

Sub-Chandrasekhar type Ia supernovae scenarios with increased pathways for neutronization

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To my parents Claudio and Jeannette. Los quiero mucho.

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Abstract

Type Ia supernovae are thermonuclear explosions of white dwarfs (WD), electron-degenerate cores of old intermediate mass stars (under $8M_{\odot}$). Reaching energies of 10^{51} erg, they outshine whole galaxies as they synthesize and distribute most of the iron group elements (IGE; V, Cr, Mn, Fe, Co, Ni) into the interstellar medium, thus being one of the main agents in cosmic chemical evolution. Also, given their notably homogeneous lightcurves, they form the last step in the cosmic distance ladder outdistancing Cepheid variables by orders of magnitude. Though calibration of said lightcurves is dependent on a high number of confirmed events, the limits of statistical significance are already being reached, causing systematics to govern errors. It is in this regard that theoretical estimations of intrinsic brightness and chemical yields can impact the astrophysical use of these standardizable candles. Though there are several possible progenitor scenarios, one of the mechanisms of explosion that has regained a measure of attention is the sub-Chandrasekhar mass Scenario (subCh): a sub-Chandrasekhar mass (under $1.4M_{\odot}$) carbon-oxygen core accretes helium from a binary companion until helium burning temperatures are reached, causing a thermonuclear runaway after ignition. It is the goal of this thesis to further investigate the constraints and ranges of this type of mechanism through 3D hydrodynamic simulations with improved nuclear kinetics via large networks.

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List of Symbols

Throughout, the cgs unit system is used unless otherwise stated.

$M_{\odot}$	Solar mass, 1.989×10^{33} g
$R_{\odot}$	Solar radius, 6.957×10^{10} cm
$L_{\odot}$	Solar luminosity, 3.828×10^{33} erg $\cdot$ s $^{-1}$
erg	10^{-7} W
Å	10^{-8} cm
Gyr	10^9 years
M_{Ch}	Chandrasekhar mass, typically $1.4 M_{\odot}$
f_{λ}/F_{λ}	Spectral flux at wavelength λ
$\Delta m_{15}(B)$	B-band magnitude decline after 15 days
$M_{B,max}$	Peak B-band luminosity
G	Gravitational constant, $6.674\,30(15)$ dyne $\cdot$ cm $^2 \cdot$ g $^{-2}$
Z	Proton number
N	Neutron number
p_{fac}	Production factor

Chapter 1

Introduction

1.1 Historical Overview

Astrometry, the measuring of positions and movements of stellar objects, has been practiced since antiquity. Every civilization has tried to measure the relative positions of bright objects above for two related reasons: practicality and culture. By accurately measuring solstices (highest and lowest points of the sun in the sky throughout the year) to determine agricultural cycles, astrometry became a fixture of sedentary civilizations. Further, the regularity of seasons and the apparent movement of the sun against the backdrop of fixed stars became a cultural mystery which, if understood, might determine other terrestrial events. It is through this grand challenge that observations became ever more rigorous, and quickly integrated the movements of the planets¹ and the discovery of transient events [140, Chapter 2].

Among transient events, apart from comets and meteors which move against the backdrop of fixed stars, multiple civilizations cataloged “novae” (from the Latin “stella novae” meaning “new stars”). These remained fixed where they appeared in the sky, and lasted weeks to months. Some of these “novae” were bright enough to be seen during daylight but they did not occur frequently, with only four events recorded between the invention of writing and the 17th century, now cataloged as SN185, SN1006, SN1572 and SN1604.² It is the last two

¹Mercury and Venus following the sun. Mars, Saturn and Jupiter exhibiting retrograde motion due to Earth’s orbit.

²modern cataloging follows SN plus year until the 19th century, which then adds an incremental letter code in order of discovery e.g. SN1987A.

that spurred a revolution in science mostly due to being close enough in time to challenge any errors in observation or scrutiny of record [103]. Alas, the invention of the telescope came after these discoveries, and further analysis of these events had to wait until the 19th century when a new one was found surreptitiously.

Now cataloged SN1885A, found in M31 (Andromeda galaxy), this nova was detected within an object which if the suggested distance to it was correct, its brightness would have been unbelievable at the time, 100 million times the brightness of the sun ($L_{\odot}$), contrasted with the most luminous stars found, which were a "mere" 10000 times $L_{\odot}$ [60]. Confirmation was achieved in 1923 with a newly developed method for measuring distances at the time. This method used a predictably variable type of bright stars which also are found in M31. [73, 56] This cemented the nature of SN1885A, and those discovered after it, which came to be known in the subsequent years as "Supernovae" (SNe) [91].

Knowing what to look for, rates of discovery increased throughout the 20th century. Larger telescopes allowed a deeper volume for discovery, and photography made detection easier. This eventually would normalize their luminosity over time or light-curves (LC) to a typical maximum, when corrected for extinction (dust and gas) ([pp 159-165 140], [also see 20, for a modern calibration]). Once pre-maxima SNe were found regularly, spectral analysis at maximum further split them into categories, which corresponded with variations in their LC post-maximum. Particularly, spectra which showed no signs of hydrogen nor helium emission or absorption came to be identified as "Type Ia Supernovae" (SNIa) (see section 1.2).

Alongside observations, developments in nuclear physics culminated in the seminal paper "B²FH" [12], which mapped every element to a particular astrophysical environment. This work tied the origin of all elements heavier than carbon to SNe based on the thermodynamic conditions for their formation. In particular, SNIa account for elements up to around iron due to them being thermonuclear, thus being limited by the binding energy threshold³. This made them a linchpin in galactic chemical evolution ([131, 27, 65]).

At the end of the 20th century, owing to the high luminosity, ubiquity and reliability of identification of SNIa (see section 1.2), several projects embarked on discovering ever

³nuclear binding energy decreases after iron-56, absorbing energy rather than yielding energy from fusion.

more distant events [44, 102]. Initially with the aim of corroborating the cosmic expansion discovered early in the century [55] at larger distances, such explorations discovered a new phenomenon: said expansion seemed to increase the further away the events happened. The crowning achievement of SNIa was the discovery of the accelerated expansion of the universe (Riess et al. [110], Perlmutter et al. [101]; for a modern accrued data collection, see Amanullah et al. [2]). This achievement relied on robust spectroscopic corroboration at or around maximum brightness and similarities in light-curves among SNIa, which allowed them to be "standardized" based on their shape. This, in essence, side-stepped any question about the event's origin or progenitors.

Efforts to understand the nature of SNIa progenitors took advantage of their increasingly available observations through the 20th century. Starting from the study of their remnants, ejection velocities of the expanding bubble, along with peak luminosity, informed the energy budget of the explosion (accounting for the interstellar dust and gas hampering the expansion). This was eventually associated with an exotic type of stellar object, the white dwarf (WD) [15, 53, also see Section 1.3]. This association was enhanced by the study of their light-curves post maximum, which could be fitted by similar masses of radioactive nickel-56, decaying to cobalt-56 and finally to iron-56 [98, 18]. Eventually, confirmation of both late time spectra of iron-56 in ratios according to the mass budget of the explosion [68], together with studies of the spatial extents of newly detected events, reduced the possibilities of the progenitors to only white dwarfs [75, 90, 9].

Another important question running along the application and observation of SNIa was their environment and possible triggers for their occurrence. Since direct observation was out of the question, computational models granted a pathway to compare theoretical models. Starting from the expected mass yields of nickel-56 from observation at around 1 solar mass ($M_{\odot}$) of nickel-56, increasingly complex models started to appear beginning from the late 20th century (see section 1.4). Observations that have the most relevance to simulations are: the ubiquitous nature of SNIa compared to other types of SNe, their compact progenitors, and their geometrically simple remnants. Ubiquity of SNIa compared to all other SNe means that they appear in both young and old stellar populations, as opposed to all others appearing in younger stellar environments. This alludes to a wide range of timescales of

formation [81]. Archival correlation of detected SNIa show that their progenitors are dim enough to discard early-type stars⁴ and the center of their remnants do not show high energy emission associated with other SNe [124, 9]. Lastly, the shape of remnants from SNIa are mostly spherical. The degree of polarization of emission from remnants is skewed at under 10% from spherical ([135], but see [74] for particular outliers).

Concurrently, SNe statistics grant special insight into possible progenitor systems. Knowledge of the principal astrophysical environment where such events occur greatly constrains the thermodynamics of the detonation, and possible triggers for the event. From total SNe counts nearing a thousand at the turn of the 20th century, a plethora of surveys and higher cadence capabilities ramped up the current discovery rate to a couple thousand *per year* [38, Chapter 2], and are expected to increase by an order of magnitude in the coming decade [58]. This has already cemented the rates at which SNIa occur with respect to other types, and the rate at which they should occur based on their host galaxy’s mass [39, 40].

Finally, a new lode of data will be discovered with space-borne gravitational wave detectors. Current Earth-based detectors suffer from seismic noise going into the frequencies required for white-dwarf mergers (10 Hz and under). This will not affect space-borne interferometers and thus will be tuned around sub-Hz frequencies. This will open up observation of double white dwarf mergers, which are difficult to detect due to their low luminosity [66]. Asserting the rate at which white-dwarfs merge directly will have a profound incidence on progenitor scenarios (see section 1.4).

1.2 Observation and classification

1.2.1 Photometry

SNIa present a steep two week-long rise to a peak visual absolute magnitude of $M_V \sim -19$ ⁵ corresponding to a peak luminosity in the range of $10^{10} L_\odot$ (4×10^{43} erg/s). Declining by 3

⁴massive, high temperature stars.

⁵*Apparent* magnitudes (m) are defined by $m = -2.5 \log(L/(4\pi d^2))$ with L the radiant flux (luminosity) of the object and d the observer-object distance. *Absolute* magnitudes (M) fix the distance to 10 parsecs (3.086×10^{14} km). Subtracting both relations yields the *distance modulus* $\mu = m - M = 5 \log(d/10)$, which sets a direct relation between the observed apparent magnitude and distance, provided the intrinsic luminosity of the object is known.

magnitudes in about 30 days, followed by a softer trailing decline for around 70 days (see figure 1.1). Expanding ejecta velocities in the range of 5000 to 10 000 $\text{km} \cdot \text{s}^{-1}$ imply a kinetic energy of 10^{51} erg, while bolometric luminosity (luminosity summed over all frequencies) integration implies a total radiated energy for the event of 10^{49} erg.

A key property of spectrally similar SNIa (see section 1.2.2) is that their peak luminosity is linked to their light curve shape, with intrinsically brighter events showing a shallower decline in their light curves. Though there are several methods to correlate these two properties, the most well known is the so called "Phillips Relation" which relates peak magnitude with the 15-day decline rate of the light curve ($\Delta m_{15}(B)$), both measured in the B-band [104]. Once the nuisance parameters are fitted with an ensemble of light curves, any new SNIa can be scaled to their *absolute* magnitude from their measured *apparent* magnitude. This "standardization" provides a distance to any SNIa, provided there's one known distance to any observed event (see footnote 5). This distance ladder teeters on the best known distance to the closest supernovae for which we also have another independent distance measurement such as Cepheid stars. To date, no SNIa have been properly observed closer than the Magellanic Clouds, barring pre-telescope events which have no reliable magnitude measurements.

While this has been tried for other types of supernovae [80, 22], SNIa have two key advantages over their siblings: first, they are the only type which shine most of their luminosity near the visible spectrum⁶, and so their relationship is tighter (less spread) and are seen further than all other types (see figure 1.1). And second, they occur in all types of galaxies, so they occur more evenly across the sky [61, p. 51].

Additionally, higher cadence surveys allow for extremely rapid response to events with hours between detection and high quality observations (e.g. Hosseinzadeh et al. [50] discovering an event 3.5 hours after explosion⁷ and performing spectroscopy a mere 12 hours later). This has lead to discovery of early bumps in luminosity, particularly in the UV-band, which imply either interaction with a companion and surrounding material of the explosion, or an ad-hoc mixing of layers of burned materials throughout the detonation [35, 13, 51].

⁶notably, type II SNe emit most of their energy as neutrinos, which are not easily detected.

⁷time to explosion is inferred from peak magnitude and a fitted model to the light curve

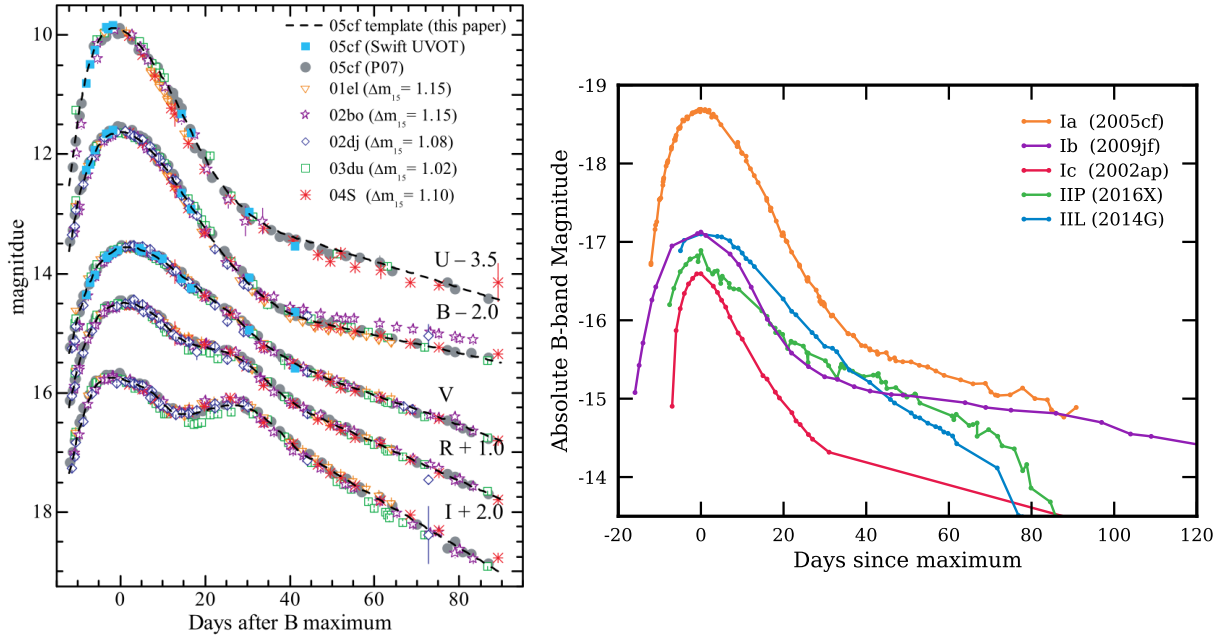


Figure 1.1: Left: Standardized group of SNIa lightcurves (adapted from [137]). Right: Light curves of other types in absolute B-band magnitude (data from Wang et al. [137](2005cf), Sahu et al. [114](2009jf), Foley et al. [32](2002ap), Huang et al. [54](2016X), Bose et al. [11](2014G)).

1.2.2 Spectrometry

According to emission lines in their optical spectra at peak brightness, SNe are split into two main groups depending on the detection of the hydrogen alpha line (Type II, SNII), or the absence of it (Type I, SNIa). Further, type I spectra split into three sub categories, subject to the particular absence of prominent lines of ionized silicon (SiII) and/or neutral helium (HeI) (see table 1.1, and figure 1.2)([29]). Line velocities for featured lines at this stage are in the range 20 000 to 25 000 km · s⁻¹

Away from peak brightness, late time spectra develop multiple iron emission lines in line with the radioactive decay of the large mass of nickel-56 produced in the detonation (see figure 1.3). At these late stages, heavy isotopes of iron group elements (IGE) show the imprint of a convolution of the initial conditions of density and temperature and the manner in which the progenitor became unbound (see section 1.4 below). Inversely, for pre-maximum spectra, intermediate mass elements (IME) show the most prominent lines of emission. Showing a large spread in both prominence and line velocities, this early developments in spectral features give rise to multiple sub-categories of SNIa, in what now known as the "SNIa Zoo" [127] (see figure 1.3).

A new venue for probing SNIa is *spectropolarimetry*, which concurrently measures the polarization of spectral features along with the slit photometry yielding the spectra [136]. So far, SNIa show little to no polarization in their continuum emission, with slightly higher values for high velocity spectral features, suggesting mostly spherically symmetric events with no particular line of sight effects [146, 16].

1.3 White Dwarfs

Progenitors of SNIa narrow down when considering the origins of the objects needed for themselves to happen. Primordially, a white dwarf has to be involved in the mechanism that generates them. Thus it is worthwhile to characterize such objects and their environments.

Table 1.1: Classification of supernovae.

Type	Hydrogen $H\alpha(\lambda 6563\text{\AA})$	Silicon $SiII(\lambda 6355\text{\AA})$	Helium $HeI(\lambda 5876\text{\AA})$	Model
Ia	No	Yes	No	Thermonuclear
Ib	No	No	Yes	Core-collapse
Ic	No	No	No	Core-collapse
II	Yes	No	No	Core-collapse

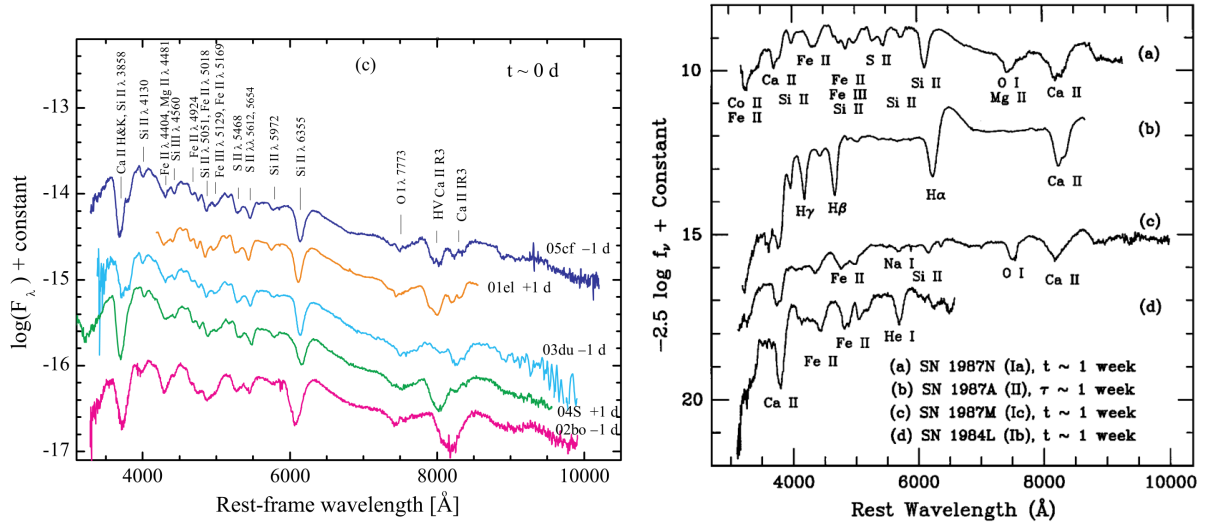


Figure 1.2: Left: Spectra of 5 different SNIa near maximum ([137]). Right: spectra of other types at maximum ([29])

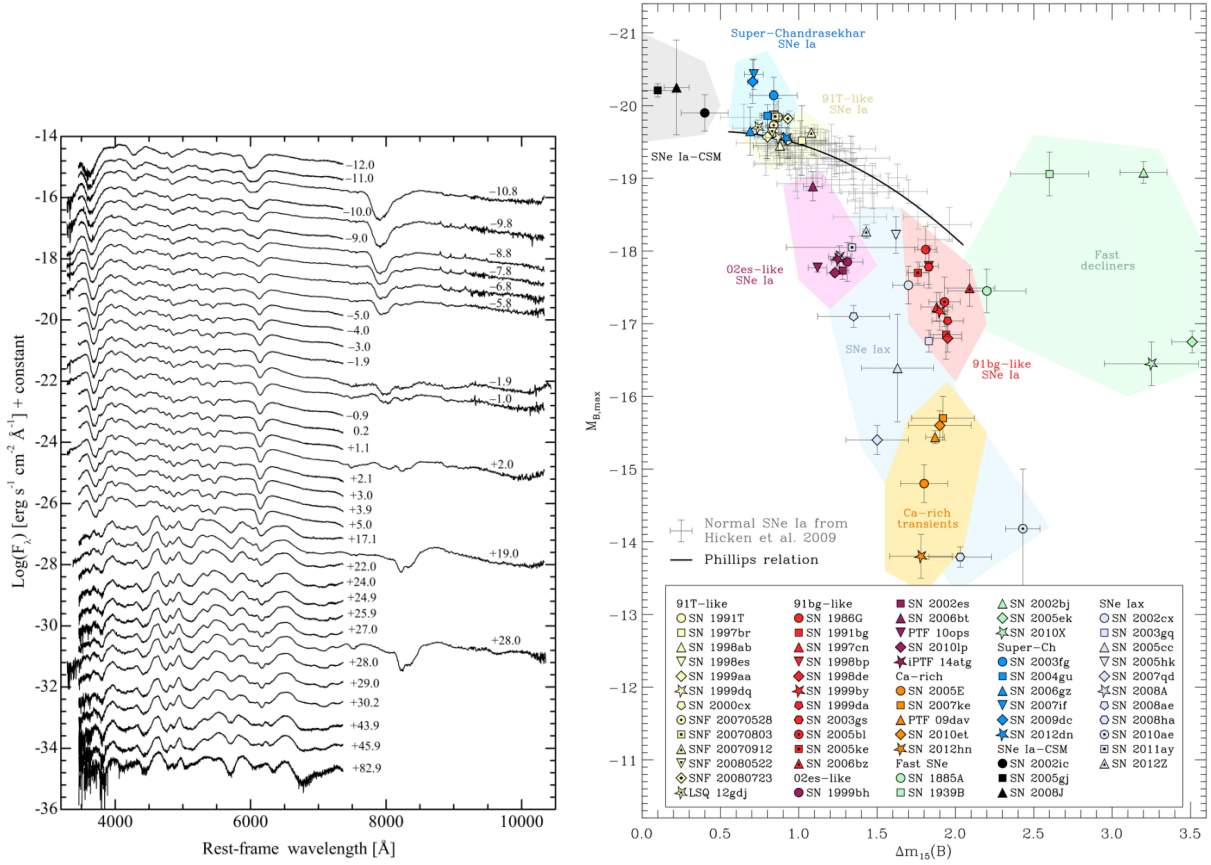


Figure 1.3: Left: Temporal evolution of spectra for a typical SNIa showing the emergence of a multitude of iron lines towards the UV ($\lesssim 5000$ Å) ([137]). Right: Plethora of SNIa subtypes, plotted by decline rate 15-days after peak in the B-band ($\Delta m_{15}(B)$) vs peak B-band brightness (M_B) ([127]).

