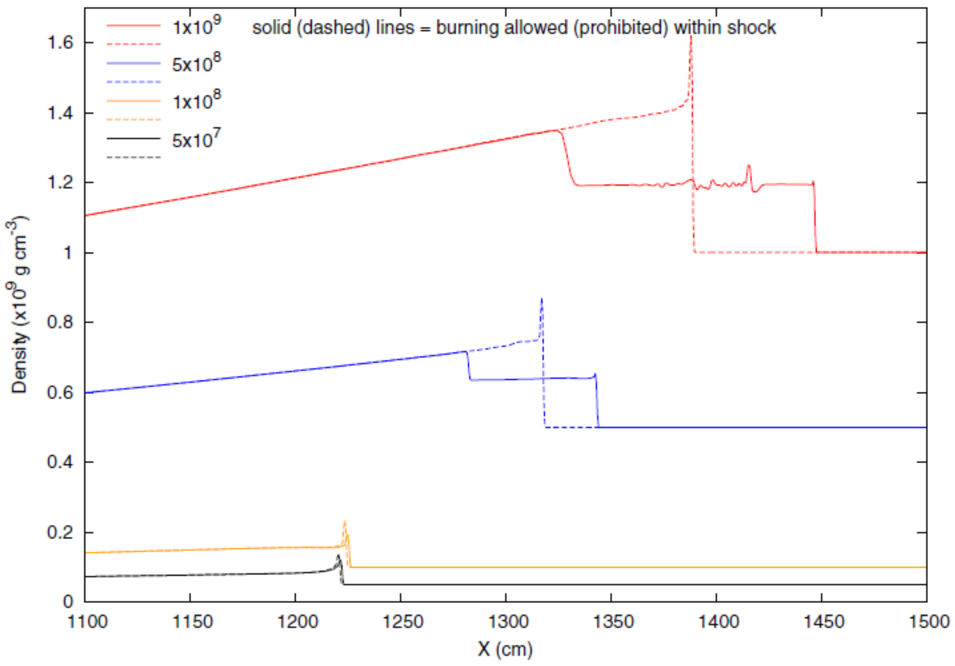
So, do you allow burning to occur within the shock?



Density Profiles

Conventional Wisdom

Fryxell et al. (1989) showed that energy deposition in the leading edge of an under-resolved carbon-burning shock can generate a secondary shock structure, which is a numerical artifact, that propagates ahead of the true shock at speeds greater than the Chapman–Jouguet velocity.



Papatheodore & Messer 2014, ApJ, 782, 12

Common prescription: prohibit burning inside of a numerical shock (Fryxell et al. 1989)

→ ensures that burning does not occur until the correct post-shock conditions are reached

→ eliminates the secondary shock structure and restores the proper detonation speed to the models

What about multi-dimensional simulations?

→ Should we still suppress burning within the shock?

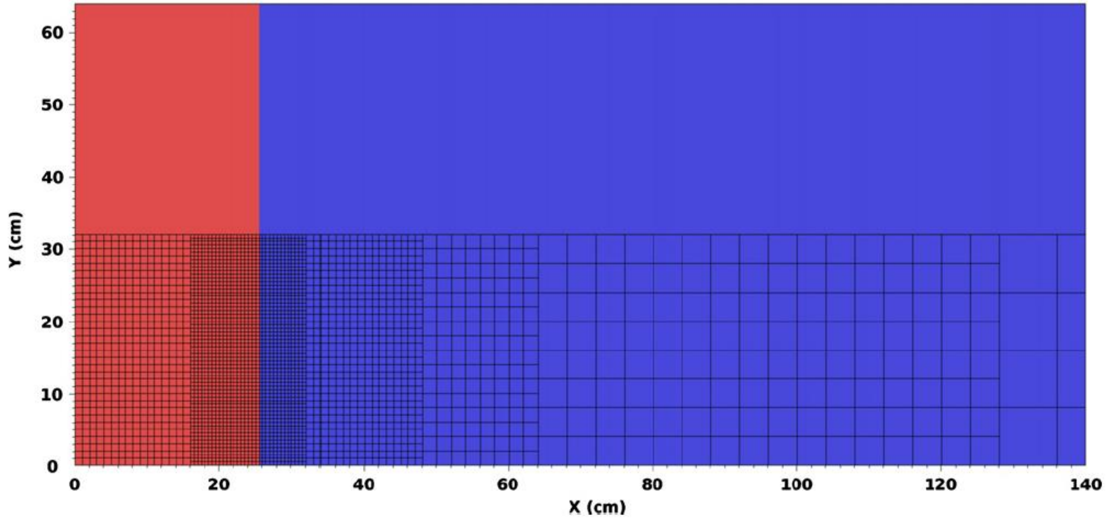
We explore the effects of modifying the burning prescription in both 1D and 2D detonation simulations in order to fully understand the ramifications of this prescription, and, in particular, its effect on cellular burning.

