

Nucleosynthesis in Self-Consistent Core-Collapse Supernova Models using Multidimensional Chimera Simulations

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Abstract

Observations of nuclear abundances in core-collapse supernova (CCSN) ejecta, highlighted by γ -ray [gamma-ray] observations of the ^{44}Ti [titanium-44] spatial distribution in the nearby supernova remnants Cassiopeia A and SN 1987A, allow nucleosynthesis calculations to place powerful constraints on conditions deep in the interiors of supernovae and their progenitor stars. This ability to probe where direct observations cannot makes such calculations an invaluable tool for understanding the CCSN mechanism. Unfortunately, despite knowing for two decades that supernovae are intrinsically multi-dimensional events, discussions of CCSN nucleosynthesis have been predominantly based on spherically symmetric (1D) models, which employ a contrived energy source to launch an explosion and often ignore important neutrino effects. As part of the effort to bridge the gap between first-principles simulations of the explosion mechanism and observations of both supernovae and supernova remnants, this dissertation investigates CCSN nucleosynthesis with self-consistent, axisymmetric (2D) simulations using the multi-dimensional radiation-hydrodynamics code CHIMERA. These models represent a necessary improvement over their parameterized counterparts in characterizing the impact of the hydrodynamically unstable, neutrino-driven supernova explosion on the ejecta composition and distribution.

Computational costs have traditionally constrained the evolution of the nuclear composition within multi-dimensional CCSN models to, at best, a 14-species α -network [alpha-network] capable of tracking only (α, γ) [(alpha,gamma)] reactions

from ${}^4\text{He}$ [helium-4] to ${}^{60}\text{Zn}$ [zinc-60]. Lagrangian tracer particles are commonly used to extend the nuclear network evolution by incorporating more realistic networks in post-processing calculations. This work presents a novel analysis of these nucleosynthesis calculations, including the impact of uncertainties therein, for four *ab initio* axisymmetric CCSN models initiated from stellar metallicity, non-rotating progenitors of 12, 15, 20, and 25 solar masses and evolved with the smaller α -network to more than a second after the launch of an explosion. The results of this analysis address many lingering concerns from parameterized 1D nucleosynthesis models. Facilitated by recent improvements to the physical approximations and computational performance of CHIMERA, future and ongoing simulations are beginning to address the implications of this analysis, highlighted by the need for larger *in situ* reaction networks and more developed explosion morphologies.

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Chapter 1

Introduction

The deaths of massive stars ($M > 8\text{--}10$ solar masses, denoted $M_{\odot}$ hereafter) as core-collapse supernovae (CCSNe) are an important link in our chain of origins from the Big Bang to the present. They are the dominant source of elements in the periodic table between oxygen and iron (Woosley and Weaver, 1995; Thielemann et al., 1996), and there is strong evidence that they are correlated with the production of half the elements heavier than iron (Argast et al., 2004). Core-collapse supernovae serve both to disperse elements synthesized in massive stars during their lifetimes and to synthesize and disperse new elements themselves.

1.1 The CCSN mechanism

Nuclear energy released by stellar nucleosynthesis is the driving force deterring a massive star from its inexorable fate of gravitational collapse. Fusion within the star consumes lighter elements, eventually producing a core rich in iron and its elemental neighbors. Surrounding the core are concentric shells composed of successively lighter elements. Unlike earlier stages of burning, wherein the ash from one burning stage serves as fuel for the next, no more nuclear energy can be released by the fusing of nuclei in the iron core. As the core approaches its maximum stable mass, defined as the Chandrasekhar limit, $M_{\text{Ch}} \equiv 1.457(2Y_{\text{e}})^2$, electrons, which are subject to the Pauli

exclusion principle, are forced into higher energy states until the pressure exerted by these ultra-relativistic particles, the electron degeneracy pressure, yields to the force of gravity and collapse ensues. For electron fractions typical of the iron core ($Y_e \approx 0.46$), $M_{\text{Ch}} \simeq 1.2 M_\odot$. It is only when nuclear densities ($\sim 10^{14} \text{ g cm}^{-3}$) are attained that the collapse of the iron core halts, forming a proto-neutron star (proto-NS). The inwardly-falling, outer layers of the iron core attain supersonic velocities before colliding with the inner core. The recoil, or core-bounce, caused by this collision launches a shock wave which propels these layers outward, ultimately disrupting the star in a supernova explosion. However, nuclear dissociation and the escape of neutrinos enervates the shock, stalling the shock in the iron core, and preventing it from driving off the envelope of the star.