1.3.1 Description

White dwarfs are low luminosity (usually less than $1 L_{\odot}$ when they are not interacting with a companion), dense ($\geq 10^6 \text{ g} \cdot \text{cm}^{-3}$ for most of their radius) stellar objects with radii comparable to Earth (around $9 \times 10^8 \text{ cm}$). They emit quiescent light from low temperature burning of helium or hydrogen on their surfaces heated by the slowly cooling hot core made of electron-degenerate matter. This core, which is overwhelmingly more massive than their envelopes, is formed from stellar fusion so it is principally made of the alpha species carbon and oxygen, with heavier white dwarfs adding neon and magnesium. Due to their extreme densities, their cores are supported by electron-degeneracy pressure, which follows a different equation of state. This forms a particular mass-radius relationship which follows roughly $M \propto R^{-1/3}$, implying that heavier white dwarfs are smaller. Further, this relationship eventually limits the maximum mass allowed by their volume to a key limit: the Chandrasekhar Mass (M_{Ch}), which set the maximum mass for any non-rotating white dwarf at $1.4 M_{\odot}$ ⁸. Currently, their best observed mass distribution favors objects of 0.5-0.8 $M_{\odot}$ [36].

1.3.2 Initial-Final Mass Relation

The initial-final mass relation (IFMR) is the semi-empirical relationship that tethers stars to their end-stages ([139, 14]; for a modern empirical calibration, see figure 3 in [26]). On one end, stars larger than $8 M_{\odot}$ sustain nuclear burning beyond the compositions of white dwarf cores and so their end-stages cannot produce them. On the other, extremely low mass stars have not yet left the main sequence⁹ so they also cannot yet become progenitors of SNIa. Now, at this mass range from near a solar mass to around $8 M_{\odot}$ the final mass of the white dwarf monotonically increases while the time to formation monotonically decreases, this sets three constraints on the progenitor problem: first, it sets a timescale for white dwarf formation and thus a timescale for SNIa to occur in galactic history at around 0.1 to

⁸this number depends on the treatment of electrons within a dense medium, but higher order corrections are around 0.01% [76]

⁹stable hydrogen burning phase at which stars spend most of their light-emitting lives. The start of this phase, the Zero Age Main Sequence (ZAMS) is a standard for timing clusters of stars, from *open clusters* with thousands of stars to *globular clusters* with hundreds of thousands.

10 Gyr. Second, it narrows the range of spectral types of objects to look for when searching for progenitors to the cooler end F,G,K spectral types¹⁰. And third, it sets a mass constraint based on the lifetime of a progenitor system, this is, if the environment of the progenitor is young when the event happens, its progenitor mass should be larger than older environments given that larger stars burn out faster than smaller ones, all things being equal.

1.3.3 Binarity and Interaction

Most stellar systems relevant to SNIa progenitors are part of binaries¹¹[109] and so, it is expected that most white dwarfs that can become progenitors of SNIa will have a companion once they have formed. And though most binary separations are large enough to not alter each of the members, a considerable fraction are sufficiently close so that the ending stages of one star can affect the evolution of its companion [100]. Stars vary their radius due to burning elements heavier than hydrogen (a phase called the asymptotic giant branch or AGB) and subsequently start shedding their outer layers (Thermally pulsating AGB or TPAGB). This affects the orbit and evolution of their companions, and for close cases, *Common Envelope*(CE) events occur where both stars mix their outer layers. CE events can significantly alter the evolution of both stars by essentially speeding up the end-stages of evolution of the star that begins to burn helium first, changing the composition of the outer layers of the companion, and reducing the angular momentum of the system causing orbits to tighten [3]. Post Common Envelope Binaries (PCEB) comprise a major group of potential SNIa progenitors since they are generally in a close enough orbit for it to decay via gravitational wave emission. This decay, though slow, eventually causes a merger between the two bodies [1].

¹⁰Stars have a direct temperature-mass relation codified by letters originally assigned to their particular spectra covered by the sequence 'OBAFGKM', with hotter(heavier) objects at 'O' and coolest(lightest) at 'M'

¹¹or systems with more stars interacting via gravitation. Systems of more than 2 similarly massive members tend to be unstable and so this work will focus only on binaries.

1.4 Explosion mechanisms

Overall, the thermonuclear disruption of white dwarfs (WD) cover all the requirements for SNIa events: Binaries containing WDs are common and prone to interactions, WDs contain the requisite high carbon content, are not hydrogen-rich, and are of compact physical size.

The archetypal progenitor introduces a common description of the event: A white dwarf surrounded by dense material compacted by an accretion stream from a donor ignites, causing the whole stellar remnant to become unbound. A clear distinction is made between the *core* made of extremely dense carbon and oxygen, with heavier masses including neon and magnesium, and the *envelope*, which is a less dense but still partially degenerate *shell* on top of the core with a varying composition made mostly of regular evolved stellar material (helium dominated), subject to mixing and compression from the donor’s envelope or accretion stream.

There’s many binary systems which can produce this outcome, outlined by the multiple combinations of three factors: the type or stage of evolution of the companion, the mass transfer rate towards the white dwarf, and the location of first ignition that starts the event (see table 1.2).

First, the nature of the donor must be such that mass transfer is possible in a manner that the receiving white dwarf can either grow in mass or immediately ignite. This allows most normal stellar objects of comparable initial mass to be donors in either their main sequence (hydrogen burning) or their red giant phases (AGB, see section 1.3.3). It also allows more exotic objects such as stripped core stars which have shed their envelopes via heavier mass loss through winds, or helium stars which are rarefied stars due to interaction via common envelopes.

Second, the build up to ignition varies from slow accretion of hydrogen-rich material from a main sequence star via Roche lobe overflow [45], to helium rich accretion from a red giant [77], then to more interacting systems such as a stripped core companion [5] or a helium star [78], and finally to another entire white dwarf colliding after a period of unstable mass transfer (a ”Double White Dwarf Merger” or DWD event)[95]. Any mass transfer has a feedback effect on the orbital separation of the system, therefore it either regulates accretion

Table 1.2: Progenitor scenarios.

Donor	Mass Transfer	First Ignition	References
Main Sequence	Accretion	Core	Han and Podsiadlowski [45]
Red giant	Accretion	Core	Liu et al. [77]
Stripped Core	Accretion	Shell/Core	Aznar-Siguán et al. [5]
He Star	Acc./Collision	Shell/Core	Liu et al. [78]
CO WD	Acc./Collision	Shell/Core	Pakmor et al. [94], Pakmor et al. [95]

or accelerates it by causing common envelope events, which may even reduce the separation to such an extent that gravitational waves can meaningfully decay the orbit to cause a merger [94].

Third, ignition can occur either as a subsonic deflagration or supersonic detonation (see appendix A) originating in the shell of the WD or via a deflagration/detonation inside the core [134, 115]. Shell ignitions are caused by the dynamics of the accretion stream (which may be as violent as a pre-merging event heating up the accreted layer) or convective heating of thicker layers on top of the white dwarf [43, 37]. Central ignition can be caused by three methods: (1) gravitational pressure within the WD provided it grows via steady burning of the accreted layer on top of it, (2) by rapid accumulation of the companion star’s material on to the white dwarf as they merge or collide, or (3) by pressure waves resulting from ignition of the shell [123]. While a central ignition guarantees the burning of the shell, the reverse is not true. If the shell ignites, it may not reach the conditions for the core to ignite, leading to a nova outburst, which does not unbind the white dwarf, though it can unbind the shell and may recur [97]. The case where the shell ignition does manage to generate a pressure wave of sufficient strength converging somewhere inside the core and causing it to also ignite is called a double-detonation scenario.

One final ingredient is the white dwarf itself, which depending on the mass at detonation alters the observable quantities of SNIa. For white dwarfs smaller than a solar mass, the term sub-Chandra (sub- M_{Ch}) is used while for heavier ones up to the Chandrasekhar mass¹², the term near-Chandra (near- M_{Ch}) is used. Historically, near- M_{Ch} scenarios took precedence due to the large luminosities needed to reproduce SNIa light curves, but the mismatch in spectral features from such large densities forced most simulations to use deflagration-to-detonation parameters, which allowed a cooler burn for the largest densities, and then evolving into a detonation for the outer layers of the white dwarf [64, 8]. More recent studies turned to subCh scenarios by adding surface detonations in the shell, which by virtue of it having a different composition can reproduce the deflagration stages of heavier models

¹²rotational or highly magnetic white dwarfs can have masses in excess of the Chandrasekhar limit, but still are included in this category

[30, 31, 141, 83]. Given that multiple mechanisms might actually take place in parallel, their overlap confounds their contributions to the overall rates of observed events [47, 52].

A particular scenario of the subCh family of simulations and a distinct focus of this work, is the double-detonation scenario (DDet). Characterized by Nomoto [88], this scenario involves a helium-rich shell detonating close to the core, developing a compression wave which eventually converges somewhere inside the core, sufficiently compressing it to start a secondary detonation within it to unbind the object. Historically, this scenario required a large mass of helium on the surface necessary for it to work [see, e.g. 79, 143, 49], leading to several signatures of the detonation matching poorly with observations [142, 49, 89, 30]

Given that the white dwarf population favors sub- M_{Ch} events, a search for working detonations with less massive shells was warranted, with many pathways to improve the outcomes of detonations including mixing heavier elements in the shell [117, 105], varying the shape and temperatures of the initial shell detonation [83], variations of when and where the double detonation occurs [106], chemical gradients [116], or sub- M_{Ch} mergers [94, 93]. Concurrently with these efforts, comparison to observations tended to align helium based detonations with the lower end of SNIa luminosities [7, 118, 121, 122].

Eventually, this scenario became versatile enough to align with a wide range of SNIa types: from normal SNIa [67, 141], to rarer calcium rich transients (see figure 1.3)[71, 59, 108], and a particular capability to emulate low luminosity SNIa [57, 42, 19, 144], albeit not clearly being the principal pathway for any specific event type [86].

Recently, a more involved mechanism that combines violent interaction with smaller helium masses has emerged where two rarefied cores with abundant helium in their shells mix their envelopes in a close orbit, causing a dynamically ignited detonation on either of the shells, which precipitates the nominal double detonation in the core [43, 120]. It is this rather involved scenario where most of the key characteristics of the progenitor event can be mixed and matched to simulations, specifically some leeway in the progenitor masses due to both members being similar, and a wide berth of accretion compositions and dynamic instabilities to form the conditions for detonation. It is within this scenario that a majority of multi-dimensional simulations today warrant initial conditions for their setups and no exception is made in this work [125, 126, 10, 96, 6, 113, 92].

1.5 Scope and Outline

The main goal of this work is to elucidate whether computational simulations which cannot resolve the enormous range in scales for the SNIa progenitor problem can properly evolve the final detonation stages of the event with consistent results. To this end, a specific type of scenario: the double detonation of a sub Chandrasekhar mass white dwarf with a slightly carbon and oxygen enhanced helium shell is evolved repeatedly with ever increasing degrees of freedom. While a fully converged solution might not appear, it is the main thrust of this thesis to build a consistent particular answer from purely theoretical simulations to confront to observations.

In Chapter 2, the computational setup is described, along with the input physics and initial progenitor properties. In Chapter 3, a two dimensional feasibility study of the computational setup is performed. Chapter 4 expands to three-dimensional setups with expanded nuclear networks.

Chapter 2

Simulation Setup and Domain

2.1 Progenitor Profiles

The starting component of the simulations, a white dwarf within a helium rich medium, is modeled by directly solving a one-dimensional hydrostatic equation at constant temperature and composition.

$$\frac{dP}{dr} = -\rho \frac{Gm(r)}{r^2} \quad (2.1)$$

$$m(r) = \rho \frac{4\pi}{3} r^3 \quad (2.2)$$

$$\frac{dP}{dm} = -\frac{Gm}{4\pi r^4} \quad (2.3)$$

with m, P, ρ, G, r , the mass, pressure, density, gravitational constant and radius, respectively. For any given step, a density is found by a Helmholtz free-energy tabulated equation of state (EoS) given an input pressure, composition and temperature. This density sets the mass, closing the solution at any given radii. This is integrated outwards increasing the radius by 10km each step with an initial condition set by fixing a central density for a starting minimum radius sphere. It is at this stage where two of the main constraints of the models are set *ab initio*, which is the target size in mass of the progenitor, and the size of the shell over the main carbon/oxygen core. A cutoff in density is decided beforehand at which the core ends and the shell begins, this splits the solution into the core and shell and can be

solved separately, provided the tail end of the core is correctly set as the initial condition for the shell.

The core is the principal mass component of the whole progenitor, with its target mass regulated by the initial condition of density at the center. On the other hand, the shell has more leeway in terms of mass and physical extension due to it being less dense and strongly affected by temperature. Further, the domain is arbitrarily extended by adding a tail exponentially declining in density subject to a scale height that allows a smooth transition in pressure from the tail end of the shell. Overall, the hydrostatic solution requires pressure equilibrium, so although there are both density and temperature jumps in the final solution, pressure follows a smooth transition into each part of the domain. This guarantees that the carrying over of the solution to the next codebase is initially stable.

Finally, picking the progenitor is bounded on the low end by the observation that most white dwarfs are in the range of $0.8 M_{\odot}$ but that the double detonation mechanism is easier to achieve on both larger masses and larger shells. Since larger shells are unrealistic as progenitors, the shell choice has to be the hottest possible without causing a direct detonation once the code is run. Following encouraging results from Fink et al. [31], a middle of the road model (model 3) is picked which sets an initial central density of $4 \times 10^7 \text{ g} \cdot \text{cm}^{-3}$ and the cutoff in density for the shell at $10^6 \text{ g} \cdot \text{cm}^{-3}$. This still leaves a selection of shells to put on top of the core, which also can be altered in composition. The final progenitor used throughout this work is shown in Chapter 3. The spatial extent of most of the progenitor covers around 8500 km including most of the mass of the shell, with the remaining very low density exponential tail accounting for less than a percent of the total mass.

2.2 Domain Scales and Physics

Since the problem pertains a white dwarf in a rarefied helium medium, the physical domain and thermodynamic gamut of the problem can be constrained. The physical extent must be such that it covers the majority of the mass of the progenitor. This is achieved quickly due to the density difference between the core and the shell, which causes the shell to decay rapidly in density within a few thousand kilometers, or around half a white dwarf radius.

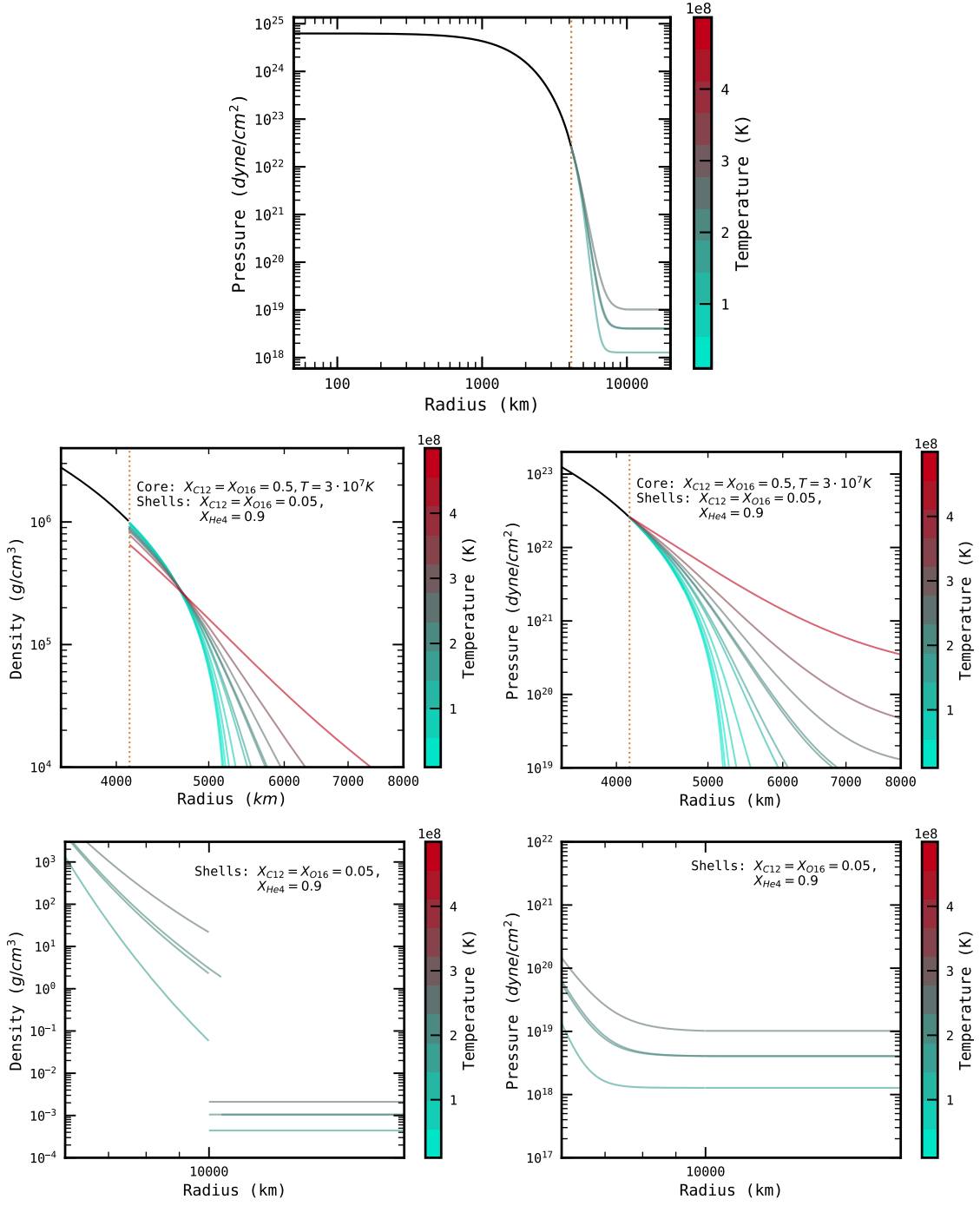


Figure 2.1: Various solutions to a spherically symmetric hydrostatic profile of a white dwarf. Top: full domain including core and three possible shells. Middle: Multiple possible temperatures for a single composition shell over the same core (Density and Pressure profiles). Bottom: Multiple exponential tails over shells of the same temperature (Density and Pressure profiles).

Now, even though the whole progenitor is included within around 9 thousand kilometers, further allowance in the domain guarantees the explosion remnants are still in the domain after the whole core becomes unbound. This allowance, though very large, cannot extend arbitrarily due to the eventual presence of the companion, which is not included in the domain. Specifically the domain becomes unrealistic at the Roche lobe overflow radius, which for a reasonable assumption of a 1.5 solar mass companion with a highly dynamical 15-minute long period around the simulated primary, comes down to around 10^5 km [25]. Next, the explosion velocities and dynamics of the problem warrant a rapid hydrodynamical treatment under Euler's equations of flow, with heating from thermonuclear products made during the progenitor becoming unbound, to wit:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (2.4)$$

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) + \nabla P = \rho \mathbf{g} \quad (2.5)$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot [(\rho E + P) \mathbf{v}] = \rho \mathbf{v} \cdot \mathbf{g} \quad (2.6)$$

$$E = \varepsilon + \frac{1}{2} |\mathbf{v}|^2 \quad (2.7)$$

$$P = \rho(\gamma - 1)\varepsilon \quad (2.8)$$

$$\text{Burn}(T, \rho)|_{dt} \implies \varepsilon, X_i \quad (2.9)$$

$$\text{EoS}|_{\rho, \varepsilon} \implies T, \gamma \quad (2.10)$$

$$\nabla^2 \phi(\mathbf{x}) = 4\pi \rho(\mathbf{x}) \quad (2.11)$$

where $\rho, \mathbf{v}, E, P, T, \mathbf{g}, \phi, \varepsilon, \gamma, X_i$ are the density, fluid velocity, total energy, pressure, temperature, gravity, gravitational potential, specific internal energy, ratio of specific heats and nuclear mass fractions, respectively. the first three equations are Euler's, while the others are auxiliary constraints for the problem to be solved. First, energy split into kinetic and internal, then, an ideal gas assumption relates pressure to internal energy. To enable compositional changes to the fluid, a nuclear network is solved to alter the internal energy of the fluid, which is then turned thermodynamically consistent by a tabulated equation of state. Finally, a Poissonian problem for gravity completes the right hand side of Euler's equations.

2.3 Source Code

Throughout this work, simulations will be run using the FLASH code [34], a modular code which can couple multiple systems of equations and perform optimizations subject to the requirements of the physics. The main modules used are:

Hydro solves the compressible Euler equations through the piece-wise parabolic method (PPM) [17], a second order Godunov finite-volume method (FVM). FVM methods are apt for unresolved shocks in the fluid due to averaging volumes before solving the equations, this in contrast with finite-difference methods which lose the shock due to it being a single point in the grid, breaking higher order solvers.

Burn calculates burning rates for a given network of species, updating the composition of the fluid and coupling the energy from said burning into the internal energy of the fluid (see section 2.4).

EoS applies a set equation of state for the simulation, updating either hydrodynamic variables or thermodynamic ones as required by their modules **Hydro** and **Burn**, respectively.

Grid uses an adaptive mesh refinement (AMR) criteria to increase the resolution of the simulation where needed (see below) [PARAMESH, see: 34, , and references therein].

Gravity solves the Poisson equation for the density distribution of the simulation via a multipole expansion, yielding an external field for the **Hydro** module.

2.3.1 Adaptive Mesh Refinement

Adaptive Mesh Refinement (AMR) consists in doubling the resolution of an existing simulation block by subdividing the block into halves in every dimension, provided some value within the original larger block triggers a certain condition. Given the vast difference in scales for the problem, namely from tens of thousands of kilometers down to sub-kilometer scales, adaptive refinement is vital to allow the simulation of the whole domain. Throughout this work, the resolutions quoted in text are the smallest zone the code is capable of resolving,

not the resolution over the whole domain. It is because of this that the refinement criteria should give utmost preference to the relevant property that is to be studied. In this case, the most important aspect of the simulations is to follow the composition changes in and near the core. This is achieved by setting three parameters to warrant a higher resolution in a particular zone of the domain: density, pressure and the molar fraction (Y_i). Density variations are particular to the large scale shape of the domain and the progenitor, most importantly they determine the changes between core and shell and shell and fluff (the lowest density envelope in the outskirts of the domain). Next, pressure allows the code to follow variations caused by the detonation and/or burning of material. And finally the molar fraction allows a higher resolution at the start of the simulation near the ignition point and along the edge of the core. Besides this, to further reduce computer load, these criteria are only allowed to reach the maximum resolution where the composition change produces a high rate of change in the internal energy, with the rest of the domain to remain at two levels of refinement behind the more active burning zones.