Numerical Laboratory

We simulated DNS of detonations in 1D and 2D (with burning allowed and prohibited within the shock)

Computational domain : 128cm by 6144cm
Fuel : C/O, 10^7 K, 0 cm s^{-1}
Match head : 10^{10} K, 10^9 cm s^{-1}

1D : ρ = 5e7, 1e8, 5e8, 1e9 g cm^{-3}
2D : ρ = 5e7 g cm^{-3}



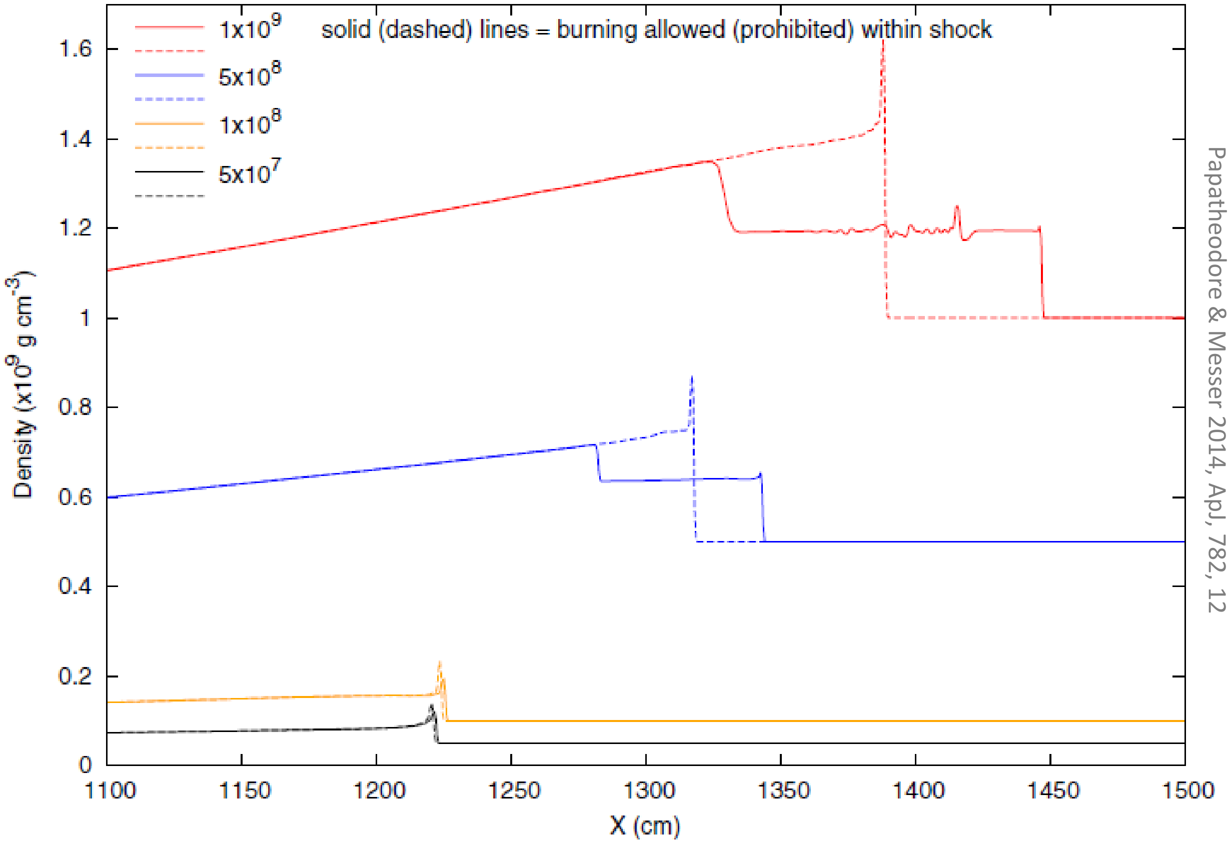
FLASH Code: Multi-physics, parallel simulation code
→ Capable of handling reactive compressible flow problems typical in astrophysical problems
→ AMR: Adaptive Mesh Refinement