Termed the *prompt mechanism*, the failure of the initial bounce shock to produce an explosion immediately lends itself to investigations of a *delayed mechanism*. Widely believed to be driving this delayed mechanism is a neutrino reheating paradigm, by which the intense neutrino flux carrying off the binding energy of the collapsed core heats the surrounding material and reenergizes the shock (Wilson, 1985; Bethe and Wilson, 1985). The stalled accretion shock eventually becomes sufficiently reenergized to overcome the gravitational force of the proto-NS and the ram pressure of infalling matter. The heated ejecta within the shock functions as a catalyst for further nucleosynthesis within the outer layers, fueling the ejection of the stellar envelope. Attempts to confirm this paradigm through spherically symmetric models have often failed to produce explosions because of an inability to sufficiently heat the envelope. This shortcoming can be attributed to the stratification imposed by the nature of spherically symmetric models (Bruenn et al., 2001). Through concentrated efforts and substantial improvements in computational resources, progress has been steadily made in better describing the neutrino transport. Spectral discretization of the neutrino radiation and implementation of spectral Boltzmann neutrino transport (Mezzacappa and Messer, 1999; Liebendörfer et al., 2004) improved upon the limitations of earlier schemes by removing the crude treatment of the transition

between an isotropic neutrino angular distribution and an outwardly streaming one. Despite these advances in the neutrino transport sophistication, spherically symmetric simulations fail to produce explosions (Rampp and Janka, 2002; Thompson et al., 2003).

By breaking the assumption of spherical symmetry, multi-dimensional models have been able to produce successful explosions, though initially restricted by computational costs to non-spectral (“gray”) neutrino transport (Herant et al., 1994; Burrows et al., 1995; Janka and Müller, 1996; Miralles et al., 2002; Bruenn et al., 2004; Fryer and Warren, 2004). Modern multi-dimensional simulations by several groups, utilizing spectral neutrino transport, have successfully produced explosions for a variety of progenitors in axisymmetry (2D) though delayed by hundreds of milliseconds compared to their non-spectral counterparts (Buras et al., 2003, 2006b,a; Burrows et al., 2006, 2007; Bruenn et al., 2006; Bruenn et al., 2009; Marek and Janka, 2009; Suwa et al., 2010; Takiwaki et al., 2012; Müller et al., 2012b,a; Bruenn et al., 2013; Mueller and Janka, 2014; Bruenn et al., 2014). Successful, fully self-consistent, spectral models have also achieved neutrino-driven explosions in three spatial dimensions (3D; Takiwaki et al., 2012, 2014; Melson et al., 2015a,b; Lentz et al., 2015). Qualitatively, the two- and three-dimensional simulations exhibit similar explosions, dominated by a small number of rising plumes that push the stalled shock outward. In both cases, explosions can be aided by enhanced neutrino luminosities due to fluid instabilities in the proto-NS (Smarr et al., 1981; Wilson and Mayle, 1993), improved neutrino-heating efficiency behind the shock as a result of fluid motions induced by convective instabilities, and the standing accretion shock instability (SASI; Blondin et al., 2003; Blondin and Mezzacappa, 2006; Foglizzo et al., 2007). However, three-dimensional models exhibit a tendency to be delayed when compared to their 2D counterparts (Hanke et al., 2013; Melson et al., 2015b; Lentz et al., 2015). The exception is Melson et al. (2015b), wherein the authors evolve a qualitatively different progenitor (zero-metallicity, $9.6 M_{\odot}$) than the models discussed here and the works cited above.

1.2 Observational evidence

The theoretically-demonstrated, highly asymmetrical behavior of CCSNe is corroborated by supernova remnant observations (see, e.g., Wang et al., 2002; DeLaney et al., 2010; Grefenstette et al., 2014; Milisavljevic and Fesen, 2015; Boggs et al., 2015). By directly imaging ^{44}Ti emission in Cassiopeia A, Grefenstette et al. (2014) revealed previously hidden asymmetries in the innermost ejecta, indicative of an explosion enhanced by low-mode instabilities (e.g. convective or SASI) rather than jet-like or bipolar behavior. Based on similar observations of ^{44}Ti ejection velocities in SN 1987A, Boggs et al. (2015) posit an even higher level of asymmetry consistent with a single-lobe explosion. These high-energy X-ray observations of large-scale anisotropies highlight the crucial role of accurate and detailed nucleosynthesis in computational models as a probe of the supernova engine.