2.4 Nuclear Networks and Nucleosynthesis

Progenitors of SNIa require an astrophysical environment capable of unbinding a white dwarf. This implies that nearly a solar mass of principally carbon and oxygen at densities around $10^5 - 5 \times 10^8 \text{ g} \cdot \text{cm}^{-3}$ must be ignited with either another similar object or a significantly less dense envelope composed of elements lighter than neon. This constrains both the available species to burn and the permissible pathways for elements to fuse.

Burning regimes are either subsonic deflagrations or supersonic detonations (see appendix A). Detonations mainly form iron group elements (iron, cobalt, nickel and neighboring species, IGE) while deflagrations result in incomplete silicon burning, producing intermediate mass elements (IME) such as calcium or titanium [82, 112]. Of note is that this dichotomy, while useful in a descriptive sense, it does not take into account any dynamical interaction, therefore the final composition of a particular parcel of material might appear representative of a deflagration when a detonation that quickly expands or mixes with colder material can

present the same outcome. This is a particular insight from multi dimensional simulations, mixing and quickly changing dynamical conditions can favor different outcomes.

The formation of new elements (species) in thermonuclear reactions is governed by three of the fundamental forces: the nuclear strong and electromagnetic for baryons, and the nuclear weak for leptons. The first two set the terms for reaction rates between species via cross-sections for interactions and electron-screening rates for each pair of colliding nuclei, while the latter, though orders of magnitude slower, is key to nuclear yields due to being the only pathway for changing the proton-neutron ratio in a medium [48]. Taking a number N of species, and assuming that the relevant nuclear burn timescales can include up to three species interacting in a timestep¹ the evolution of species i is given by:

$$\dot{Y}_i = \sum_j^N \mathcal{N}_j^i \lambda_j Y_j + \sum_{j,k}^N \mathcal{N}_{jk}^i \rho N_A Y_j Y_k \langle jk \rangle + \sum_{j,k,l}^N \mathcal{N}_{jkl}^i (\rho N_A)^2 Y_j Y_k Y_l \langle jkl \rangle \quad (2.12)$$

where $Y_i = n_i/(\rho N_A)$ is called the nuclear molar abundance (in $\text{g} \cdot \text{mol}$), which normalizes the number of particles of type i (n_i) to the overall density of the medium², ρ is the local density of the studied parcel of the simulation, N_A is Avogadro's number, the $\langle ij(k) \rangle$ quantities are the velocity-averaged cross sections for two(three) species (including Coulomb screening factors), λ_j are decay rates for single particles (β decays, electron capture and photo-disintegration) and the $\mathcal{N}^i$ are stoichiometric values for each reaction, weighted by repeating species counting [85, pp. 419].

Once each abundance change is computed, it is linked to the hydrodynamics in two ways. First, locally through the energy released by the reactions ε_{nuc} :

$$\dot{\varepsilon}_{\text{nuc}} = - \sum_i N_A M_i c^2 \dot{Y}_i [\text{MeV} \cdot \text{s}^{-1} \cdot \text{g}^{-1}] \quad (2.13)$$

¹the most important resonant three-body interaction is the Saltpeter-Hoyle (triple-alpha) process since it involves the key element Helium and is extremely sensitive to temperature (T^{40}).

²therefore, a group of different kind of particles with atomic weights A_i multiplied by their respective abundances, sum up to one ($\sum A_i Y_i = 1$), no matter the volume. It is customary to use the mass fraction $X_i = A_i Y_i$ which is dimensionless.

where $M_i c^2$ is the rest mass of species i . And second, via an indirect non-local coupling due to species diffusion, convective mixing and advection of species through the fluid equations [85, pp. 425].

There are many situation specific networks [128], of which the most relevant for SNIa are those which focus on alpha capture with emphasis on neutron-capture processes. This is due to the events being realized in older stellar environments, where hydrogen burning is already extinct or negligible, and also due to the relatively high initial densities of the detonation, forcing a high level of neutronization [145]. Due to these considerations, a reaction network for calculating abundance yields during a detonation must consider all the species attainable through an environment similar to *Fe*-core forming in massive stars.

To this end, a customizable network of species is used: **XNet** is a "softwired"³ nuclear network integrated to the **FLASH** code, which can include an arbitrarily large net of reactions and isotopes. Through it, the typical 13 isotope network can be expanded *a gusto*, to treat specific relevant species for the detonation (see figure(2.2)).

Given the thermodynamic gamut of the problem, two compositions at distinct densities are subject to a range of temperatures, which based on nuclear burning alone can be broadly understood by their peak burning temperatures. Shown in figure 2.3, the envelope composition (90% helium-4 with 5% carbon and 5% oxygen at $10^6 \text{ g} \cdot \text{cm}^{-3}$) shows a quick transition from IME to IGE elements granted by the carbon and oxygen already present in the envelope in an alpha-rich environment. Higher temperatures allow a greater share of the end result composition to remain in lower proton species such as iron-54.

On the core composition case (50% carbon 50% oxygen at $40 \times 10^6 \text{ g} \cdot \text{cm}^{-3}$) burning timescales are longer due to the lack of initial helium-4 and less energy release from carbon/oxygen burning. Contrary to the envelope case, higher temperatures do not change the final outcome, only the timescales.

³meaning independent and expandable code, as opposed to "hardwired" in which the code is intrinsic to the main program.

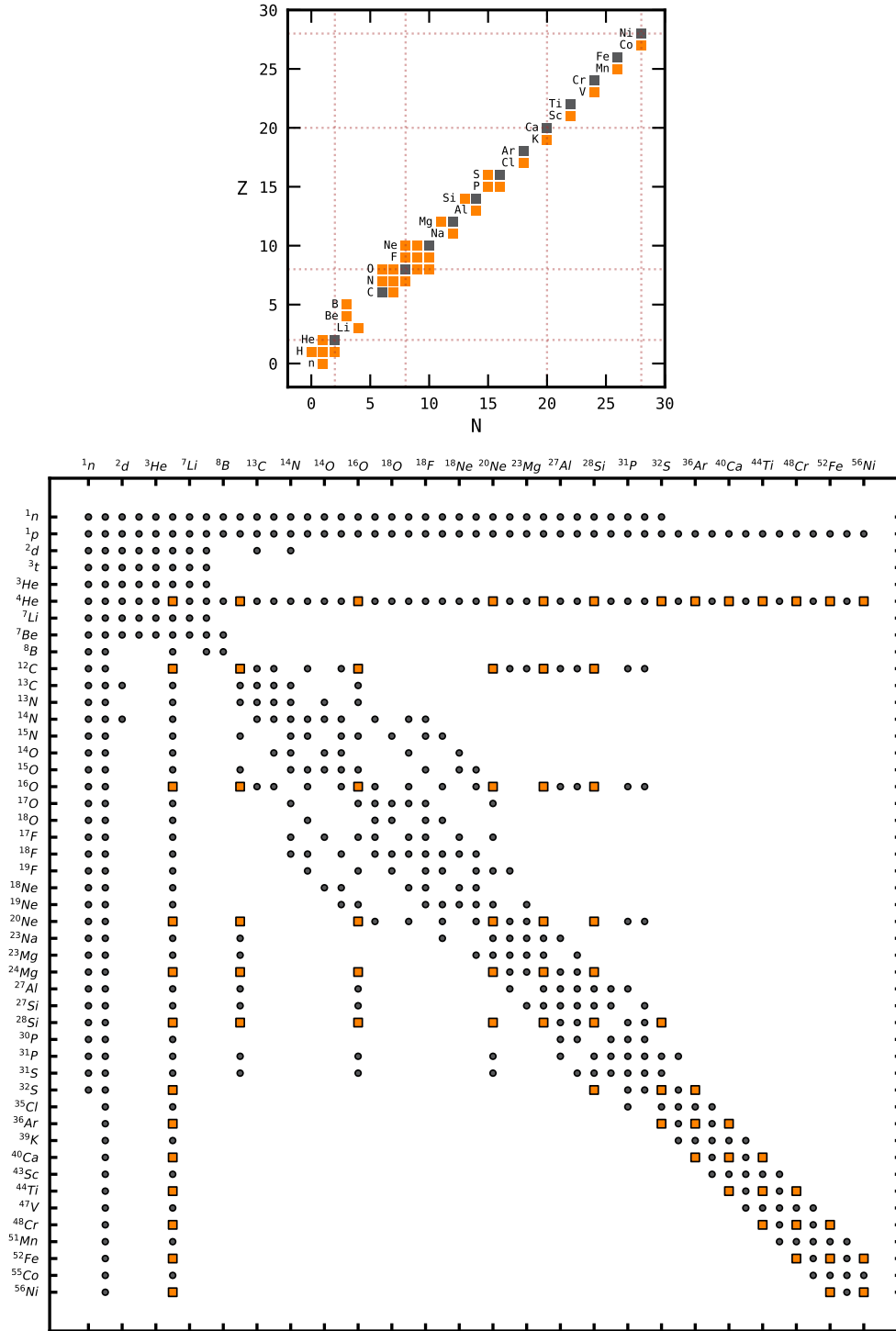


Figure 2.2: Top: XNet Isotope grid for 47 species with a 13 isotope alpha chain overlay (orange). Bottom: Rates active in the 47-isotope grid, with the alpha chain grid overlaid (orange).

Table 2.1: Relevant scales for the problem.

Property Ranges	
White dwarf size/mass	$5 - 7 \times 10^8$ cm, $1.9 - 2.3 \times 10^{33}$ g ($1.0 - 1.2 M_{\odot}$)
Envelope size/mass	$2 - 5 \times 10^8$ cm, $1.9 \times 10^{30} - 0.4 \times 10^{33}$ g ($0.001 - 0.2 M_{\odot}$)
Temperatures	$10^6 - 10^{10}$ K
Densities	$10^{-2} - 10^6$ g $\cdot$ cm $^{-3}$
Pressures	$10^{17} - 10^{27}$ dyne $\cdot$ cm $^{-2}$
Detonation timescale	~ 1.0 s
Detonation speeds	$10^7 - 10^9$ cm $\cdot$ s $^{-1}$
Rayleigh Number	$> 10^{11}$

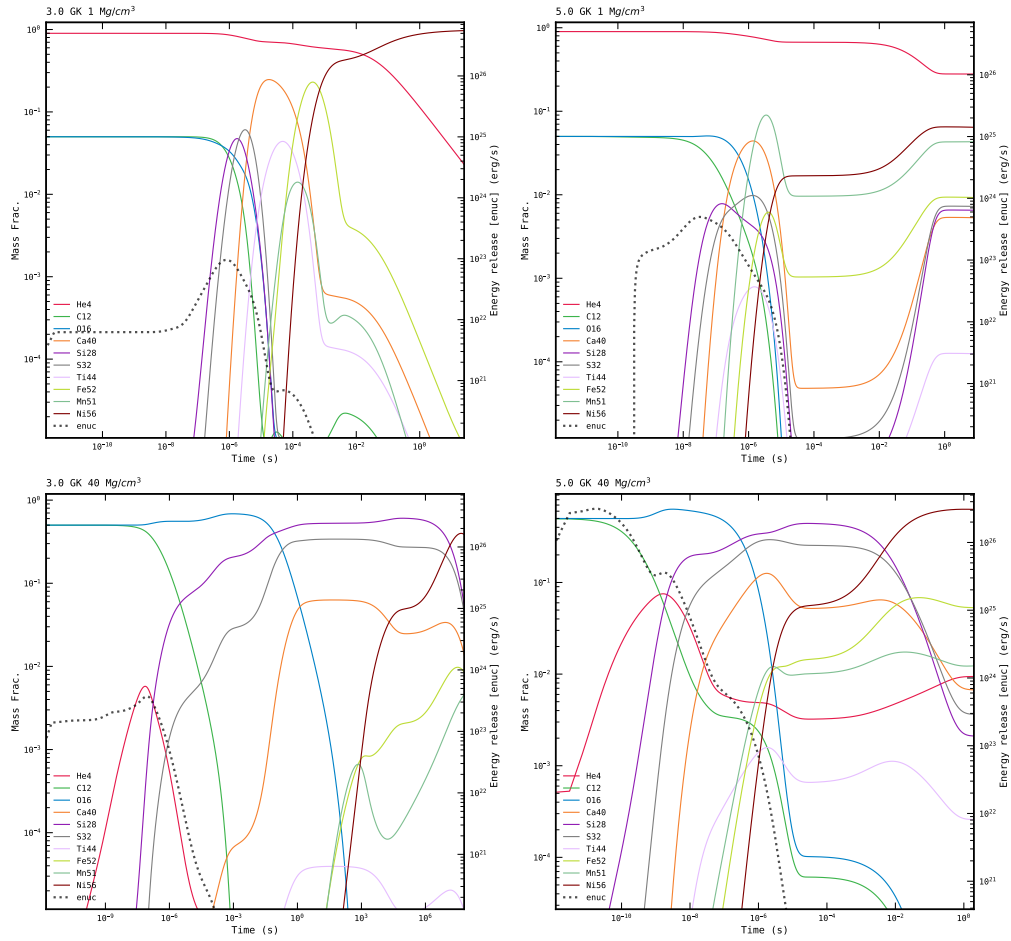


Figure 2.3: Single cell burning examples on a 47-isotope network (selection of isotopes plotted). Top: envelope composition starting with 90% helium-4 with 5% carbon-12 and 5% oxygen-16 at 10^6 g $\cdot$ cm $^{-3}$ at two temperatures (3 GK left and 5 GK right). Bottom: core composition starting with 50% carbon-12 and 50% oxygen-16 at 10^6 g $\cdot$ cm $^{-3}$ at two temperatures (3 GK left and 5 GK right).

Chapter 3

Two Dimensional Resolution Study

Statement of disclosure: This chapter is an attached version of the published journal article [111]. The author of this work is the primary author of this article.

3.1 Abstract

Thermonuclear supernovae are the result of the violent unbinding of a white dwarf, but the precise nature of the explosion mechanism(s) is a matter of active debate. To this end, several specific scenarios have been proposed to explain the observable traits of SNe Ia. A promising pathway is the double-detonation scenario, where a white dwarf accretes a shell of helium-rich material from a companion and a detonation in the resulting helium shell is the primary cause of the explosion. Through a set of two-dimensional grid-based simulations of this scenario we clearly distinguish three phases of evolution: external helium-rich detonation, core compressive heating, and a final core carbon burn. Though final disruption of the whole system is achieved at all resolutions, only models with minimum resolutions of 4 km and better exhibit all three phases. Particularly, core compression detonation is only observed for higher resolutions, producing qualitatively different nucleosynthetic outcomes. We identify the effect of finer spatial resolution on the mixing of hot silicon at the interface between the detonating helium layer and the underlying C/O WD as a primary driver of these dynamic differences.

3.2 Introduction

Type Ia supernovae (SNIa) are among the most highly luminous of stellar transients, occurring in both old and young stellar populations [81]. Their number, distribution, and a tight relation between their peak luminosity and brightness decay have made them useful for cosmological scale distance measurements ([101], [110], [4]). They also play an important part in the chemical enrichment of galaxies ([131], [27], [65]). Given their importance to these and other open questions, it is frustrating that our understanding of the details of the explosion mechanism is still incomplete. The production of large amounts of ^{56}Ni has been known to power their lightcurves for half a century at this point [98, 18], but details of the progenitor systems and the particulars of the nuclear burning that produce the radioactive nickel are a matter of active inquiry today.

In addition to the aforementioned production of ^{56}Ni , Type Ia supernovae are distinguished by the lack of H and He and the presence of distinct Si, Ca, and Fe features in their spectra. These spectroscopic features and the timescales over which they evolve have led to a strong consensus that their origin is the thermonuclear explosion of a C-O white dwarf [81]. Several scenarios have been invoked to explain the details of the explosion mechanism, including models with Chandrasekhar-mass white dwarfs (M_{Ch}) accreting material from both degenerate and non-degenerate companions and involving nuclear burning occurring in both subsonic (deflagrations) and supersonic (detonation) modes. However, in recent years, considerable attention has been paid to models of sub-Chandrasekhar-mass (sub- M_{Ch}) systems as potential progenitors that can produce results consistent with observations.

Here we focus on one specific model of this type: the double-detonation scenario. This scenario [87, 88, 143], involves accretion of helium from a rarefied donor onto the surface of a sub- M_{Ch} white dwarf. A detonation in the accreted shell leads to the disruption of the white dwarf either through an *edge-lit* ignition of the underlying C-O core [87, 88] or via the inward propagation of a shock into the core that eventually compresses a region of the core sufficiently to start a secondary *core detonation* [79, 143, 119]. The large amount (roughly $0.1 M_{\odot}$) of helium that was originally believed to be necessary for this model to work [see, e.g. 79, 143, 49] typically resulted in models with a significant overproduction of iron-group

elements [49, 89]. This led to studies of the viability of less massive shells [7, 122] and [31] did realize core detonations in two-dimensional models with shells with masses less than $0.1 M_{\odot}$. [83] also produced explosions in three-dimensional models using different ignition starting points and sizes, and helium shells enriched with some heavier elements. These models produce reasonable candidates for the lower-luminosity edge of SNIa [122]. Some recent work [120] has been centered on binary white dwarfs as progenitor systems for the double-detonation scenario. This scenario (the so-called 'D6' scenario) has been shown to be robust for a range of configurations while producing observational signatures that are roughly consistent with nucleosynthetic yields and ejecta velocities.

More recent studies have included the use of Lagrangian codes: [125, 126] studied close double white dwarf binaries and the effects of the detonation on the donor star. [41] investigated similar models to [31], but in three dimensions using a Lagrangian grid, a relaxation phase which mixes some of the shell and envelope, and somewhat coarser effective resolution. [41] also implemented a nuclear network to model the energy release and isotopic composition of the burned material. Core detonation is realized for all nine of their considered model systems, which include varying the ignition spot, using different masses, and varying the amount of carbon mixing into the shell. [132] exhibited similar results using an Eulerian code. [107] performed a parameter study at around the similar resolutions, but in one spatial dimension. Importantly, for some combinations of shell and core mass and initial detonation position, [107] note that edge-lit detonations result. They found that varying the ignition point position could instead produce a core detonation for the same shell and core masses and spatial resolutions.

This variety of edge-lit and core detonation outcomes and the seeming sensitivity to initial conditions motivates our work here. The differences between these two double-detonation sub-types could alter both the final composition of the remnant and the spatial distribution of that composition [28]. A source of uncertainty that has not been investigated systematically through parameter studies is the differing evolution of the detonation front at varying spatial resolution. To this end, we investigate the hydrodynamic evolution of a double-detonation through over an order of magnitude in spatial resolution. We find that spatial resolution, in the context of an Eulerian, adaptive-mesh-refinement code without additional methods to

control physical and numerical diffusion, does qualitatively impact the particulars of double-detonation explosion models, including the dynamics and other primary outcomes.

This paper is structured as follows: Our methods and setup are described in Section 3.3. Section 3.4 presents results of the simulations and a description of the observed phases of the explosion, whose duration and importance are functions of the grid resolution. In Section 3.5 we discuss the implications of our results to future simulations of this scenario, including those in three spatial dimensions.

3.3 Methodology

All of the simulations we describe here were carried out using the multiphysics code Flash-X [23, 46], an evolution of the widely-used FLASH code [34] for exascale computer systems. This modular code solves the compressible Euler’s equations on a Eulerian grid via a finite volume method. We also employ a small nuclear network (approx13, [129]) to compute the energy release and change in composition of the stellar material as the detonation propagates. The system of equations we must solve is completed using the Helmholtz tabulated equation of state [130]. Finally, the effect of gravity is computed via a multipole solver using 8 moments [21].

In addition to these particular choices of included physical modules, Flash-X uses adaptive grid refinement (AMR) to produce higher resolutions in key areas while maintaining a lower computational load elsewhere. In the simulations described here, refinement is triggered by tracking gradients in density, pressure, and molar fractions of the fluid. The resolution of density gradients are used because they mark the important features of the initial configuration, including the edge of the underlying white dwarf. Refining on pressure gradients allows the model to accurately track the position of the detonation shock and the compression wave that is observed in the stellar core. Finally, gradients in the mass fractions pinpoint the details of initial setup in a manner that guarantees a higher resolution around the shell-core interface from the start of the simulation. Additionally, 2 more refinement levels are allowed where energy release (ϵ_{nuc}) is sufficiently large ($|\epsilon_{nuc}| > 10^{16} \text{erg} \cdot \text{s}^{-1}$), yielding the maximum refinement level only where burning is vigorously occurring (meaning its rate

is enough to alter the dynamics of the simulation). Burning within cells that fall within the numerically thickened shock is not allowed, as per [33] and [99] to prevent numerical diffusion from affecting the propagation of the reaction front. [133] have shown that this practice reproduces the steady-state detonation speed and does not affect the extended reaction structure beyond the initial carbon burning stage in the FLASH code.

We note that burning is moderated via the Flash-X runtime parameter `enucDtfactor` (ε) which restricts the time step to be a constant fraction of the nuclear energy release timescale, calculated as the ratio of the internal energy (E_B) and the nuclear energy from burning per unit time (ϵ_{nuc}) over the hydrodynamical timestep $\left(\varepsilon \frac{E_B}{\epsilon_{nuc}}\right)$. A method of restricting the energy release from nuclear burning has been suggested by [70], and this scheme has been used in several studies with physical parameters like the ones described here [e.g., 10]. This technique evolves the simulation at the CFL-limited time step, relaxing the restriction imposed from fully resolving the nuclear burning timescale by renormalizing all of the burning rates within a cell if the energy delivered in a time step exceeds some fraction of the cell’s internal energy. This prevents sudden changes in the nuclear energy release at the onset of a detonation in the context of an operator-split scheme from sharply reducing the overall time step. [62] caution that the use of such a limiter may lead to unexpected suppression of burning in regions where ignition should occur. However, [69] argue that this finding and many of the details in [62] are not generic to the use of the limiter, but, rather, depend on specifics of the simulations carried out therein. Because we do not require the use of the limiter here and our desire is to restrict our study only to the particular effects of spatial resolution in our Eulerian code, the limiter of [70] is not implemented in our simulations.