Results

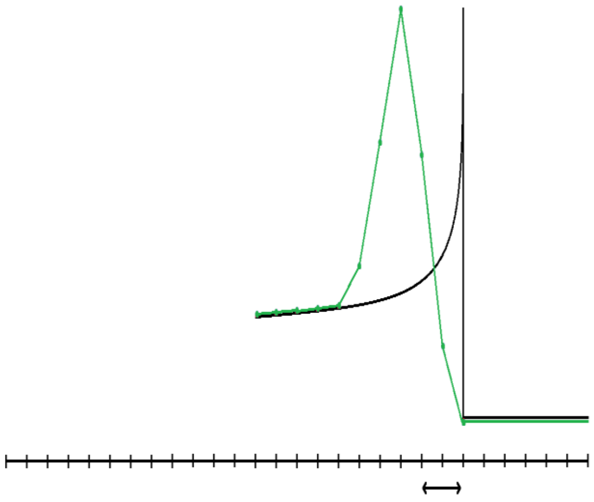
In 1D we find that prohibition of shock burning is important when significant amount of fuel will burn within shock, consistent with FMA.

Sufficiently resolved shock does not require this prescription but its use ensures integrity without search for adequate refinement for different fuel densities.

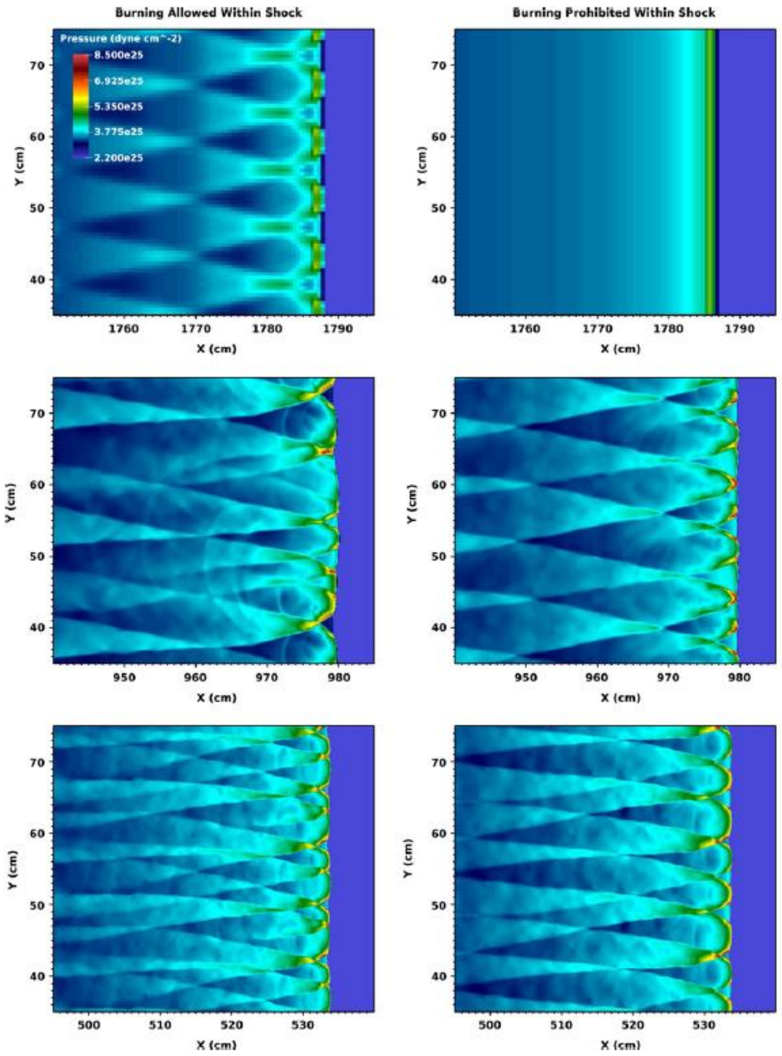
Hence, the well known recommendation to prevent burning within simulated shock