γ -ray observations, like those of ^{44}Ti , are particularly useful for supernova nucleosynthesis theory, as they are able to measure both isotopic and elemental production in the deepest layers of the ejecta (Diehl and Timmes, 1998). Only neutrino and/or gravitational wave detection can probe deeper within the explosion. Observations of both SN 1987A and Cassiopeia A, using the Compton Gamma-Ray Observatory (CGRO), reveal a nuclear composition yet to be reproduced by stellar nucleosynthesis simulations (Clayton et al., 1992; Renaud et al., 2006) and, alongside ongoing γ -ray observations with the International Gamma Ray Astrophysics Laboratory (INTEGRAL), provide an excellent constraint for CCSN nucleosynthesis studies. This data must eventually be explained by extending first-principles explosion models to the interstellar medium (ISM). The extent to which such models can reproduce the wealth of observational data provides a unique look into the otherwise hidden explosion mechanism and its impact on galactic chemical evolution.

The wealth of supernova spectroscopic and photometric observations at longer wavelengths reveals a consistent pattern of extensive, large-scale mixing of the chemical elements (see, e.g., Wang and Wheeler, 2008). Mazzali et al. (2007) infer

from observations that the Type Ic supernova SN 2002ap had an oxygen-rich inner core with ^{56}Ni at higher velocity, a strong indication of large-scale overturn. The case is particularly persuasive for SN 1987A. Observed asymmetries in iron lines are most easily explained by the concentration of iron-peak elements into high-velocity “bullets” (Spyromilio et al., 1990). The *Bochum event*, the rapid development of fine structure in the H_α line from SN 1987A roughly two weeks after the explosion (Hanuschik et al., 1988), was interpreted by Utrobin et al. (1995) as an indication that a large ($\sim 10^{-3} M_\odot$) clump of nickel was ejected at high velocity ($\approx 4,700 \text{ km s}^{-1}$) into the far hemisphere of the supernova. Similarly, near-IR observations of He I lines arising roughly two months after explosion were interpreted by Fassia and Meikle (1999) as indications of dense clumps of nickel mixed into the hydrogen envelope of SN 1987A. Such evidence for asymmetries in SN 1987A motivated the first multi-dimensional studies of the propagation of the supernova shock through the star (see, e.g., Hachisu et al., 1990; Müller et al., 1991; Herant and Benz, 1992). These studies found that Rayleigh-Taylor instabilities developing as the shock encounters the stellar compositional interfaces were not sufficient to explain the observed asymmetries, pointing to asymmetries as part of the explosion mechanism itself.

1.3 Nucleosynthesis in CCSNe

Clearly, the deaths of massive stars are rife with instabilities. In fact, the existence of asymmetries, even in the pre-supernova core, has been known for some time (Kane et al., 2000; Meakin and Arnett, 2006), though these asymmetries have yet to be followed through core-collapse and bounce and into supernova explosions in a consistent fashion. However, Couch and Ott (2013) do show that artificially imposed but physically reasonable asphericities in the pre-collapse progenitor can qualitatively alter the post-bounce evolution. Despite the fundamentally multi-dimensional nature of a supernova explosion from its earliest moments, relatively limited work has addressed the impact of multi-dimensional behavior on the nucleosynthesis. We

have, however, learned that multi-dimensional effects produce significant differences in the fraction of ejecta which experiences α -rich freeze-out (Nagataki et al., 1998; Maeda et al., 2002) and larger ejecta velocities, characterized by metal-rich clumps (Kitaura et al., 2006; Hammer et al., 2010; Ellinger et al., 2012; Wongwathanarat et al., 2013, 2015a). Unfortunately, the complexity and cost of self-consistent CCSN models (abetted by their past, frequent failures to produce explosions) has led the community to largely continue to rely on nucleosynthesis predictions for CCSNe from models using a parameterized kinetic energy piston (Rauscher et al., 2002; Woosley and Heger, 2007; Magkotsios et al., 2010) or thermal energy bomb (Nagataki et al., 1998; Maeda et al., 2002; Umeda and Nomoto, 2008).