3.3.1 Numerical Setup

The domain uses cylindrical symmetry and is sized to encompass both the white dwarf itself and its immediate surroundings, reaching an extent of $\{r, z\} = \{6.5536 \times 10^4 \text{ km}, 13.1072 \times 10^4 \text{ km}\}$. This domain size is required (indeed, it is likely the minimum useful extent) because the envelope is expelled considerably outwards before the onset of any core detonation. At the same time, upper limits for the domain size must be chosen so as to avoid the accretion disk and inclusion of the companion, given our ignorance of how the accretion process actually

impacts the dynamics. The burning module uses Flash-X’s approx13 13-species network with ^4He , ^{12}C , ^{16}O , ^{20}Ne , ^{24}Mg , ^{28}Si , ^{32}S , ^{36}Ar , ^{40}Ca , ^{44}Ti , ^{48}V , ^{52}Cr and ^{56}Ni . This network uses effective rates tuned to more accurately capture nuclear energy generation and captures the bulk behaviors of isotopic flow and hydrodynamic feedback for the thermodynamic conditions and timescales encountered in the simulations we considered.

The initial 1D profile is based on Model 3 from [31]. We construct the model by directly querying Flash-X’s equation of state with an initial central density of $4.15 \times 10^7 \text{ g} \cdot \text{cm}^{-3}$ and a composition for the white dwarf of $X_{^{12}\text{C}} = X_{^{16}\text{O}} = 0.5$. This is integrated outward subject to hydrostatic equilibrium and assuming spherical symmetry to a density of $10^6 \text{ g} \cdot \text{cm}^{-3}$, where the composition is changed to a mixed value of $X_{^4\text{He}} = 0.90$, $X_{^{12}\text{C}} = X_{^{16}\text{O}} = 0.05$ to start the shell. Outward integration continues until the shell reaches densities of roughly $20 \text{ g} \cdot \text{cm}^{-3}$. Finally, for numerical stability purposes, a hot, exponential density scale height tail is added above the shell extending to the domain limits. This tail is read into the initial conditions in Flash-X as an isothermal fluff.

A total of five simulations were performed at maximum resolutions of 16 km, 8 km, 4 km, 2 km, and 0.5 km. These resolutions represent the highest levels of grid refinement reached by the AMR and cover salient regions of burning in the domain. All five simulations are initialized with the analytical profile shown in Figure 3.1, which amounts to a C-O core mass of $0.981 M_{\odot}$ with an overlying ^4He -shell mixed with 5% ^{12}C and 5% ^{16}O by mass fraction adding a total additional $0.058 M_{\odot}$ to the domain. This envelope split into $0.050 M_{\odot}$ forming the shell proper out to 8410 km, and $0.008 M_{\odot}$ in the low-density “fluff” filling the rest of the domain. The assumed carbon-oxygen pollution in the envelope stems from multiple mechanisms before ignition: the companion’s accretion stream composition, burning of some helium in the shell, and dredge-up from the core into the envelope [84, 122]. Our choice for initial enrichment of the fuel (5% ^{12}C and 5% ^{16}O) is motivated primarily from the results of [84], where this choice produced detonation velocities and burning length scales that were roughly the median of the values considered therein.

To achieve ignition in the accreted layer, sufficient energy must be deposited in a small enough area to produce a self-sustaining detonation in the helium-rich shell. This is done by directly altering the thermodynamic state of a selected set of zones in the shell. An increased

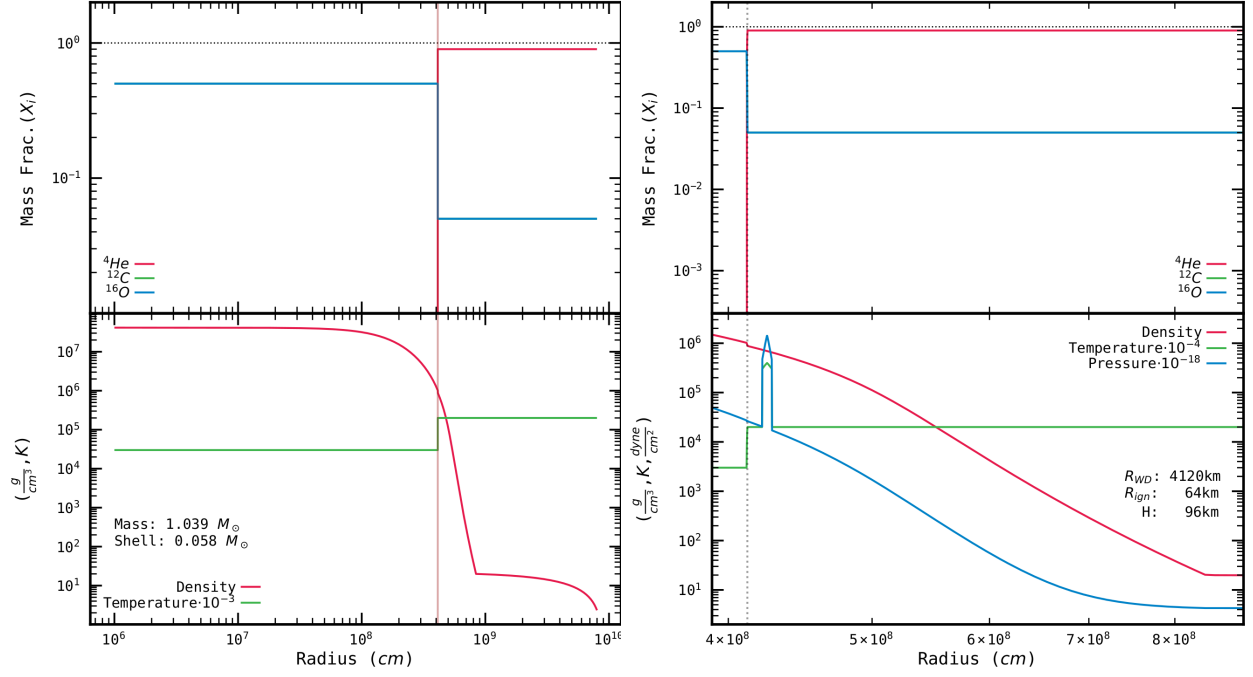


Figure 3.1: Left: Spherically symmetric, hydrostatic analytical profile made with initial conditions for a central density and composition and closed with the Helmholtz equation of state. Right: Magnified line-out of the initial profile above the WD surface in Flash-X with the heated bubble added to ignite the detonation.

temperature at a given density is typically used to start detonations of this type, but this does not guarantee the detonation will be self-sustaining. Therefore, the spatial extent of the heated region and the gradients in various values must also be chosen carefully. [83] achieve self-sustaining detonations in their least massive, pure-helium shell ($0.045 M_{\odot}$), 2D axisymmetric model by increasing the temperature in zones within a radius of 25 km from the ignition point using a peak ignition temperature of 2 GK that has a slight linear decline towards the edge of the region. Notably, [83] achieve detonation propagation only when the resolution reaches 2 km, with coarser resolutions not able to sustain the detonation. [37] model convection of accreting helium onto the core with a 2D wedge centered around the core-shell interface. While convection mixes the helium with the carbon-oxygen core blurring the interface, detonation conditions (burning timescales faster than both hydrodynamical and convective timescales) are achieved at around 100 km above the closest pure carbon-oxygen composition boundary. Finally, [31], do not achieve a detonation for a small (of order a few 8 km cells) 3 GK ignition zone. Considering these previous studies, we set the initial ignition condition as a heated bubble at the pole, centered at 100 km above the surface of the C-O core. This region has a radius of 32 km, regardless of resolution, to achieve a relevant size in the 16 km case. Within this region, temperature is set to 3 GK and linearly increases towards the center of the bubble to 4 GK to ensure a detonation in the shell at all tried resolutions. A line-out through the central ignition point of this 2D initial configuration is shown in the right panel of Figure 3.1.

3.4 Results

3.4.1 Dynamics

For all resolutions tested here, the entire star is unbound within three seconds of the initial helium-shell ignition, however the process of the explosion depends on resolution. The principal features of the highest resolution scenario are shown in figure 3.2. The initial edge-lit detonation is not strong enough to ignite the core outright, but rather the detonation front makes its way around the shell, quickly enveloping the C-O core and generating mostly

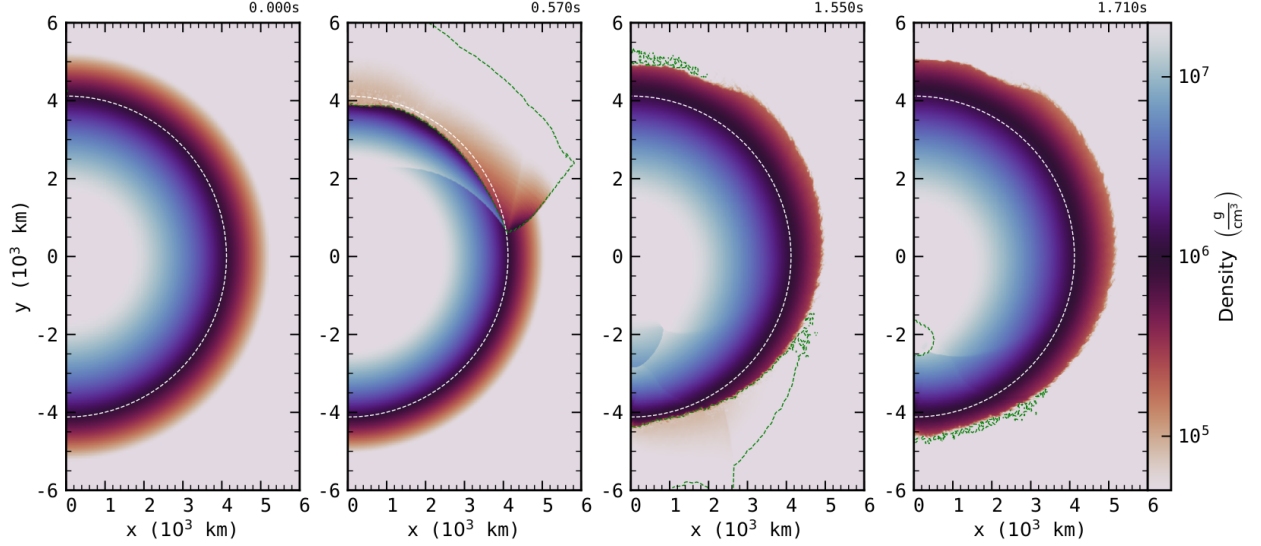


Figure 3.2: Key features in the evolution in density for the maximum resolution case (0.5 km). The white contour marks the initial edge of the WD (4120 km), while the green contour traces a temperature of 1 GK. To start the detonation, a small region is artificially heated above the WD along the axis of symmetry as described in Section 3.3.1. Initially, a supersonic front propagates around the edge of the core, burning mostly shell material with some incursion into the core via mixing. After reaching the antipodal point at 1.2 s, shell burning subsides. Throughout this stage, the core is compressed due to the initial shock of the ignition aided by the surrounding burning front. These compression waves converge at an off-center point inside the core at around 1.6 s, causing a secondary carbon detonation that unbinds the system. A single panel animation of the time evolution is available. The animation shows the density, covers the same spatial extent and runs from 0 to 2.6 s highlighting the same contours as shown in the figure.

intermediate mass elements as products of explosive helium burning. The detonation propagates along the limb of the core (shown as the green contour in Figure 3.2), increasing the lateral pressure and creating a pressure wave directed inward, but not strictly radially. After ≈ 1.5 s, the shell, the initial innermost extent of which is marked by the white contour in Figure 3.2, has expanded sufficiently to quench any relevant composition changes and the shell detonation subsides. Shortly after this time, the initial inward pressure wave converges at an off-center point in the core, igniting a second detonation via compressional heating. This detonation is strong enough to unbind the white dwarf, as shown in the last panel of figure 3.2. We refer to this outcome as Case 1 and note that it only obtains in simulations with minimum cell widths of less than or equal to 2 km.

A pivotal difference appears at resolutions of 4 km and above, as shown in figure 3.3. The wake of burned material behind the detonation front deposits a threshold amount of energy at a point on the limb of the WD when the front reaches the symmetry axis, causing a secondary antipodal (with respect to the original ignition point) detonation, which ignites the core at its edge. This detonation immediately propagates into the core. It obviates the effect of the compressional heating from the earlier stages of burning by burning through the convergence point before the pressure wave reaches that locus (Case 2). This is in contrast to higher-resolution runs, where the shell burning is quenched by the expansion of the envelope and does not produce a secondary shell detonation. In these higher-resolution simulations, the only process producing a core detonation is a separate ignition through compression (Case 1, as described above). We once again note that due to the asymmetric ignition condition, the convergence point is far from the geometric center of the WD; namely, over 2000 km from the center for all examined resolutions.

The core-shell-interface detonation observed in the lower-resolution cases is driven by the compression of hot, partially burned and significantly mixed material as the initial shell detonation front collides with itself at the reflecting boundary at the second pole of the configuration. This material has been swept up during the earlier progress of the detonation front around the edge of the WD. The coarse resolution of the less-resolved cases produce a mass of compressed material at this focus point that is considerably large than in the higher-resolution cases because of the relative lack of spatial resolution (see figures 3.4 and

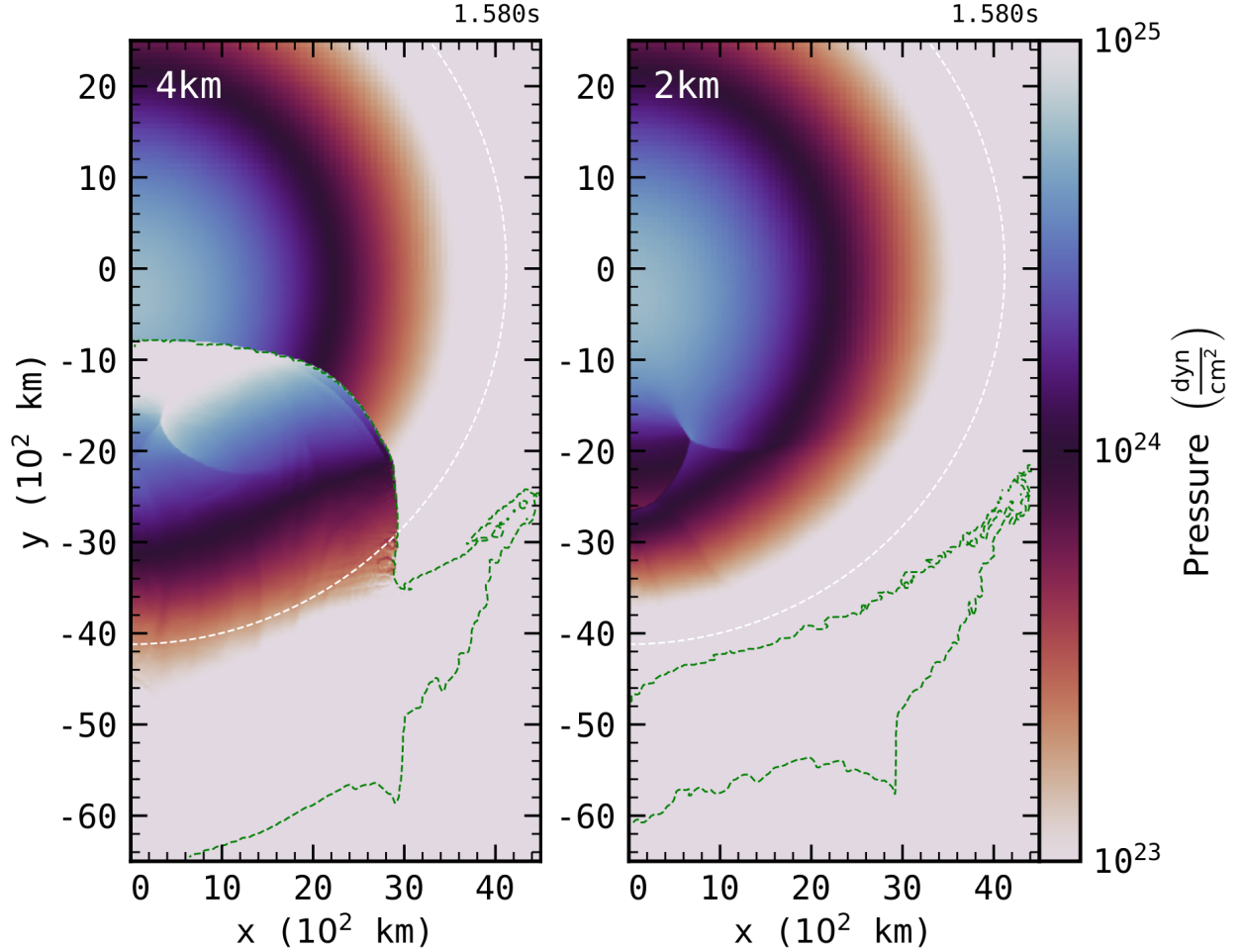


Figure 3.3: A magnified view of the antipodal point for two different maximum resolutions. As in the previous figure, the white contour marks the WD extent while the green contour demarcates a temperature of 1 GK. Left: The four-kilometer resolution case is driven not by a core ignition but rather an antipodal detonation. In this case, shell burning continuously mixes and progressively burns some mixed core material. Right: The two-kilometer case driven by off-center compression. This case burns the core after a distinct pause in shell burning, and separates the two detonations spatially and therefore also in terms of density.

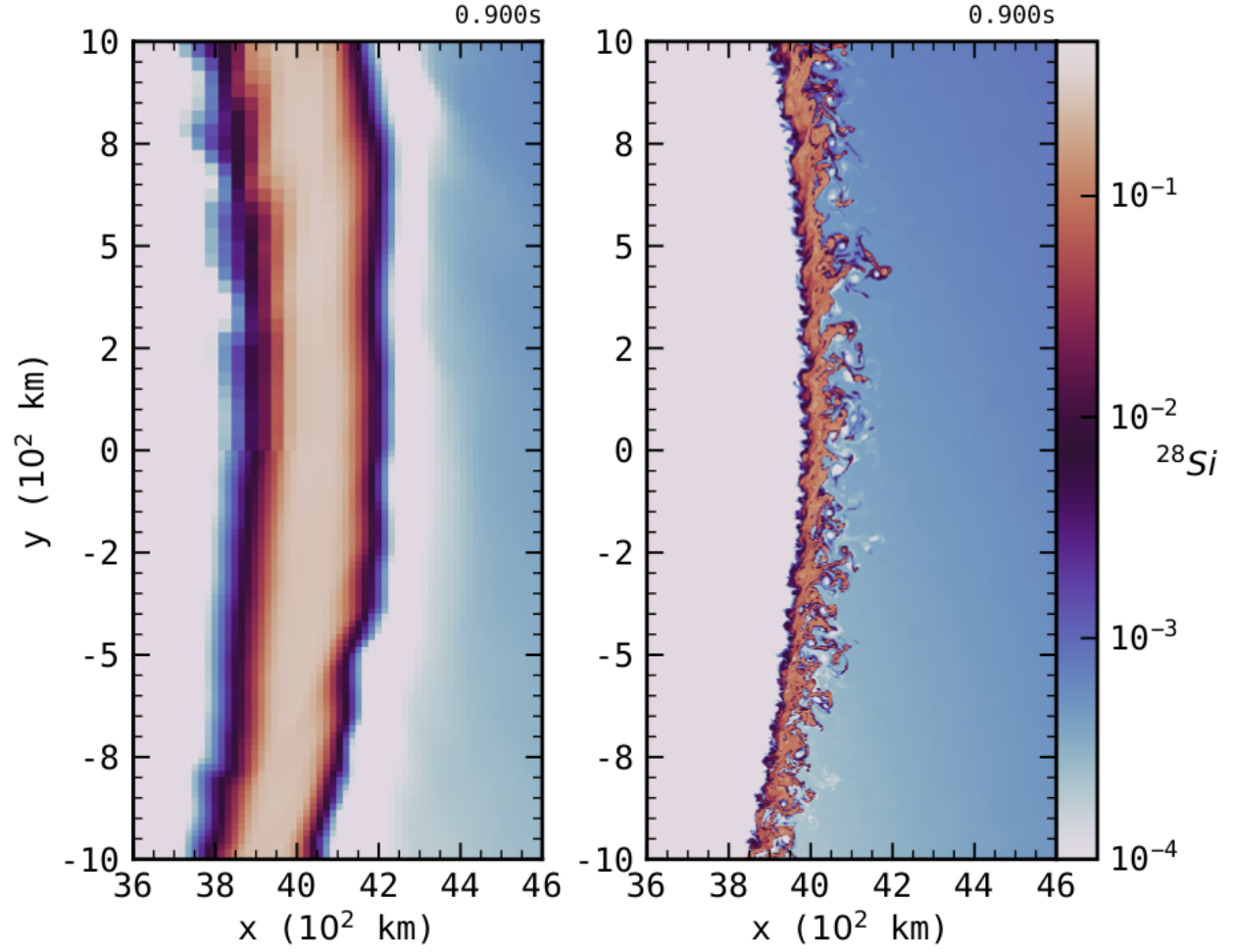


Figure 3.4: Outer shell burning remnants: equatorial slice of mass fraction of silicon-28 at the WD limb after shell burning traverses the whole cutout. At 16 km resolution (left), the thickness of the expanding band is 4 times larger than in the highest resolution case (0.5 km, right). Additionally, mixing is far more complex and evolved even at scales which do not represent the actual length scales of burning.