Papatheodore & Messer 2014, ApJ, 782, 12



Results

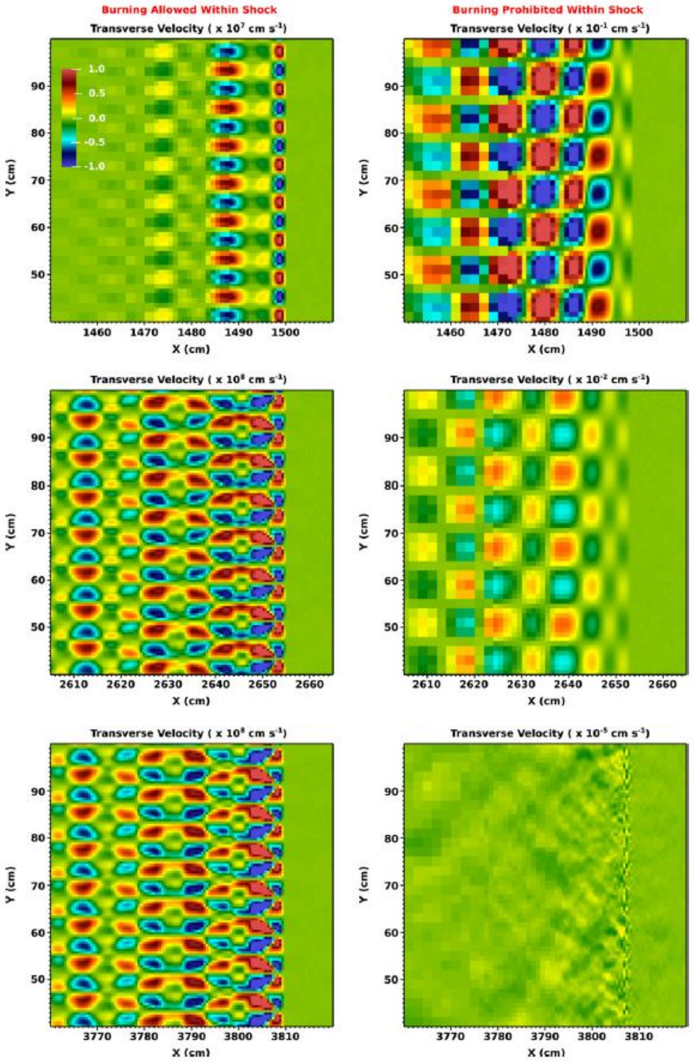


Papatheodore & Messer 2014, ApJ, 782, 12

In 2D we find that this treatment can unintentionally inhibit the formation of cellular structure by displacing energy release to region behind a coarsely resolved shock

→ obstructing the development of transverse perturbations

We also find that the strength of the triple-points, as well as energy release realized in triple-points, is affected by treatment of shock burning.



Papatheodore & Messer 2014, ApJ, 782, 12

Conclusions

How can cellular structure influence our understanding of SNe Ia explosion mechanisms?