Beyond multi-dimensional effects, these parameterizations fall short in the inner region of the star, where interactions with the intense neutrino flux from the proto-NS are strong (Fryer et al., 2008). This is important because virtually all simulations utilizing spectral neutrino transport (e.g. Rampp and Janka, 2002; Buras et al., 2006b; Marek and Janka, 2009; Bruenn et al., 2014) exhibit decreased neutronization, increasing the electron fraction in the outer neutrino-reheating region as a result of these interactions, a feature which the parameterized bomb/piston models cannot replicate. In the neutrino-reheating paradigm, neutrino interactions also directly affect the *multi-dimensional mass-cut*—the amorphous, discontinuous boundaries separating regions of matter by their fate as either part of the interstellar medium or the proto-NS—and fundamentally alter the chemical composition of the ejecta.

Fröhlich et al. (2006a) and Pruet et al. (2005) have shown that nucleosynthesis from spectral, neutrino-driven explosions is qualitatively different in composition from both parameterized models and gray (mean energy) neutrino transport models, with the possibility of neutrino-driven flows to $Y_e > 0.5$ producing isotopes with mass number $A > 64$. This makes the innermost regions of CCSNe a candidate production site for light p -process nuclei via the νp -process. The spherically symmetric models of Fröhlich et al. (2006a,b) were explicitly neutrino-driven with a self-consistent determination of the mass-cut. These models (and the more recent models of

Perego et al., 2015) rely on an artificial increase in neutrino heating to produce explosions, which otherwise do not occur in such one-dimensional (1D) models. Pruet et al. (2005) achieved similar results with key neutrino opacities modified to favor a stronger explosion (see Buras et al., 2006b, for details of this model). Both Fröhlich et al. (2006a) and Pruet et al. (2005) successfully resolved the common problem of over-production of neutron-rich nickel and iron isotopes in bomb/piston models and increased Ti, Sc, Cu and Zn production, overcoming a shortcoming of previous models as compared to metal-poor stars (Gratton and Sneden, 1991; Cayrel et al., 2004). Recently, Perego et al. (2015) have demonstrated the ability to successfully reproduce ^{56}Ni yields in SN 1987A by retroactively extending the mass-cut to include late time fallback, but at the cost of under-producing ^{44}Ti —a direct consequence of the imposed spherical symmetry, since α -rich freeze-out occurs most strongly in the innermost ejecta in such stratified models.

The combination of a neutrino-driven explosion and multi-dimensional fluid flow by Pruet et al. (2005) hinted at the importance of departing from stratified 1D simulations. However, despite the profusion of exploding first-principles models with spectral neutrino transport in recent years, very little investigation of CCSN nucleosynthesis from these models has been conducted. This curious deficit can be partially attributed to the prolonged times after bounce the models must be evolved in order to fully characterize the ejecta and, therefore, compute the nucleosynthesis.

Nucleosynthesis studies of electron-capture supernovae (ECSNe), which arise from the collapse of oxygen-neon cores, are more mature, as these explosions trigger and complete more rapidly than in Fe-core SNe and can be obtained even in 1D simulations. Multi-dimensional investigations of ECSN nucleosynthesis (Wanajo et al., 2011, 2013a,b) using spectral neutrino transport find only modest impact from multi-dimensional effects, which is unsurprising given the successful 1D explosions. In these axisymmetric simulations, the authors describe a small amount of neutron-rich matter being dredged up from near the proto-NS during the early stages of the explosion, a phenomenon not seen in similar 1D simulations. As a result, the

models of [Wanajo et al. \(2011\)](#) are characterized by lower minimum values of Y_e , ultimately enhancing the production of As, Se, Br, Kr, Rb, Sr, and Y relative to that of spherically symmetric simulations, but leaving the ejected masses of ^{56}Ni and other iron-group elements unaffected. Multi-dimensional Fe-core CCSN models also exhibit convective overturn near the outer proto-NS layers, potentially with even greater affect on the nucleosynthesis and, given the necessity of multi-dimensionality to engender these explosions, occurs merely as a subset of other multi-dimensional effects. Consequently, the lessons learned from ECSN nucleosynthesis studies, with respect to multi-dimensional effects, provide only modest insight into the CCSN problem.