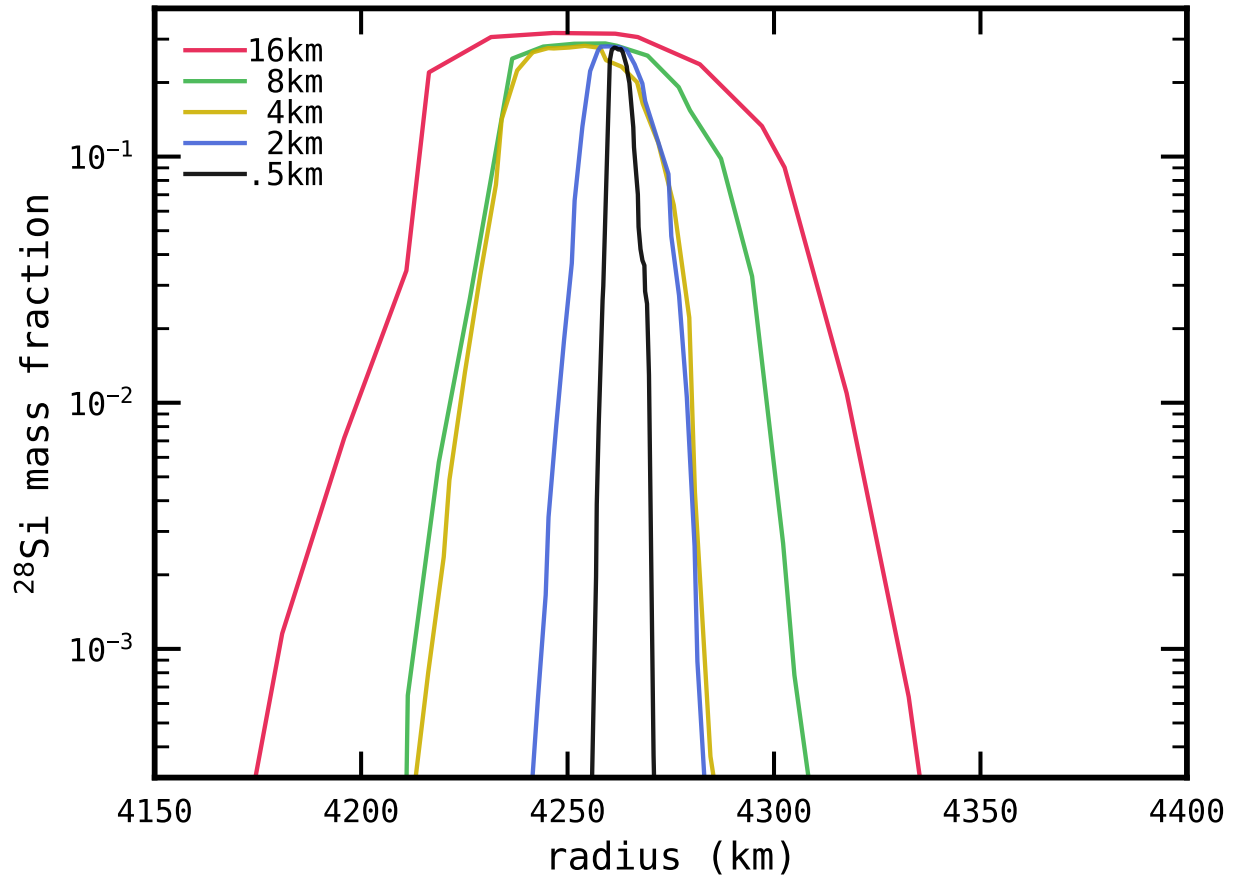


Figure 3.5: Silicon burning front thickness for all cases, measured at 20 degrees from the antipode.

3.5). In addition, this material is preconditioned for explosion via the artificial mixing of hot, partially burned shell material and underlying core material. This numerical effect is apparent in Figure 3.4. The coarser resolution spuriously smooths sharp gradients in composition at the shell-core interface, causing the suppression of fluid instabilities that are clearly visible in the higher-resolution cases. Without this additional numerical mixing, the antipodal material is insufficiently compressed and heated by encountering the reflecting boundary at the second pole, allowing time for the off-center core detonation to be triggered deeper in the core of the WD. More quantitatively, we calculate the internal energy of the matter for the domain within 4×10^8 cm of the center of the system (the 'core') and outside of said radius (the 'shell'). Both the peak energy release as a function of position and the total overall energy being deposited in the matter are shown in figure 3.6. The left figure shows the explicit separation of shell and core burning and the transition in the nature of this distinction as resolution is increased. Evident is a distinct shift of approximately 0.5 s in core ignition for case 1. The right figure further reinforces this separation by showing that at resolutions finer than 4 km, burning subsides in the shell before the core can be ignited at the limb by the original detonation wave. In all of the simulations we find that the detonation speeds during the burning of the envelope agrees well with other simulations at around $10\,500 \text{ km} \cdot \text{s}^{-1}$ [31, 41]. We also find consistent detonation speeds in simpler configurations (i.e. two-dimensional burning tubes) using the same reactive flow code, also agreeing with earlier work [134]. The curvature of the propagating front in all simulations described here tends to $0.05 \times 10^{-7} \text{ cm}^{-1}$, which according to the analytical solutions given by [24] for similar densities and a pure helium fuel correspond to speeds in a range of $10\,000 - 12\,000 \text{ km} \cdot \text{s}^{-1}$.

We note that previous investigators have also obtained a variety of outcomes that are qualitatively similar to our Cases 1 and 2. [31] used a level set with two advected scalars to model burning in their simulations, effectively preventing core burning until the core reaches a certain temperature. Their results are very much like our Case 1: off-center detonation due to converging waves from the initial shell detonation. [83] probed multiple initial detonation sites in both two and three dimensions, obtaining an off center hotspot in all simulations. More recently, [10] running with a similar codebase in two dimensions obtained Case 1 scenarios for all but the heaviest shell they investigated ($0.1 M_{\odot}$). That heaviest case is very

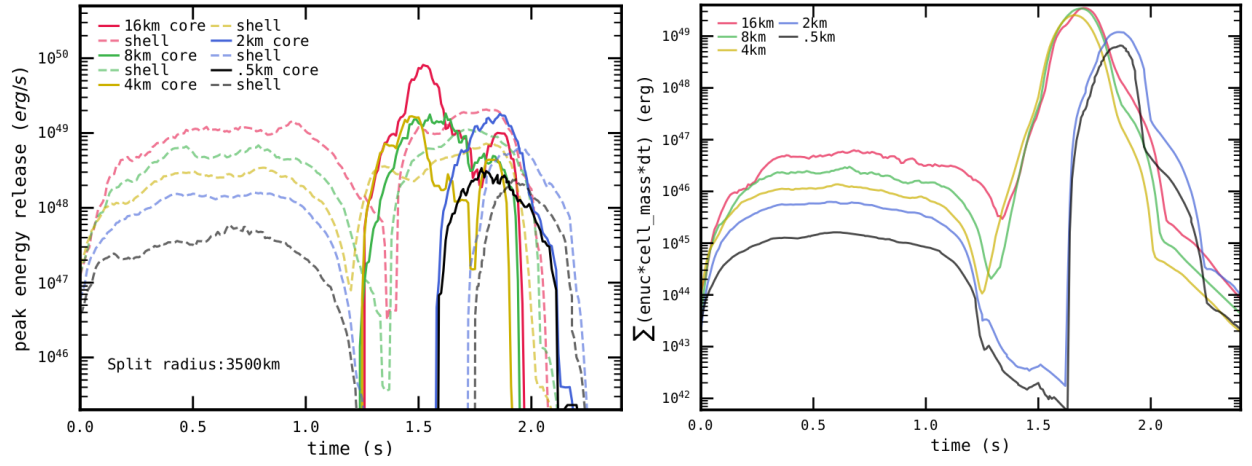


Figure 3.6: Left: Peak positive energy release within the domain, split into values for the 'core' and 'shell' based on radial distance from the domain center (split radius). Right: Total energy added to the domain via burning. Two families of solutions emerge based on the dynamics of the event: a direct shell to core burning at resolutions over 4 km, and a case with clearly separated shell and core burning stages at finer maximum resolutions.

similar in origin and evolution to our Case 2. [125, 126], modeling a large three dimensional domain that includes both progenitor and companion, also obtain outcomes very similar to our Case 1 and notably show a distinct thick silicon shell which maintains its shape well out into the domain. A notable counterpoint is found in the three-dimensional simulations of [41]. In a setup similar to ours on a Lagrangian grid, they find a Case 2-like scenario with a distinct antipodal detonation (they dub this a “scissor mechanism”) where the shell burning front crosses over itself at the antipode, pinching the partially mixed limb of the core enough to start a detonation. Following the pinch, this limb detonation reaches the expected core ignition point before a Case 1 scenario occurs.

3.4.2 Nucleosynthesis

Final yields from the modeled explosions are shown in Figure 3.7, taken at a time where the energy release falls by ten orders of magnitude from shell-burning levels. Using the two higher-resolution cases as fiducial (2 and 0.5 km), their relative differences in yields vary by less than 10% except in 2 species: Mg(11%) and Ne(18%). With respect to differences that appear across both cases, larger and distinct differences are seen when comparing the 4 km vs the 2 km case. In this comparison, the largest differences arise in magnesium(62%), neon(30%), silicon(13%), and oxygen(20%). Shell burning is remarkably similar in all cases, regardless of resolution, particularly in terms of the velocity of the burning front (where the detonation velocity differs by no more than 2%). However, as previously discussed, there is significant variation in the thickness of the mixing layer between the burning shell and the underlying core, with coarser resolutions mixing the edge of the core as the detonation goes around it. These thicker fronts produce a higher mass of intermediate elements as opposed to higher resolution cases, which do not mix and burn as much core material under shell burning conditions (Figure 7). Since shell burning is the principal contributor of neon, the effect of the artificial thickening of the burning front due to resolution is best observed in this species, where the difference in yield from our coarsest to finest resolution cases is roughly a factor of two.

Other intermediate species (Mg, Si, S) show a large variation with resolution, not only in their yields but also in their spatial extent (see figure 3.4). This is a direct effect of

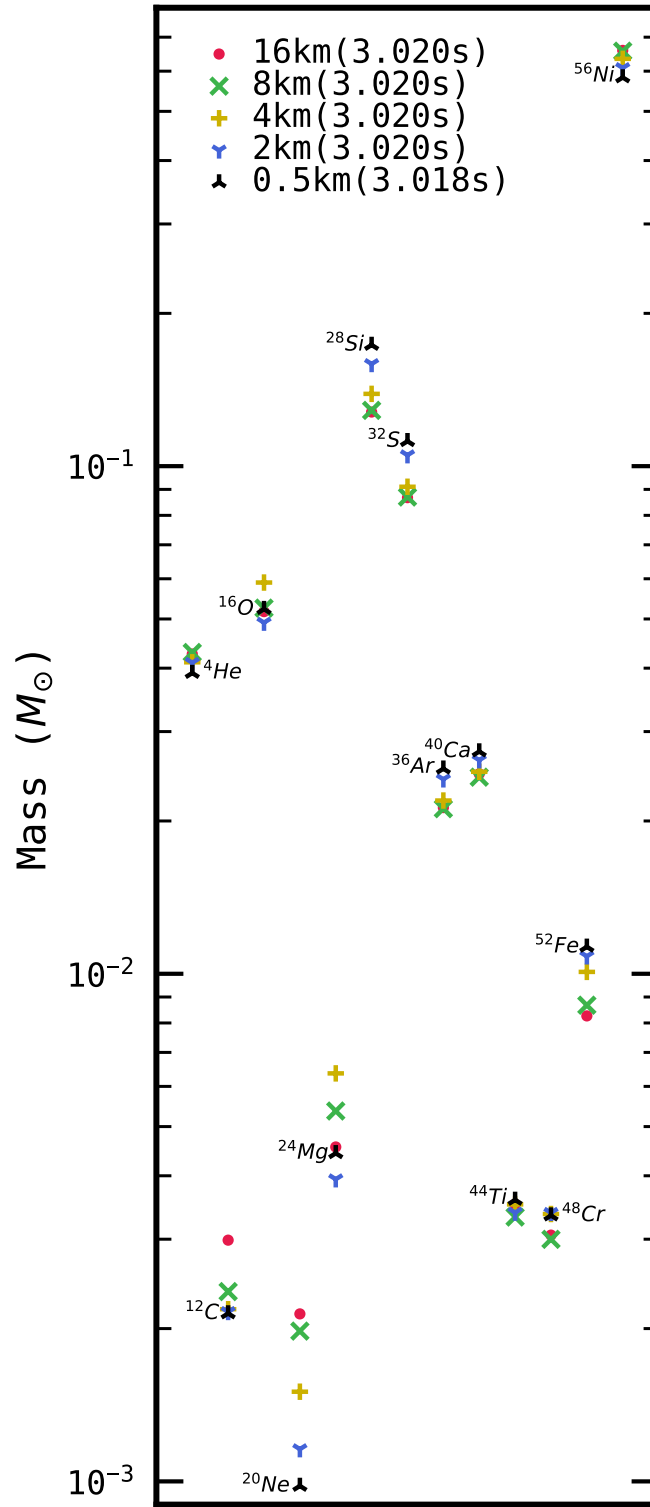


Figure 3.7: Final yields from all simulations.

improving resolution in a problem where the real burning front is never resolved, and results in a distinctly thinly layered composition as opposed to a thick, more thoroughly mixed composition.

Coarser resolutions burn from the limb of the WD, causing the core to burn at progressively higher densities towards the center and compressing the material closer to the center. On the other hand, finer resolutions manage to ignite the core from a near-central position, causing core burning to start at a higher density and progress towards the lower densities at the edge of the WD. This difference in the cases causes what is shown in figure 3.8. Further clarity can be seen in figure 3.9. For Case 2, due to the secondary detonation starting at a lower density near the edge of the white dwarf, a substantial portion of the core is burned while the front is climbing the density gradient towards the center of the core. This material is burned at lower temperatures yielding more intermediate mass elements. This behavior is exhibited via the silicon mass fraction, shown in the left group of figure 3.9 for two representative resolutions. On the other hand, Case 1 begins its secondary detonation closer to the center of the core at a much higher density. This burning front starts at high temperatures and propagates outward, down the density gradient of the core. But, because the front starts inside the core, much more material (at higher density) is quickly burned to nickel. The front eventually reaches most of the material that Case 2 burned, but encounters this material at a higher temperature than was realized in Case 2, burning most of that material all the way to nickel (shown in the right panels of figure 3.9). In Case 2, the detonation starts at a lower density and climbs the core density gradient, yielding comparatively less nickel. As for Case 1, the detonation starts at higher densities than the coarser resolution cases.

3.4.3 Ejecta structure

The final simulation ejecta structures are shown in Figure 3.10. Shown are velocity distributions of three 30 degree sized wedges fanning out into the domain from the geometrical center with their angular center aimed at 3 specific angles (θ) each measured from the center of the core hemisphere ($\{x, y\} = \{0, 0\}$, and defined such that positive angles point towards positive y): one pointing towards the equator ($\theta = 0^\circ$), one at 45

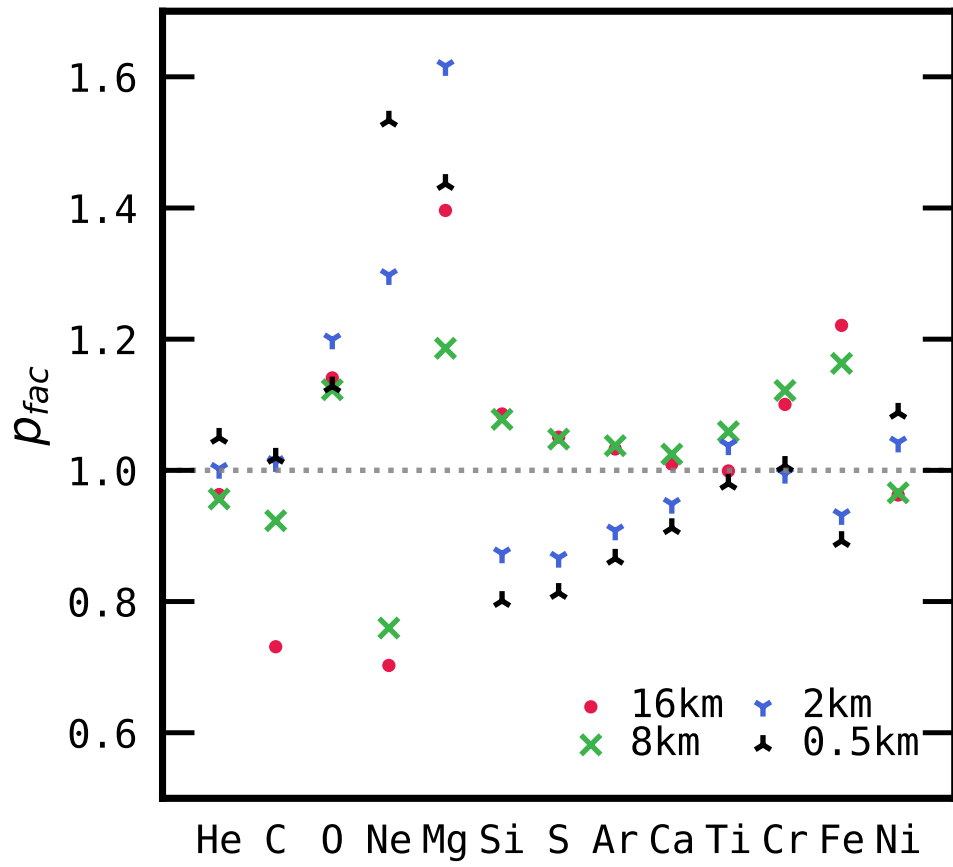


Figure 3.8: Relative yields for simulations compared to the 4km case.

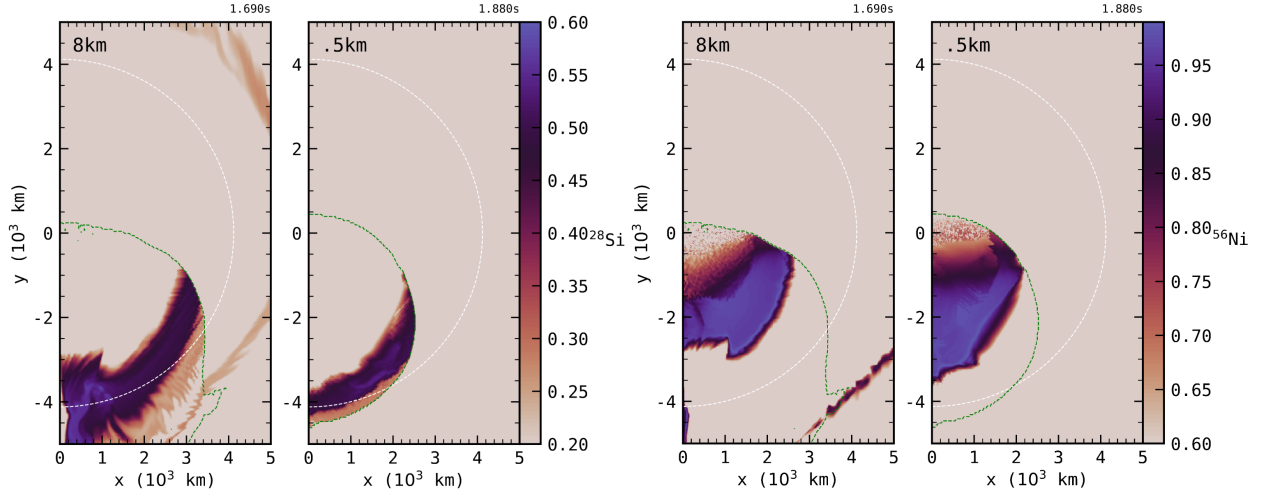


Figure 3.9: Silicon and nickel compositions around the core at the time of peak energy release for both cases. Left: A large amount of low density material is burned to silicon at coarser resolutions due to the secondary detonation starting at the edge of the white dwarf. Right: Burning to nickel in coarser resolutions is localized to the front climbing the density gradient of the core, while for higher resolutions (case 1), the off-center detonation starts at a higher density resulting in more complete burning over the lower hemisphere of the core. Subsequently, both cases evolve similarly over the rest of the domain.

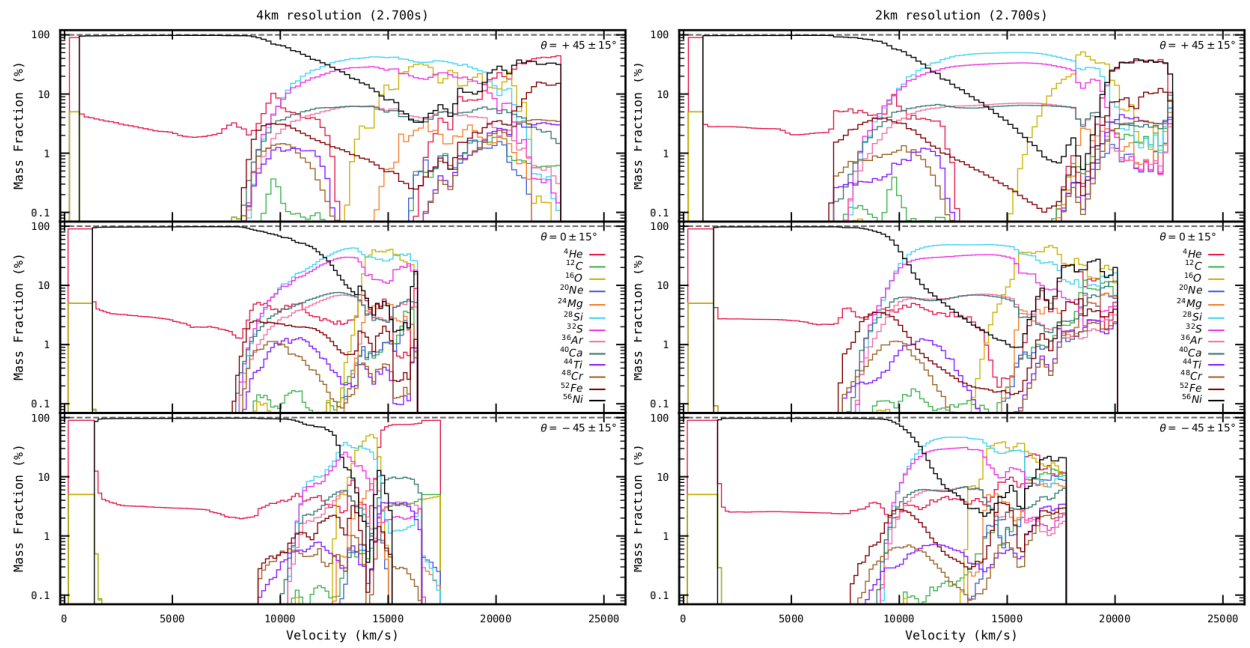


Figure 3.10: Ejecta composition by mass fractions sliced by angle of view. Top, middle and bottom enclose 30 degree wide slices in the domain centered at noted angles (θ , further description in section 3.4.3). Left: Described slices for the 4 km case. Right: Described slices for the 2 km case.

degrees ($\theta = 45^\circ$) north of the equator, and one at 45° south of it. Though at the plotted times homology has not yet been reached, all burning has already subsided and most mixing has already taken place. Given this, some of the principal characteristics and the overall structure of the ejecta can be seen at these early times and are not expected to change in character at later times.

First, aside from the focusing and compressional effect of axisymmetry that was noted earlier, another consequence of the reflecting boundary along the polar axis can be discerned. The reflecting boundary condition diverts material hitting it, pushing the material along the polar axis and causing a boost in velocities at the poles. Though this happens in both cases, the surface detonation of Case 2 imparts an additional acceleration to the diverted envelope material along the axis. This same sort of behavior is evident above and around the initial polar detonation. For Case 1, there's no additional energy release at the antipode, leading to lower polar velocities in this case. Additionally, the secondary detonation in Case 1 pushes against a significant overburden of core material between the ignition and the envelope, causing a comparably smaller boost at the antipode. Second, though nuclear burning has subsided, there is still a significant amount of helium on the grid. Notably for Case 2, helium is not evenly mixed throughout the ejecta. In addition, a large fraction of this high-velocity helium is accelerated from its initial location just above the antipodal, core-shell explosion site. Conversely in Case 1, the central detonation, even when off-center, causes a symmetrical mixing of the ejecta along all lines of sight, distributing both helium and nickel among all layers of the ejecta.