Due to disparity of length scales in SNe Ia, sub-grid models are used to approximate burning in full-star simulations
→ DNS needed to build the sub-grid models

DNS of multi-D detonation fronts in SNe Ia (Boisseau et al. 1996, Gamezo et al. 1999b, Timmes et al. 2000, work presented here)
→ pockets of incompletely burned material (created by cellular structure)
→ *can increase effective size of burning regions relative to 1D results*

Gamezo et al. (1999b) argued:
→ production of IMEs would be possible at higher densities (elongated burning lengths)

→ ***Increase the critical density at which DDT can occur***

Can our findings affect these results? Probably not.
→ If building a sub-grid model from DNS in multi-D, you are doing so specifically to include the effects of cellular structure.

However, it does show how the small-scale effects of cellular structure can influence large-scale models that are used in comparison with observation.

Conclusions

In general, full-star simulations which employ sub-grid models will not likely be affected by our results
→ Any small-scale effects (including those resulting from cellular structure) will be included in sub-grid model

However…
→ many full-star simulations do not have the sophistication of sub-grid models
→ many simulations that model large regions of WD, but not full-star
→ large-scale convective motions
→ He shell burning

Under-resolved DNS
→ Here shock burning will almost always need to be prohibited

Our results are particularly relevant for simulations of sub-Chandrasekhar-mass explosions
→ Here we may be under-resolved but low densities allow for resolved cellular structure (albeit coarsely)

Conclusions

Until recently, observations of unburned C in Type Ia spectra was thought to be rare (confined to super-Ch events)

→ However, increased interest in Type Ia has led to more telescopes and early detection

→ Observing more Type Ia at earlier times

→ Find unburned C at early times (outer ejecta) in significant number of all events (~30%)

→ *Still unsure where this unburned C comes from*

<u>Sub-Ch explosion</u>: Unburned C trapped in cellular pockets might remain

→ if nuclear burning is arrested due to expansion in low-density material

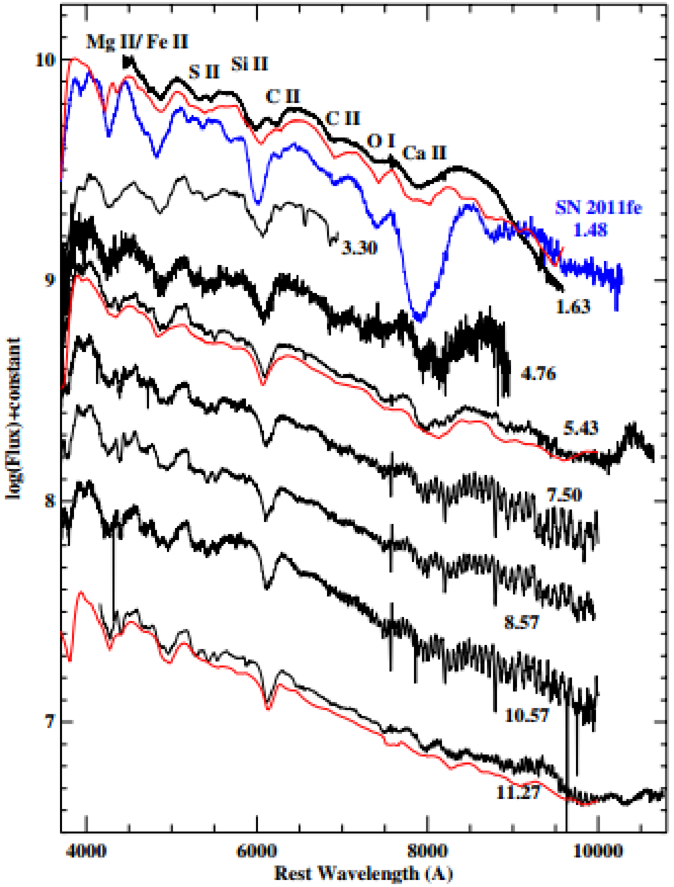
→ ***essentially "freezing out" carbon in outer ejecta***