This work aims to address the effects of multi-dimensionality and realistic nuclear burning as they relate to CCSN nucleosynthesis simulations. In Chapter 2, I provide a description of the relevant numerical methods and key physical approximations employed by the CHIMERA code and subsequent post-processing calculations relating to the nucleosynthesis (for a more thorough discussion of methods in CHIMERA, see [Bruenn et al., 2014](#)). In Chapter 3, I quantify the impact of several factors which introduce uncertainties in the context of multi-dimensional models of CCSN nucleosynthesis and is the continuation of an earlier study which examined these uncertainties for one of the CHIMERA models ([Harris et al., 2014](#)). This uncertainty analysis ([Harris et al., 2015b](#), in prep) provides a proper framework for the detailed nucleosynthesis calculations presented in Chapter 4. The full extent of these results constitutes the subject of a forthcoming publication ([Harris et al., 2015a](#), in prep). Finally, in Chapter 5, I discuss recent improvements to the physical approximations and computational performance of CHIMERA ([Dong et al., 2014](#)), which have enabled future and ongoing studies to examine the effects of realistic nuclear networks in CHIMERA simulations.

Chapter 2

Simulating CCSNe

2.1 Overview of B-series models

Defined by a shared set of numerical methods and physical approximations, the B-Series simulations originate from solar-metallicity, non-rotating progenitors calculated by [Woosley and Heger \(2007\)](#) for $12 M_{\odot}$ (B12-WH07), $15 M_{\odot}$ (B15-WH07), $20 M_{\odot}$ (B20-WH07) and $25 M_{\odot}$ (B25-WH07) stars. These simulations were evolved with the CHIMERA code described in Section 2.2, incorporating modern neutrino-matter interactions, self-consistent luminosities and neutrino spectra, and coupled nuclear burning. The B-Series simulations extend to 1.2–1.4 seconds after bounce and were carried out in axisymmetry from the onset of collapse, with the very small post-bounce roundoff errors supplying the perturbations that seed the growth of fluid instabilities. The long times after bounce to which the B-Series simulations were evolved make them a unique resource for investigations of the uncertainties stemming from ongoing hydrodynamic activity that can impact post-processing nucleosynthesis results, even at these late epochs. All times reported hereafter are relative to core-bounce, or equivalently as time post-bounce (t_{pb}).

2.2 Methodology

CHIMERA is a multi-dimensional, radiation-hydrodynamics code for stellar core-collapse with five principal components: hydrodynamics, neutrino transport, self-gravity, a nuclear reaction network, and a nuclear equation of state (EoS; see [Bruenn et al., 2014](#), for details). In the following sub-sections, the points most relevant to this nucleosynthesis study are summarized.

2.2.1 Radiation hydrodynamics

Hydrodynamics is evolved via a dimensionally-split, Lagrangian-plus-remap scheme with piecewise parabolic reconstruction (PPMLR; [Colella and Woodward, 1984](#)) as implemented in VH1 ([Hawley et al., 2012](#)), modified to include the consistent multi-fluid advection of [Plewa and Müller \(1999\)](#). The self-gravity is computed using a multi-pole expansion ([Müller and Steinmetz, 1995](#)), replacing the Newtonian monopole with a general relativistic (GR) monopole ([Marek et al., 2006](#), Case A). The neutrino transport solver is an improved and updated version of the multi-group (frequency), flux-limited diffusion (MGFLD) implementation of [Bruenn \(1985\)](#), which uses near-complete physics, solving for four neutrino species ($\nu_e, \bar{\nu}_e, \nu_{\mu\tau} = \{\nu_\mu, \nu_\tau\}, \bar{\nu}_{\mu\tau} = \{\bar{\nu}_\mu, \bar{\nu}_\tau\}$) while allowing for neutrino-neutrino scattering, pair exchange and different opacities.

2.2.2 Nucleosynthesis in Chimera

B-Series simulations (see Section [2.1](#)) utilize the $K = 220$ MeV incompressibility version of the [Lattimer and Swesty \(1991\)](#) EoS for nuclear-matter densities ($\rho > 10^{11} \text{ g cm}^{-3}$) and an enhanced version of the [Cooperstein \(1985\)](#) EoS for $\rho < 10^{11} \text{ g cm}^{-3}$ where nuclear statistical equilibrium (NSE) applies. These provide a 4-species representation of the chemical composition, consisting of free neutrons, free protons, α -particles, and a representative heavy nucleus. To improve the fidelity of

the composition of matter that may eventually become part of the ejecta, in regions of NSE where $Y_e \geq {}^{26}/_{56}$ (the value of Z/A for ${}^{56}\text{Fe}$), a 17-species representation of the composition is used, including free neutrons, free protons, the 14 even- Z and even- A nuclei between ${}^4\text{He}$ and ${}^{60}\text{Zn}$ which constitute an α -network, as well as ${}^{56}\text{Fe}$ to conserve Y_e .