3.5 Conclusions

Examining the dynamic evolution of the double-detonation scenario subject to increasing spatial resolution highlights a divergence in outcomes with respect to the particular mode of explosion. In both cases, a generally credible thermonuclear supernova occurs, but the paths to explosion are different at a qualitative level and lead to significant quantitative differences in nucleosynthetic yields and the distribution of those yields. At coarser resolutions, burning proceeds in a continuous fashion with no particular separation in burning regimes other than

the type of fuel being burned. Shell burning proceeds around the limb of the white dwarf without causing the core to ignite until burning reaches the antipodal point of ignition, forming a pinch at the limb of the core which begins carbon burning towards the center. This edge ignition of the core overwhelms the inward compression wave caused by shell burning, blurring the difference with direct edge-lit cases. However, at finer resolutions – 2 km and better – a new picture emerges: shell burning proceeds in the same qualitative manner as coarser cases, but it reaches the antipodal point with less heated mass and therefore avoids an antipodal edge ignition. This causes shell burning to subside, and pressure waves set in motion earlier by shell burning move through the core, prompting a new stage where there is little nuclear burning occurring throughout the domain for approximately 300 milliseconds. Once the pressure waves converge off-center in the core, burning ignites a secondary detonation within it, away from shell burning remnants. The combined effect of a distinct core detonation in both time and space yields clear differences in nucleosynthetic yields from the burning of the core and the symmetry of the ejecta which should be borne out in observations, specifically for line-of-sight arguments and intermediate mass element yields. Though burning length scales involved in the physical events are still out of reach for the stated resolutions, the emergence of three clear stages at resolutions under 4 kilometers warrants a minimal resolution for consistency of the general scenario. This notion can be extended to full 3d simulations given that the three stages, though connected, are sufficiently independent from each other to conflate symmetry axis effects or nuclear network picked (energy deposition dependence).

Chapter 4

3D exploratory work

4.1 Setup, Domain and Extent of Work

Starting from the same profile as in Chapter 3, an equally sized axis is added, placing the same ignition point along the z-axis at the same altitude relative to the surface of the core, and using same linear temperature gradient and size. The `burn` module now utilizing `XNet` has an expanded 47-species network.

Based on the conclusions of Chapter 3, a starting hypothesis for running a three dimensional case should be that a resolution of 2km or better, the ignition of the shell should not immediately burn the core at its edge when it engulfs the core at the antipode. Given the large jump in computational resources needed to increase dimensionality (see Appendix B), a conservative 8 km run is performed, along with an ambitious attempt for a 2 km case to correlate with the two dimensional case.

Due to time constraints, neither attempt reached the unbinding of the system, with the 8 km case reaching the antipodal point of the core and the 2 km case reaching stable shell burning at around 45 degrees from the ignition point. The additional species used have not yet caused a significant difference in the dynamic evolution of the configuration. This due to the high density environment of the core not having detonated yet to utilize the breadth of the expanded network towards more neutron-rich species (see Figure 2.3).

4.2 Dynamics

Shell burning develops in a markedly different way than in two dimensions, both in terms of speed and features. While two dimensional domains reduce the curl of the velocity to a scalar field, in three dimensions, this vector is allowed to change and actively alters the dynamics of the fluid [138]. This is easier to see by for example, taking the Lagrangian form of the momentum conservation in Euler's equations (Equation 2.5) and re-writing via the material derivative¹. From $\frac{\partial \rho \vec{v}}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) + \nabla P = \rho \vec{g}$, the first term expands into:

$$\begin{aligned} & \frac{\partial \rho}{\partial t} \vec{v} + \rho \frac{\partial \vec{v}}{\partial t} \\ & \frac{\partial \rho}{\partial t} \vec{v} + \rho \left[\frac{D \vec{v}}{Dt} - \vec{v} \cdot \nabla \vec{v} \right] \\ & \frac{\partial \rho}{\partial t} \vec{v} + \rho \left[\frac{D \vec{v}}{Dt} - \nabla \frac{||\vec{v}||^2}{2} + \vec{v} \times (\nabla \times \vec{u}) \right] \end{aligned}$$

this last term now fully affecting the flow throughout the hydrodynamical evolution. This new interaction within the fluid changes the behaviour of the burning front, the wake of ashes mixing into the shell, the energy input of the burning into the fluid, and the velocities and timescales of the event. As shown in figures 4.1 and 4.2, the capacity of the three dimensional simulation to mix evenly and faster prompts the burning front to lengthen along the surface of the core, speeding it up and also making it thinner, building a shallow annulus converging towards the antipode. The wake of the front also mixes thoroughly forming a smooth surface of ashes instead of a dendritic structure of well burnt material mixed with colder shell material. The core pressure wave also differs in the three dimensional case, mostly at the central axis which is bounded in the two dimensional case, making the wave move faster along the symmetry axis, flattening the arc of the overall inward pressure wave.

The 2 km case in two dimensions most closely resembles the evolution in the three dimensional 8 km case in terms of the structure of the propagating burning front (fig 4.2), more than the two dimensional 8 km case (4.1), managing to resolve the surface burning better than the 8 km case but still forming non-smooth structures in its wake. Specifically, (1)

¹also called the Lagrangian derivative since it changes the derivative reference to a parcel of fluid along its path instead of relative to the general flow velocity.

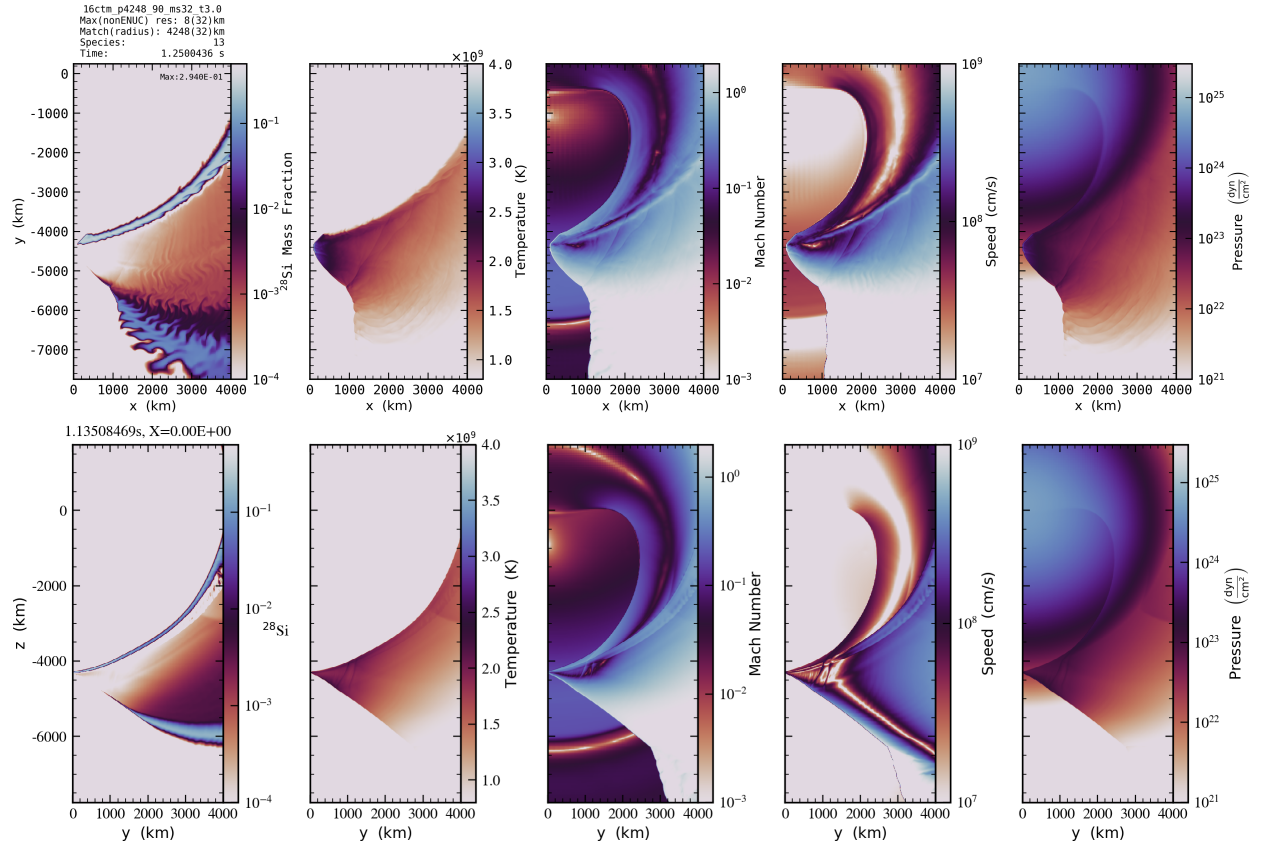


Figure 4.1: Multiple domain bulk properties at the point of antipodal contact for the 8 km case in two dimensions (top) and three dimensions (bottom).

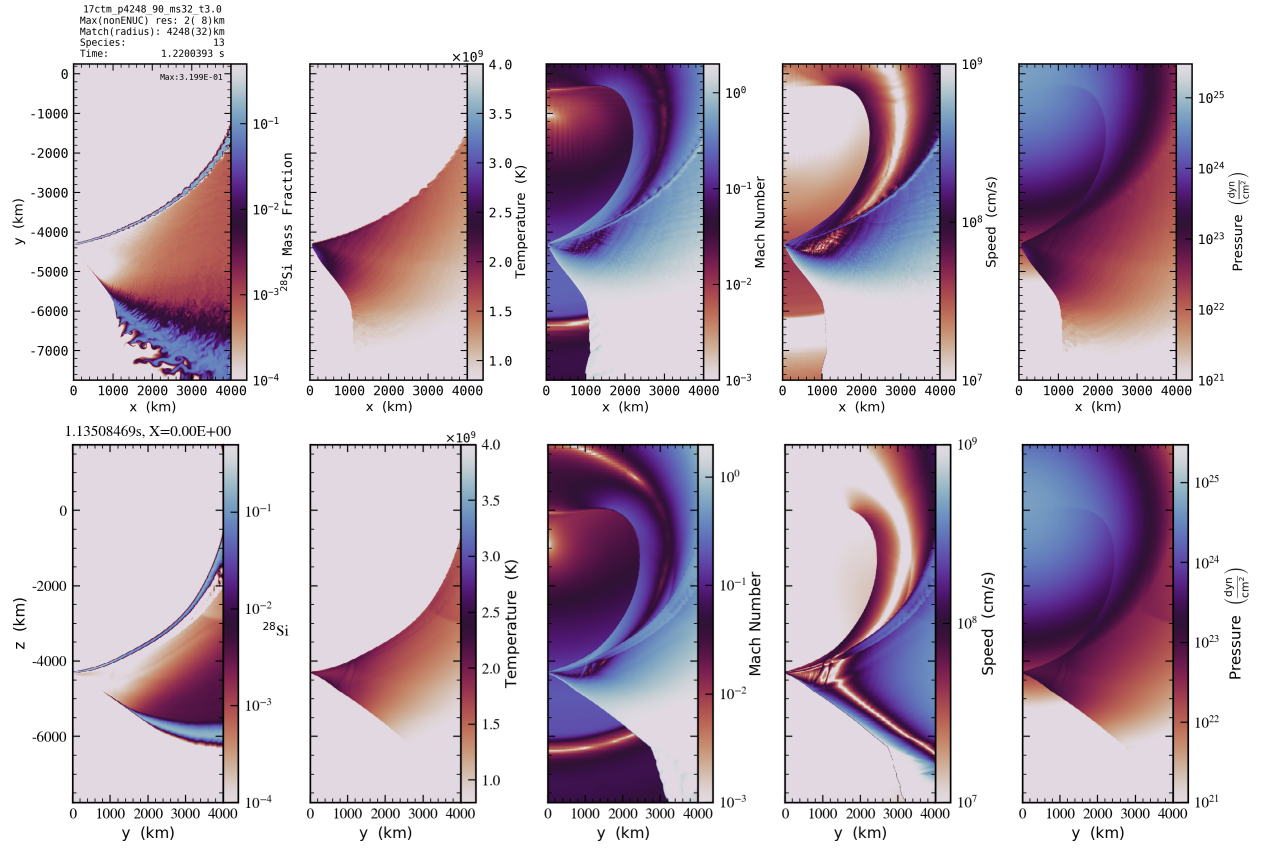


Figure 4.2: Same as figure 4.1, but compared to the two dimensional 2 km case (top).

the 8 km three dimensional case exhibits considerably less mixing of shell burning products and underlying core material than in two dimensions and (2) the most advanced portion of the three dimensional burning front along the limb of the white dwarf is far more localized than in the two dimensional case at the same resolution.

4.2.1 Energies and Speeds

As shown in figure 4.3, the additional degree of freedom from the increased dimensionality for the simulation changes energy deposition into the domain. With an additional dimension, burning imparts into the domain a similar energy as in the two dimensional case only at early times, falling off once shell burning stabilizes going around the core. Late in the shell burning evolution, the rate at which burning is depositing energy in the domain falls below the rate of the two dimensional case with maximum resolution of 2 km, strongly suggesting it will fail to ignite the core at the antipode. This can be attributed to the thinner, more thoroughly mixed burning front stemming from differences in turbulent fluid flow behavior evolved by the hydrodynamical evolution (see sections below).

Figure 4.4 shows the inward pressure wave speed taken at a 45 degree angle from the expected core ignition point (taken from the two dimensional simulation), with the 3d case showing a steeper decline early on but a shallower slowing curve once it settles after the initial polar explosion. This overall increases the speed by around 16%, implying there is a stronger inward pressure wave going towards the convergence point. On the other hand, the shell burning detonation speeds are also faster but by a smaller margin of around 7%.

4.3 Species Kinematics

In terms of species distribution, though the three dimensional runs include 47 species, since no run managed to reach core burning, most of the neutron heavy species have had no dense medium in which to be produced (see Figure 2.3). Nonetheless, thorough mixing of the ashes and increased velocity of the front already create a stark contrast in the velocity distribution compared to the two dimensional case, as shown in figures 4.5 to 4.10. Throughout in two dimensions, the dendritic structure of the physical domain maps onto the velocities achieved

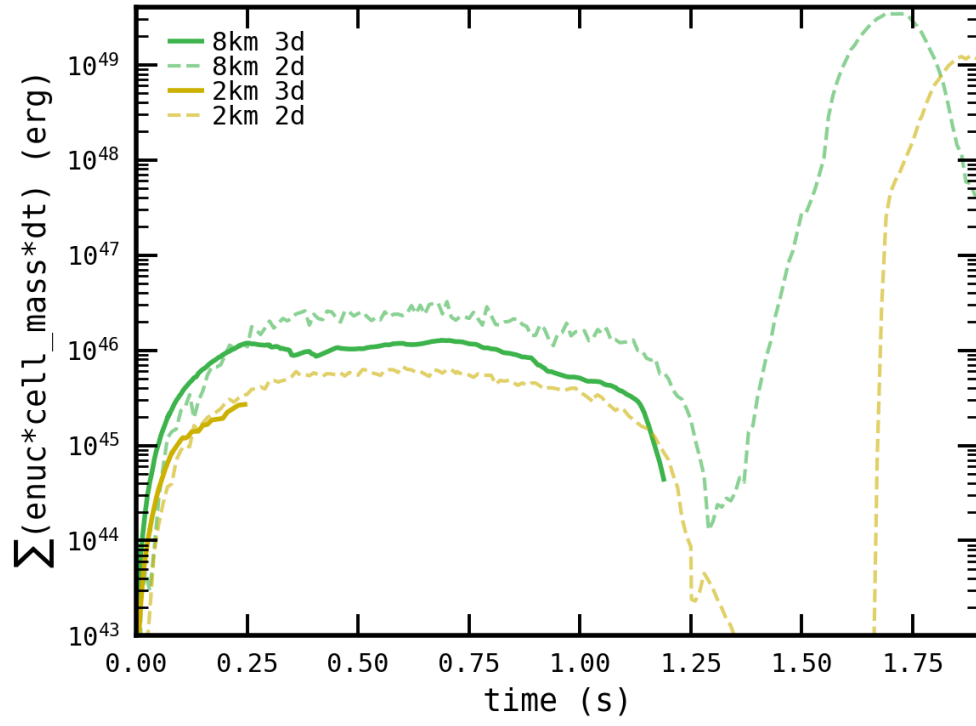


Figure 4.3: Total nuclear burning energy being added to the domain through time for two three dimensional runs, compared to their respective two dimensional iterations at the same maximal resolution.

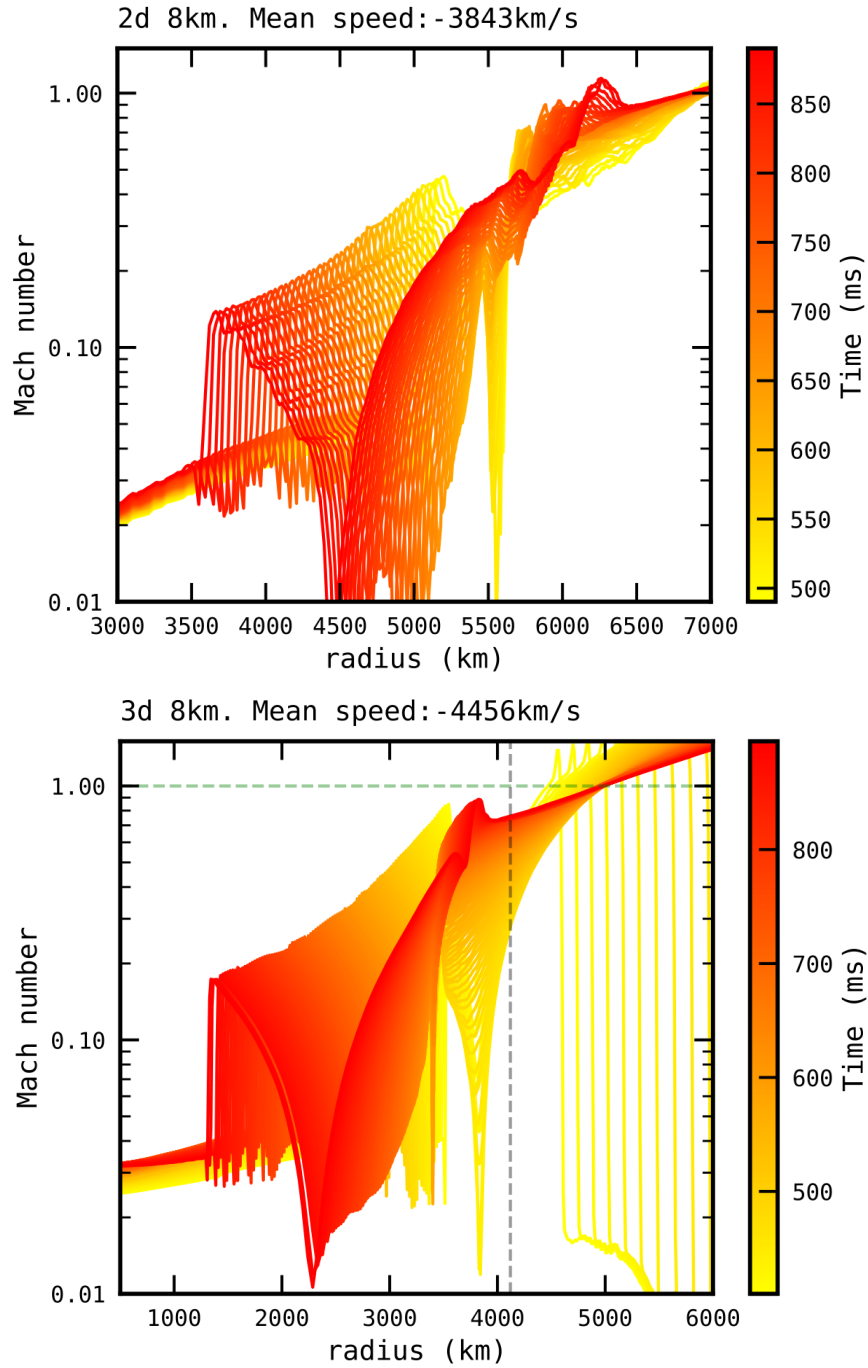


Figure 4.4: Inward pressure wave velocity for the 8 km case probed over a settled shell burning regime. Each lineout is at a fixed 45 degree angle from the ignition point and stem from 2000 km below the center of the core. For the three dimensional case, the lineout is at a fixed azimuth of 90 degrees.

by the ashes, distributing them evenly in velocity space. While for three dimensions, there is clear clumping (in velocity space) of would-be ejecta compactly following the thin and smooth burning front and wake.

In the initial stages, the symmetry axis in two dimensions dominates the distribution, while in three dimensions, there is a continuous transition from burning front to wake, leading to the bi-modal distribution of species in velocity space. Also for at this stage, a comparison between 8 km and 2 km can be made (figures 4.5 and 4.7), which shows that with increasing resolution, the boundary between core and shell that is mixing and burning gets smaller, while the rest of the detonation becomes more defined, with the velocity distribution of species having even more than two ranges of well mixed ashes.

Further in the evolution, when the front reaches a steadier burning state near the equator of the white dwarf (figures 4.9 and 4.10), there is more similarity between the dimensionality cases. But still, the edge-burning thickness is thinner, and the bi-modal velocity distribution shows up clearly in contrast with the two dimensional case, which has a single, rather small range of velocities for its ashes.

4.3.1 Antipodal Hit

Lastly, the 8 km case reached the antipode of the ignition point. The annular shaped burning front collapsing onto itself without causing a significant enough spike in temperature, nor amassing enough ash to directly ignite the core at its edge as shown in figure 4.11. This is warranted by the low energy deposition achieved through shell-burning and thin surface-burning thickness, meaning less mixing of the core's carbon/oxygen into the shell burning front and is contrasted by the increased velocity of the tip of the burning front.