Full-Star/Sub-Grid: small-scale features need to be accounted for in sub-grid model if this is to be captured

→ probably not affected by our results

Under-Resolved Large-Scale: cellular structure may well be resolved (albeit coarsely)

→ Our results imply that these features could be unintentionally inhibited by treatment of shock burning

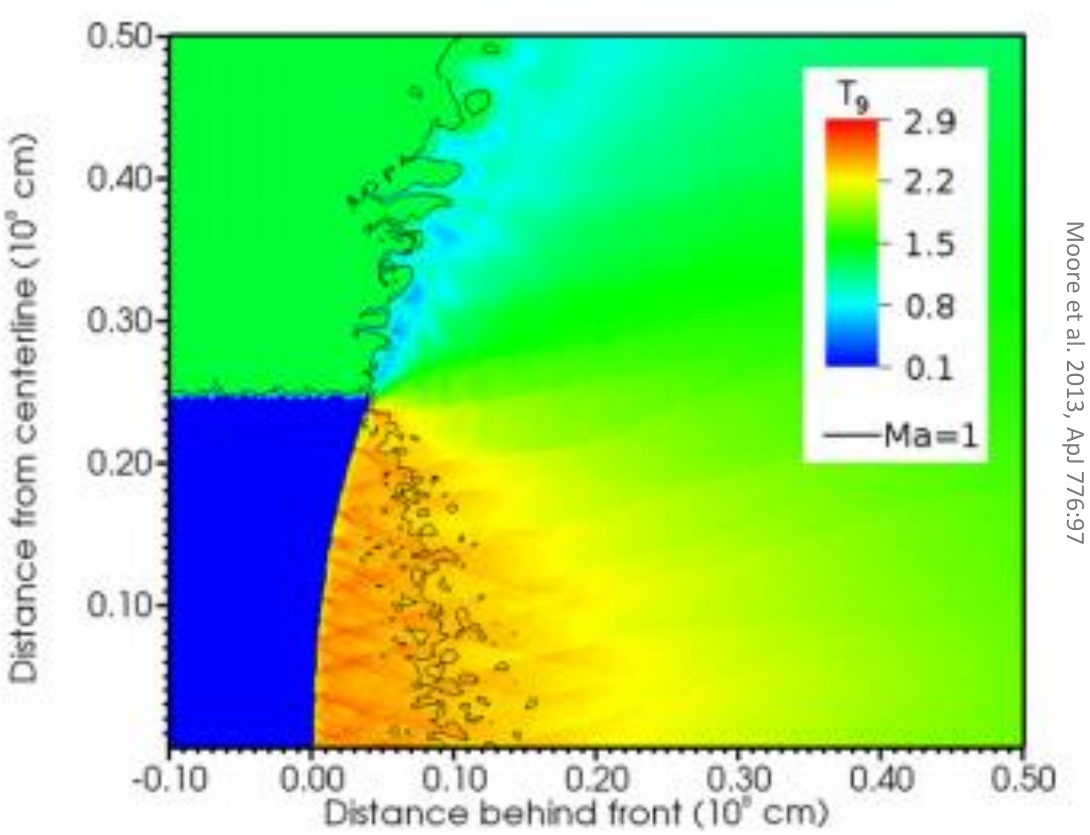


Zheng et al. 2013, ApJ 778:L15

Conclusions

Under-resolved DNS of detonation in low-density He shell
→ burning should be prohibited within the shock
→ but presence of cellular structure

Prohibition of burning inside of a shock can lead to inhibition of cellular structure if not treated carefully.



Moore et al. 2013, ApJ 776:97

Conclusions

Final Thoughts

Although geared toward Type Ia SNe, these results are relevant for many astrophysical events posited to involve detonations

→ Novae, X-ray bursts

The prohibition of burning inside reactive shocks will have different outcomes, depending on the simulation

→ Then, these results serve as caution

In multi-dimensional simulations, specifically at low densities, our results should be considered on a case-by-case basis.

Questions?