4.4 Conclusions

The jump from two dimensions to three immediately changes the dynamics of the simulation: (1) faster burning front speeds, due to more efficient transfer of energy to the self-sustaining burning front, (2) a stronger pressure wave towards the center of the core, (3) thinner burning

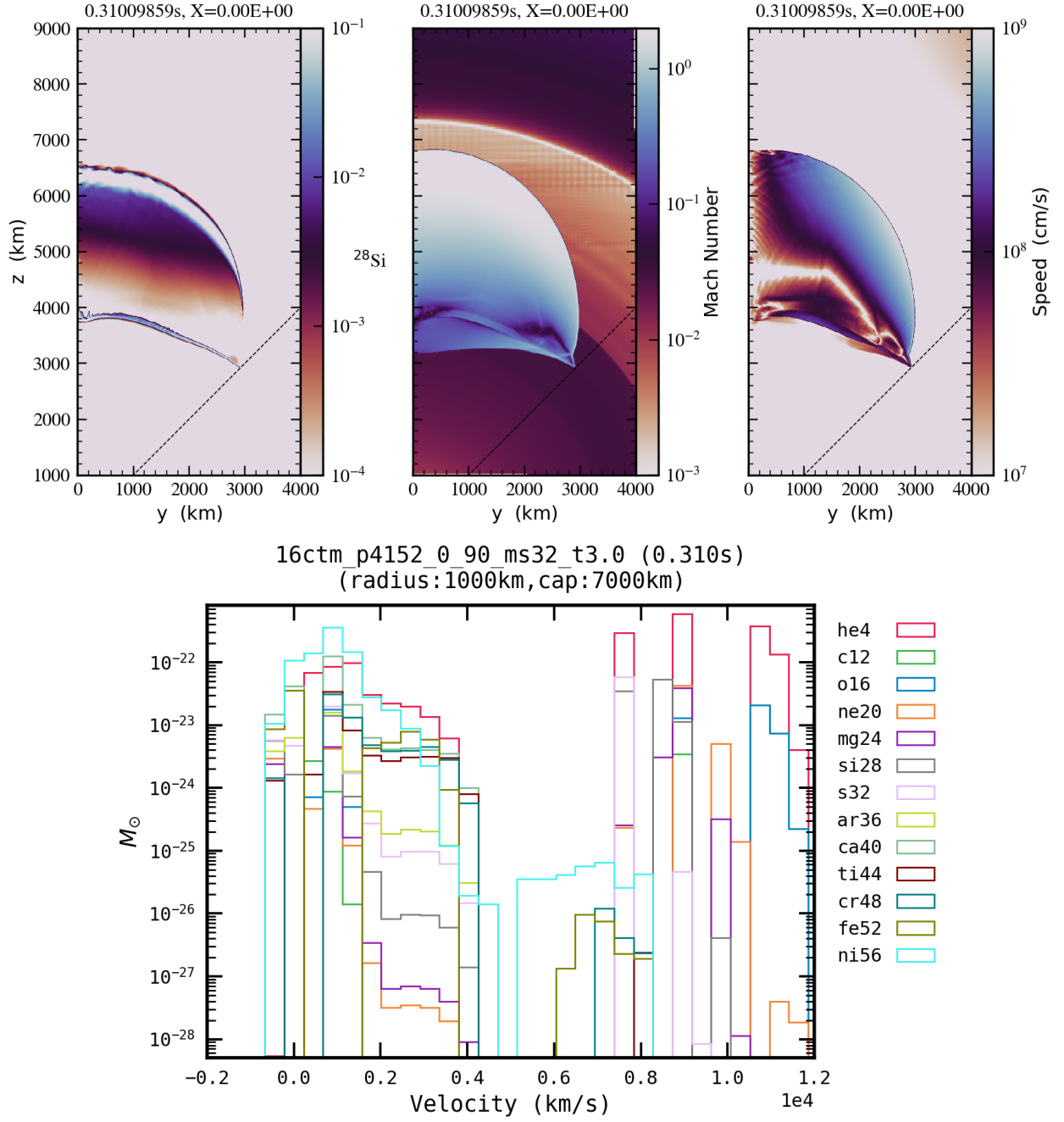


Figure 4.5: Bulk properties (Silicon mass fraction, mach number and speed. Top) and velocity distribution of species (bottom) for a representative volume of the domain at the point where the burning front reaches 45 degrees from the ignition point. Three dimensional 8 km case.

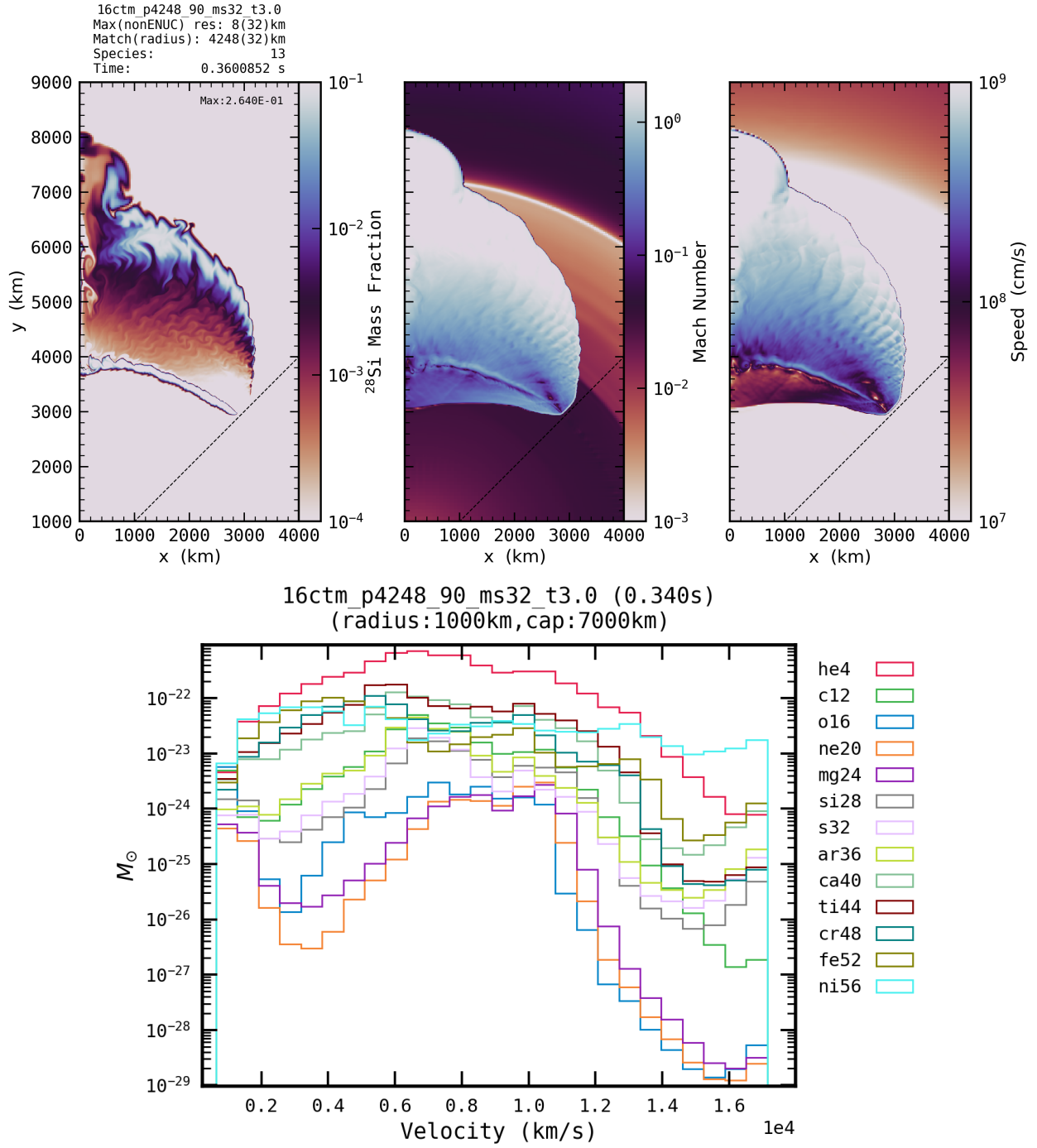


Figure 4.6: Same as Figure 4.5.
 Two dimensional 8 km case.

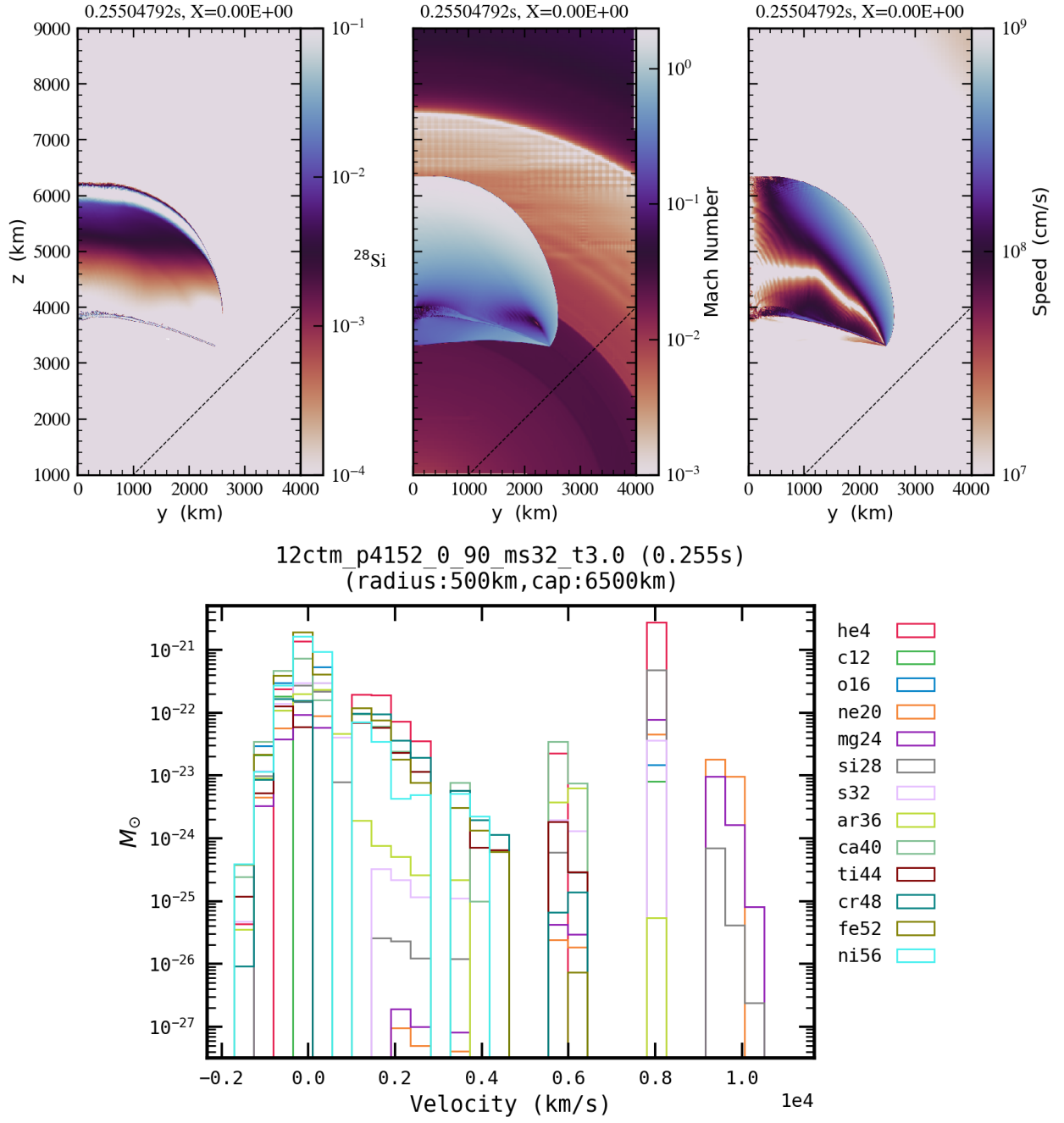


Figure 4.7: Same as Figure 4.5.
Three dimensional 2 km case.

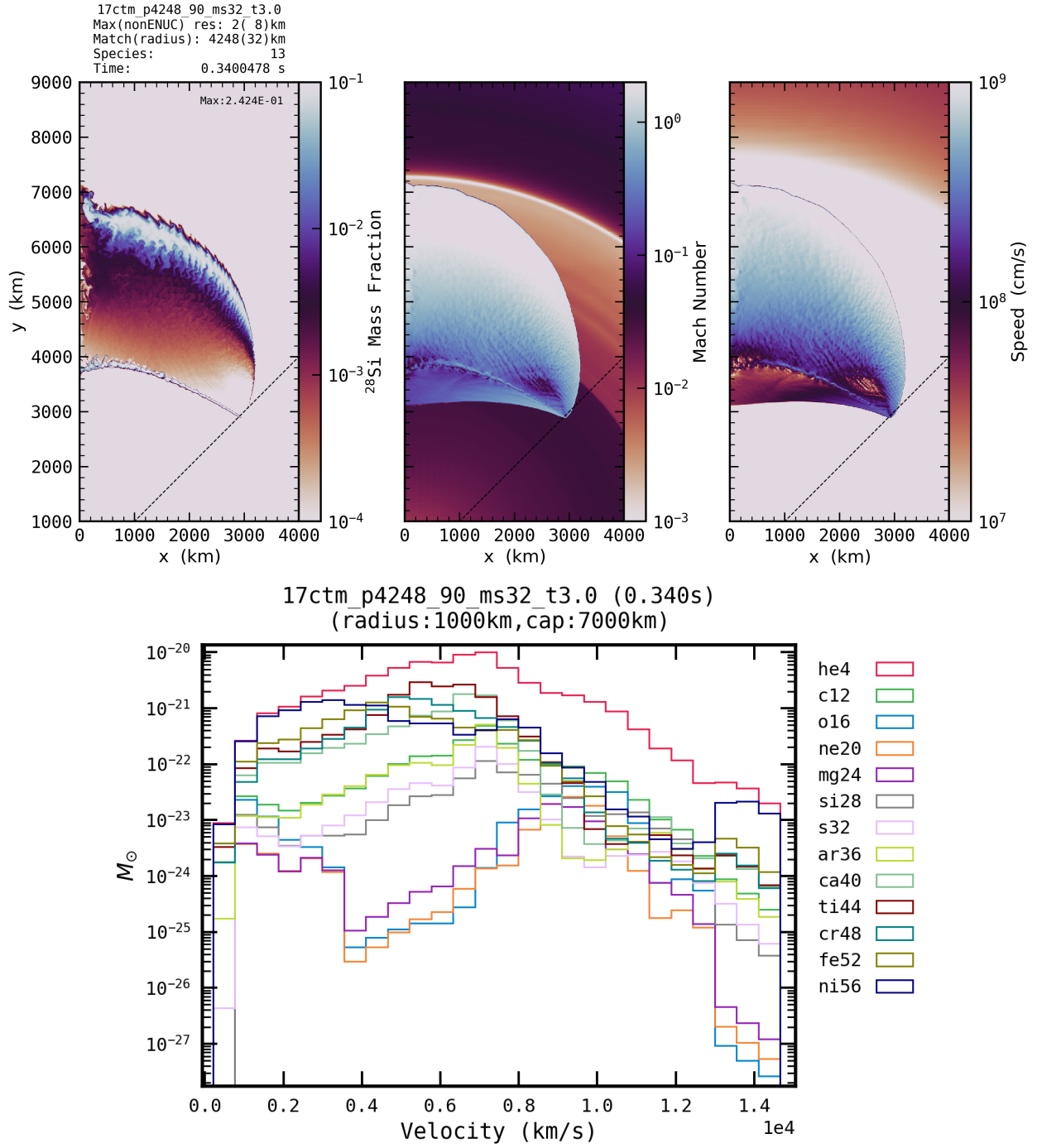


Figure 4.8: Same as Figure 4.5.
 Two dimensional 2 km case.

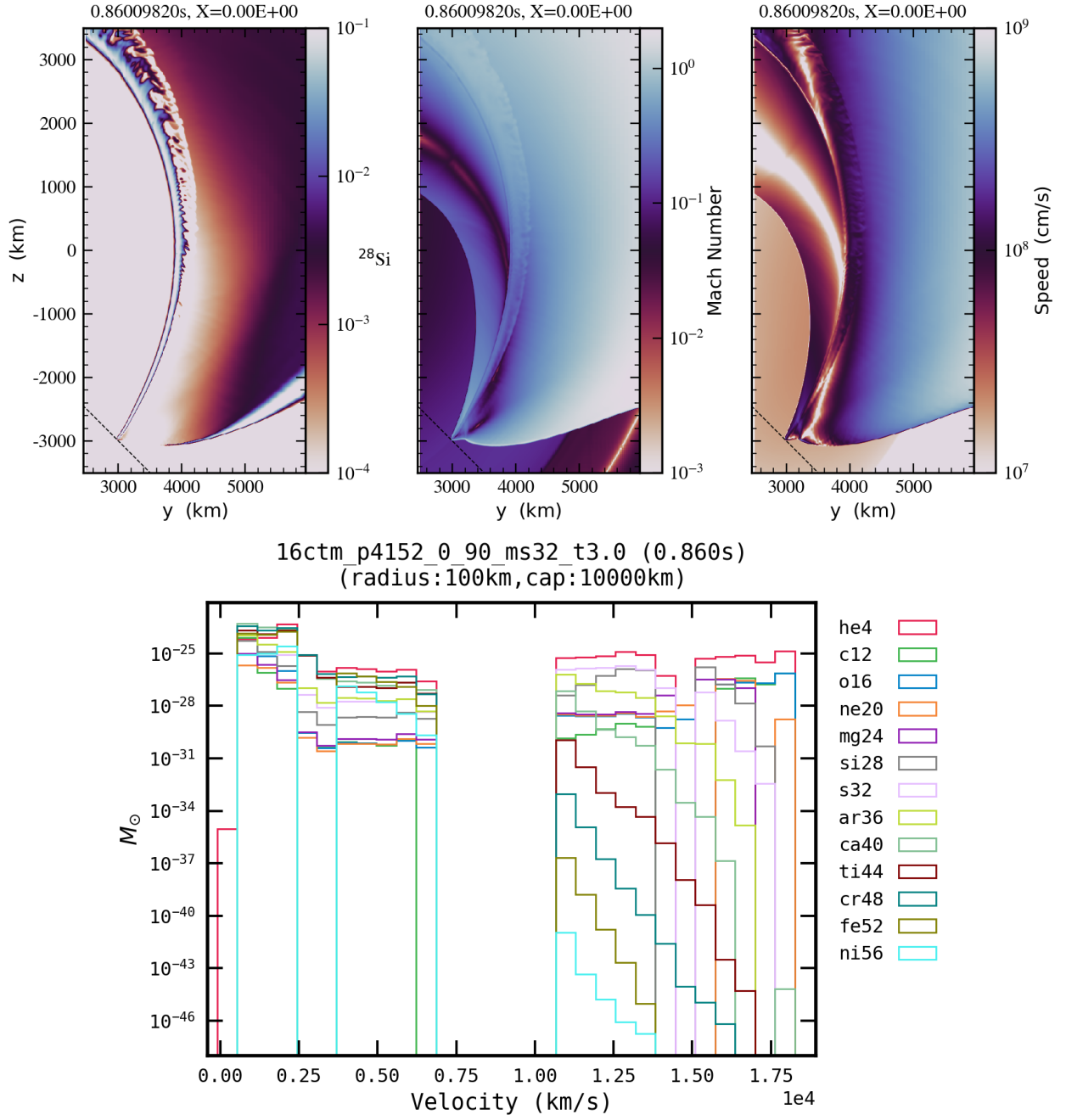


Figure 4.9: Bulk properties (Silicon mass fraction, mach number and speed. Top) and velocity distribution of species (bottom) for a representative volume of the domain at the point where the burning front reaches 135 degrees from the ignition point. Three dimensional 8 km case.

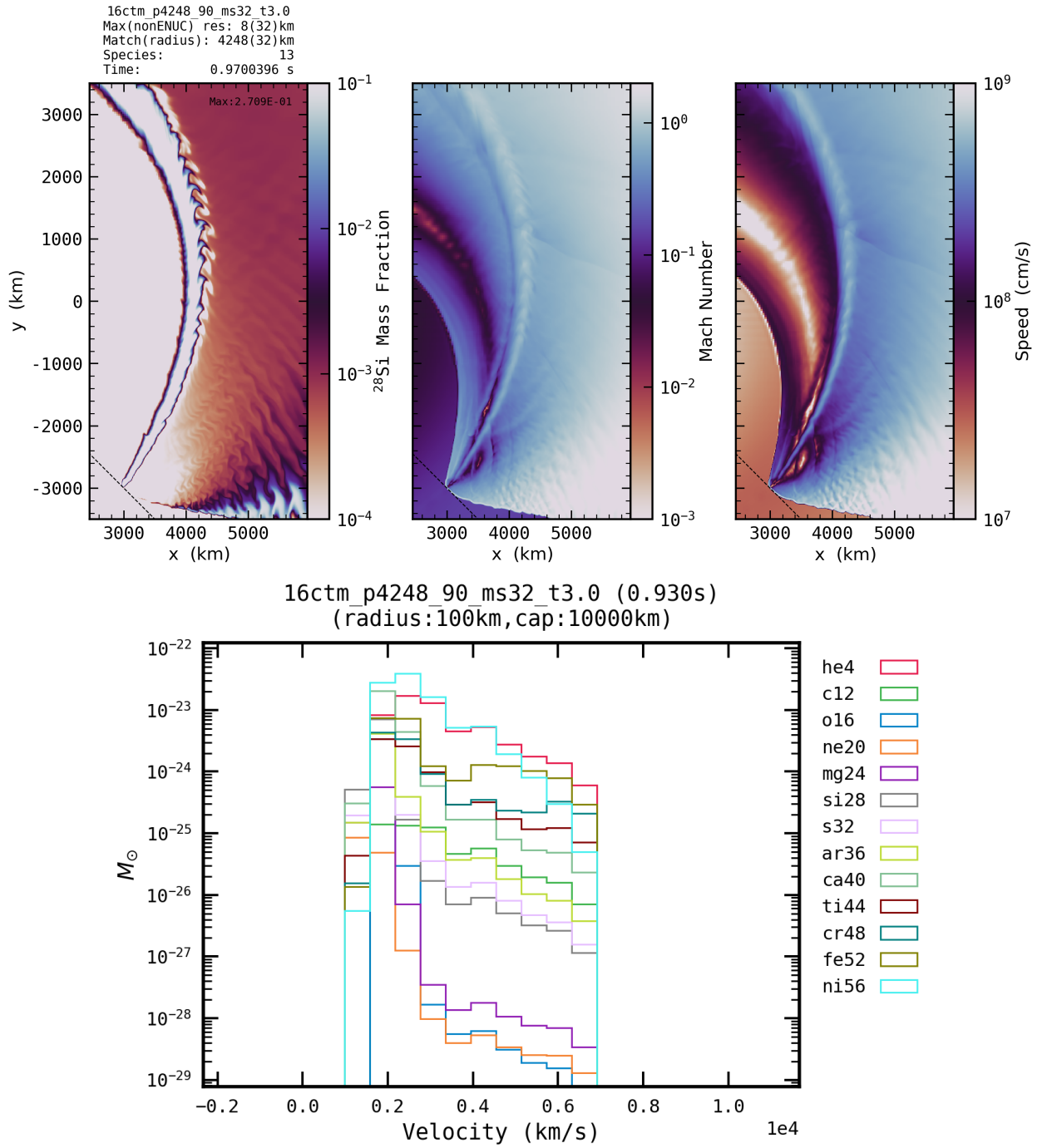


Figure 4.10: Same as Figure 4.9.
Two dimensional 8 km case.

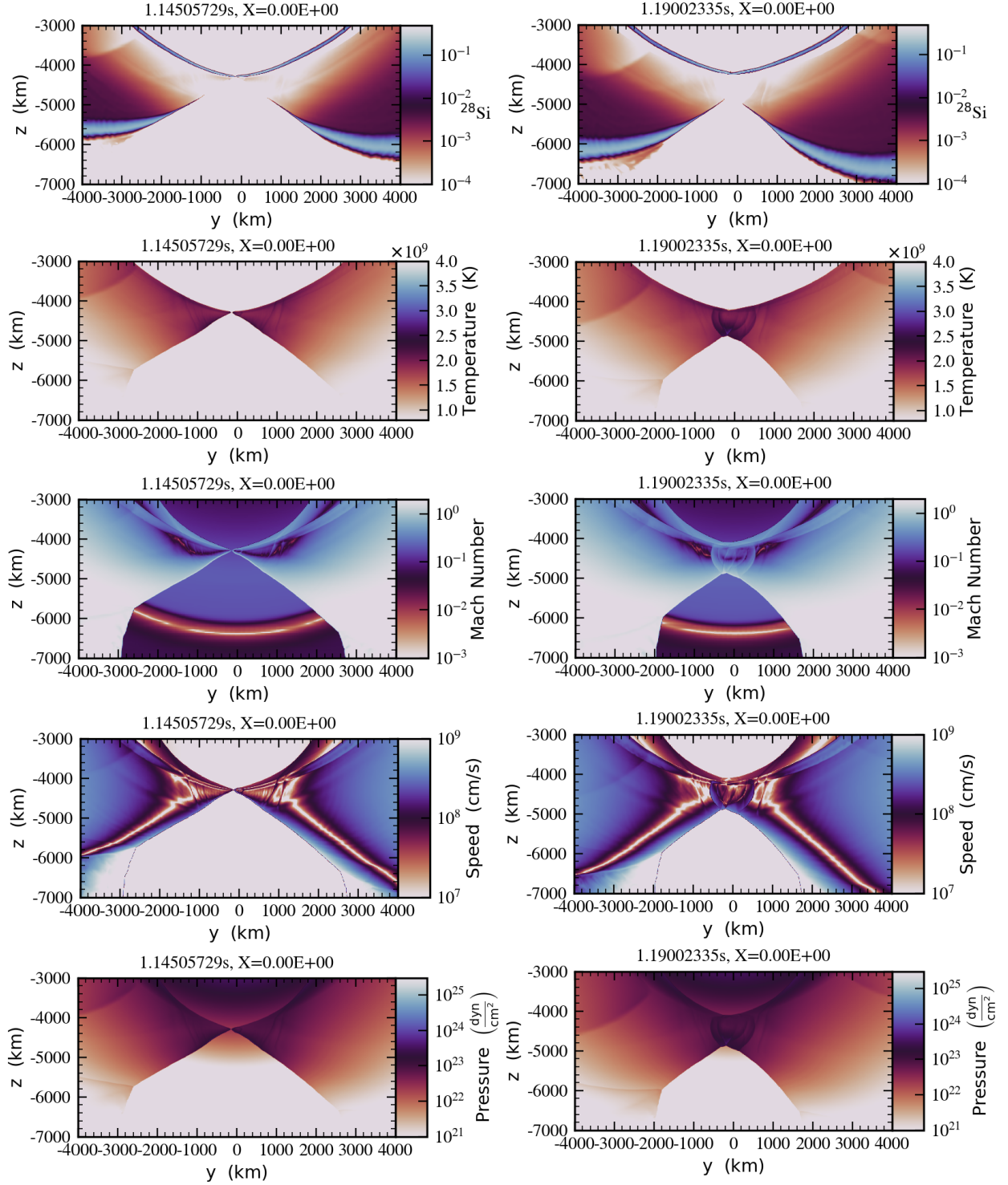


Figure 4.11: Bulk domain properties at the convergence point for the shell burning front at 8km maximum resolution. Left: closest to convergence. Right: 45 ms after convergence.

surface at the core-shell interface, (4) almost immediate mixing of the ashes in the burning wake.

The antipodal hit not igniting the core directly at the a maximum 8 km resolution becomes a reference point, allowing future simulations to run on even coarser grids up to the point where an edge lit detonation is found.

Though there is an apparent transition in burning thickness between a higher resolution two dimensional case, and a coarser three dimensional one, the basis for this notion is not warranted due to the outcomes of the kinematics of species borne out by the runs so far. There is a seminal difference in the interaction between heated material from burning and the shell that two dimensional simulations cannot capture, no matter the resolution. Though if the eventual final yields of the simulations are comparable, only proper analysis of the velocity distribution of species could discern whether these types of three dimensional simulations are to be further developed.

The development of the computationally faster 8 km run has shown that three dimensional simulations have an easier path to achieving a within-core double-detonation, and thus future work will not develop the 2 km case unless a core ignition is not achieved.

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Appendices

A Detonation Dynamics

The physics of thermonuclear burning allow two regimes, separated by the relevant scale: the speed of sound in the medium (c_s). A subsonic burning front is called a deflagration, while for sonic or supersonic velocities, the front becomes a detonation. Following [72], the conditions for the speed of burning can be understood from first principles if there are no dimensionality effects, i.e., if the burning front is flat and is negligibly small. Under these assumptions, the burning of matter within a fluid is a simple discontinuity between the pre-burned fuel (subscript 1) and the ashes left by the flame front (subscript 2), which can be solved via typical mass, momentum and energy conservation at the interface (the burning front), yielding the Hugoniot Equation:

$$e_2 - e_1 = \frac{1}{2}(p_1 + p_2)(\nu_1 + \nu_2) \quad (1)$$

where e_i, p_i , and ν_i are the specific internal energy, pressure and specific volume of the pre (1) and post (2) burn states. Given this relation, the adiabats of different pre- and post-burn states can be compared, primarily through Rayleigh lines (lines of constant speed) joining both, determining the thermodynamic path for burning as shown in figure (A.1, left). Starting from point A (the original fluid), the red shock adiabat heats the fluid up to point B, where it burns through the Rayleigh line down to point C, the ash state. Of note is the Chapman-Jouguet point, where the Rayleigh line is tangent to the adiabat, and burning is at it's most efficient state (smallest thermodynamic path). This method can be used further to constrain the types of burning, as in figure (A.1, right). Given that the transition between two states can only be joined through a Rayleigh line, there is a geometrical range

of possibilities for a given two state burning scenario. For final pressures above point (a), we have that the speed of burning with respect to the ashes (v_2) is lower than the soundspeed in them (c_2), while the speed with respect to the fuel (v_1) is greater than the speed inside it (c_1) thus this detonation is *overdriven* [63]. Point (a) is the mentioned Chapman-Jouguet point, at which $v_2 = c_2$ while $v_1 > c_1$, implying a shocked detonation (burning and shock are spatially matched). Further 'down' from point (a) both v_1 and v_2 tend to infinity and are both supersonic, up to point (b), where the volume doesn't change. Between points (b) and (c), there are no physically realizable states due pressure and specific volume both increasing. At point (c), we have no change in pressure, so $v_1 = v_2 = 0$. After point (c), both speeds gradually increase from zero, therefore subsonically, and thus only deflagrations can occur, with the tangent at point (d) being the last stable (and quickest) deflagration solution for the starting condition.

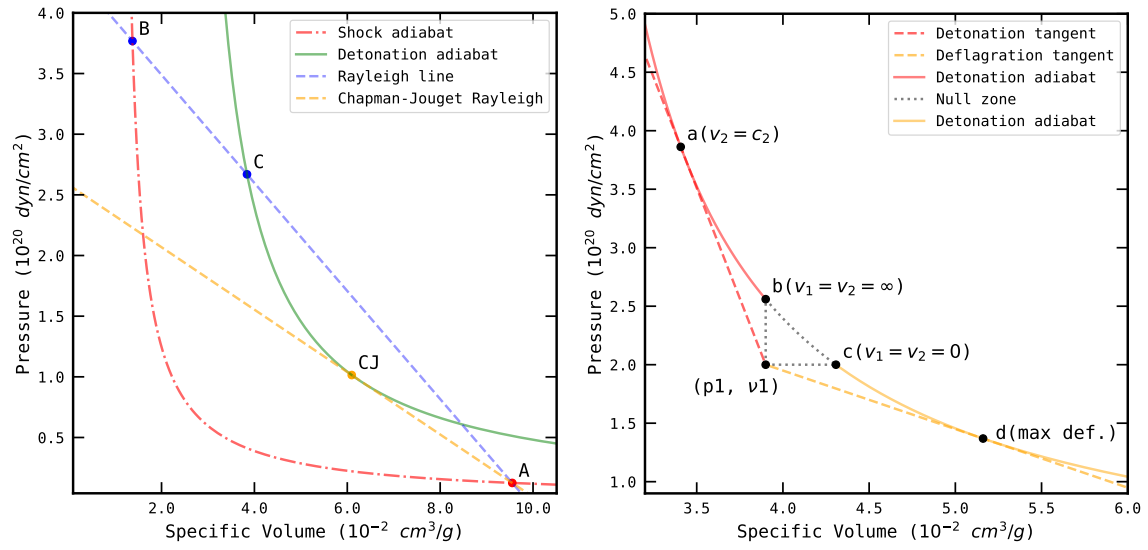


Figure A.1: Left: Detonation Cycle. Right: Available outcomes for a fuel state (p_1, v_1)

B Computing Resources

All simulations were performed with the Summit machine at the Oak Ridge Leadership Computing Facility (OLCF)². Properties of the machine are outlined in table B.1.

Scaling of increasingly more resolved simulations quickly ramp up the capacity needed to perform them. Initially, two-dimensional simulations utilized from a few to a dozen nodes, implying somewhere around 500 CPUs to run.³

Three dimensional attempts included an expanded network which also utilized the GPUs on each node. While this offloads the burning from the CPUs, the additional dimension still amounts to utilizing at least an order of magnitude more nodes to perform, reaching around ten thousand cores/ranks.

Machine utilization vs actual simulation time achieved can be seen in figure B.2, where two simulations at the same resolution in both two and three dimensional cases are shown. Though ranks are 3 orders of magnitude more in the three-dimensional case, the real-time timestep (IRL) is still the same 3 orders of magnitude more than the two-dimensional case. Even with GPUs handling the load of burning, pure hydrodynamical evolution trumps the computational cost of running the simulation, suggesting carrying more species in the simulation is only hampered by memory and bandwidth, not actual computational speed.

Proper distribution of workloads across all ranks becomes an issue at scale. The computational problem involves a large domain where for most of the simulation time, only a small part of the domain is burning, which might cause ranks to accumulate hot blocks while most of the other ranks solve much faster non-burning blocks and idle while most of the work is done by a few ranks. This is shown in figure B.1, where between figures an improved workload balancing criterion has been adopted⁴. Though simulation times are not the same, the burning regimes are the same, thus the only difference in between snapshots is the amount of cells in the domain that are refined or burning (i.e., the number of total blocks). Proper handling of a large amount of ranks solves both having empty ranks and ranks with too many hot burning blocks.

²<https://www.olcf.ornl.gov/summit/>

³Specifically requiring roughly 500 MPI ranks, each of which can straightforwardly be mapped to a CPU core.

⁴<https://github.com/Flash-X/Bittree>

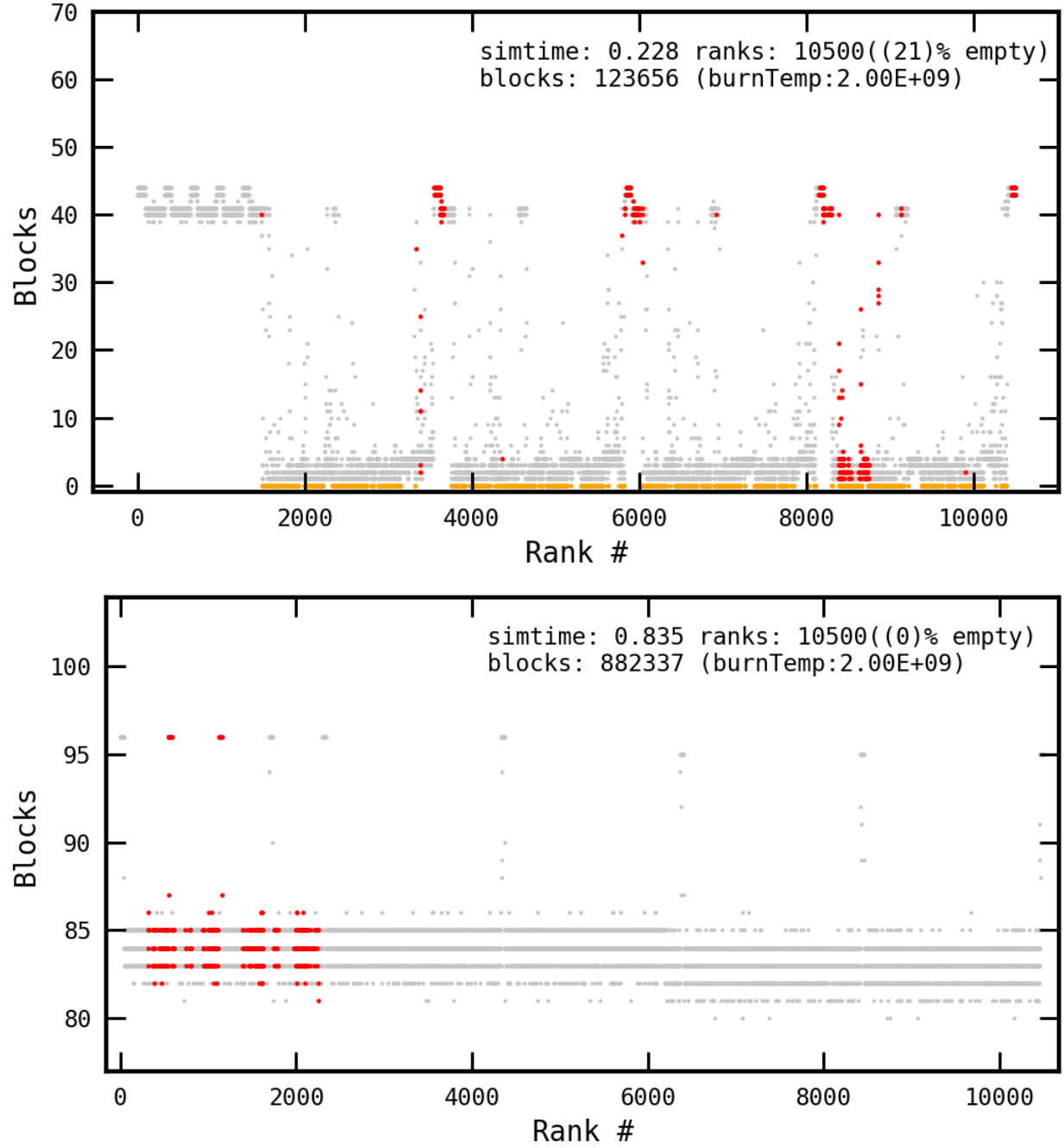


Figure B.1: Blocks assigned to each rank within simulations at a determined time. Yellow points are ranks without work, while red points are ranks with hot blocks (blocks that have cells hotter than 2 GK). Top: early simulation without load balancing measures in place. Bottom: evolved simulation with proper load balancing.

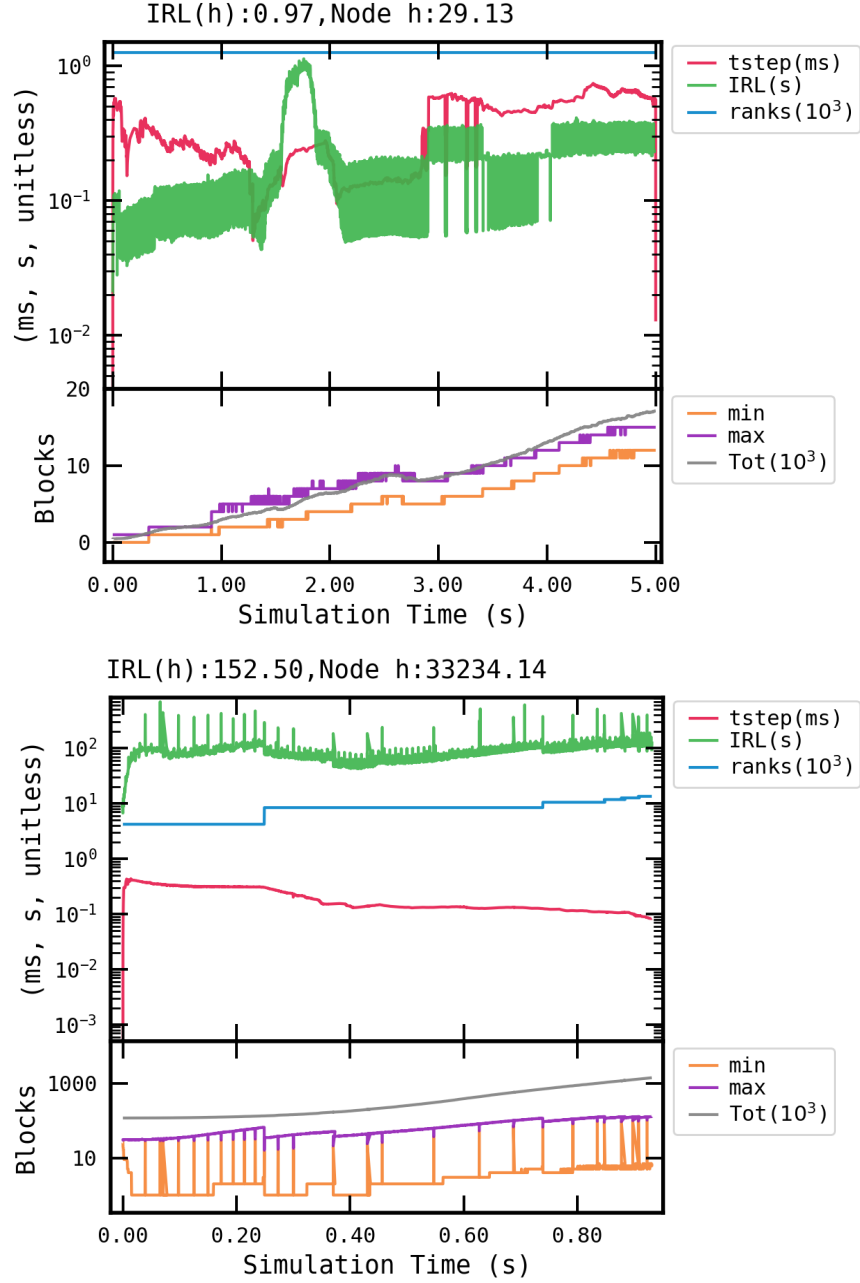


Figure B.2: Main computational properties of two equally refined simulations. Top: 8km two dimensional simulation. Bottom: 8km three dimensional simulation. Large peaking features in real-time (IRL, green) correspond to checkpoint writes while peaking minimum blocks (orange) correspond to reorganization of the block distributions by the load balancing criterion.

Table B.1: Bulk Machine Properties for Summit (IBM AC922 node)

CPU	2 x 21 core IBM POWER9 with SMT (4 threads/core) 2.8GHz (3.1GHz Turbo) with L1/L2/L3 caches of 32kB/512kB/10MB
GPU	6 x NVIDIA V100 (16GB) 2560 double precision CUDA cores at 1530 MHz clock frequency
Memory	512 GB DDR4

C FLASHy Data Interface

Throughout this work, the large scale of output data from simulations demanded ad-hoc tools and resources to enable analysis. To this end, a bespoke toolkit was developed: FLASHy (<https://github.com/frivasa/flashy.git>). This toolkit can produce publication quality figures on large scale datasets both interactively or in parallelizable batch jobs. Written completely in Python, it relies on general packages found in typical distributions, most importantly YT⁵, which greatly simplifies both the geometric considerations and adaptive mesh refinement organizational tree for data analysis.

It consists mainly of 3 branches of modules, a data handling branch, a plotting branch, and an auxiliary branch with both IO for file handling and general nuclear physics functions.

The data handling branch controls the input data from hdf5 files either by directly probing its contents or going through YT to manage mesh data. Additionally, it handles parameters and metadata for simulations to allow comparisons between iterations of both codebase and simulation performance.

The plotting branch develops into two sub branches: first, a one-dimensional plots both for simulation metadata such as block distribution(load balancing) or time step overview, and integrated quantities of higher dimensional simulations such as line of sight composition or total energy produced in the domain through time. The second sub-branch yields 2-dimensional plots for any required variable in 2d and 3d files (planar slices of 3d datasets).

The final auxiliary branch deals with either essential physics such as solving polytropes, hydrostatic profiles and nuclear properties of species, or analyzes data coming from the simulations, allowing calculation of CJ velocities, or velocity distributions of mass fractions.

This whole suite of tools can be deployed in-situ at the machine where simulations are run via anaconda⁶, creating an interface between remote clusters and the user, avoiding the transfer of large data checkpoints elsewhere for analysis.

⁵<https://yt-project.org/>

⁶<https://www.anaconda.com/>

Vita

Fernando Hernan Rivas Aguilera was born in Santiago, Chile on January 14th, 1988 to parents Claudio Rivas and Jeannette Aguilera as the youngest of four siblings, along sisters Jeannette and Claudia, and a brother, Claudio. After graduating from San Gabriel High School in 2005, Fernando attended *Universidad de Chile* in Santiago, graduating with a Bachelor's degree in Astronomy in July 2012. Beginning Fall 2015, Fernando began his graduate studies in Physics at the University of Tennessee in Knoxville.