For regions not in NSE, the nucleosynthesis is computed within the constraints of an α -network (α , ${}^{12}\text{C}$ – ${}^{60}\text{Zn}$) by XNet, a fully implicit thermonuclear reaction network code (for details, see [Hix and Thielemann, 1999a](#)). In these regions, the initial composition is determined by mapping the abundances of free nucleons and the α -network species directly from the stellar progenitor to the computational grid in CHIMERA. To account for neutron-rich nuclei in the stellar progenitor, abundances of all nuclei which are not part of the α -network are bundled into an inert, representative auxiliary nucleus to conserve Y_e .

To determine whether a zone is in NSE, and may therefore be omitted from nuclear burning, CHIMERA applies an empirically determined linear relationship between the NSE transition temperature, T_{NSE} , and density:

$$T_{\text{NSE}}(\rho) = \begin{cases} C_1\rho + C_2 & \text{if } \rho < 2 \times 10^8 \text{ g cm}^{-3}; \\ 6.5 \times 10^9 \text{ K} & \text{otherwise,} \end{cases} \quad (2.1)$$

where $C_1 \equiv 5.333 \text{ K g}^{-1} \text{ cm}^3$ and $C_2 \equiv 5.433 \times 10^9 \text{ K}$. At the beginning of a global timestep, any non-NSE zone for which $T \geq T_{\text{NSE}}$ is transitioned to NSE. A zone which is in NSE at the beginning of a timestep will be transitioned out of NSE if $T < T_{\text{NSE}} - 2 \times 10^8 \text{ K}$ and if the representative heavy nucleus, split into ${}^{56}\text{Ni}$ and ${}^{56}\text{Fe}$, will result in less than half of the mass fraction being ${}^{56}\text{Fe}$. Otherwise, the transition out of NSE occurs if $T < 4.9 \times 10^9 \text{ K}$. The details of this transition out of NSE have a significant impact on the final composition of the ejecta (see Section [3.1.5](#)).

2.2.3 Domain decomposition

Two-dimensional CHIMERA simulations employ a polar axisymmetric grid of N_r non-equally spaced radial zones and N_θ uniformly-sized angular zones from 0 to π . For the B-Series models, a grid of $N_r = 512$ non-equally spaced radial zones covers from the stellar center into the oxygen-rich layers with an angular resolution of 0.70° ($N_\theta = 256$). The spacing of the moving radial grid is chosen such that relative density changes in the inner zones are small ($\Delta\rho/\rho \lesssim 0.1$), guaranteeing that the neutrino-emitting proto-NS surface is sufficiently resolved. Otherwise, the radial resolution is defined by limiting changes in the relative zone width, $\Delta r/r$, such that the grid cells are approximately square.

The individual modules of CHIMERA are algorithmically coupled in an operator split approach. The thermonuclear kinetics is evolved after the radial sweep in the directionally-split hydrodynamics, leaving each processor with the data along a single ray (see Figure 2.1). Thus, thermonuclear burning is computed zone-by-zone along each radial ray, using only data that is local to that ray and, therefore, local to the current process. This combination of directionally-split hydrodynamics and operator-split local physics provides the backdrop for the communication and computation patterns found in CHIMERA. Currently, each 2D CHIMERA simulation uses N_θ parallel MPI tasks on N_θ processor cores with one task/core for each radial ray. With this scheme, no off-node communication is required for the operator-split local physics calculations along a single ray of zones.

2.2.4 Tracer particle method

We provide a brief description of the implementation of the tracer particle method (TPM) in CHIMERA, wherein passive, Lagrangian tracer particles record the thermodynamic histories of individual mass elements, which may then be used for post-processing nucleosynthesis calculations (see, e.g., Nagataki et al., 1997; Nishimura et al., 2006; Seitenzahl et al., 2010; Nishimura et al., 2015). Following

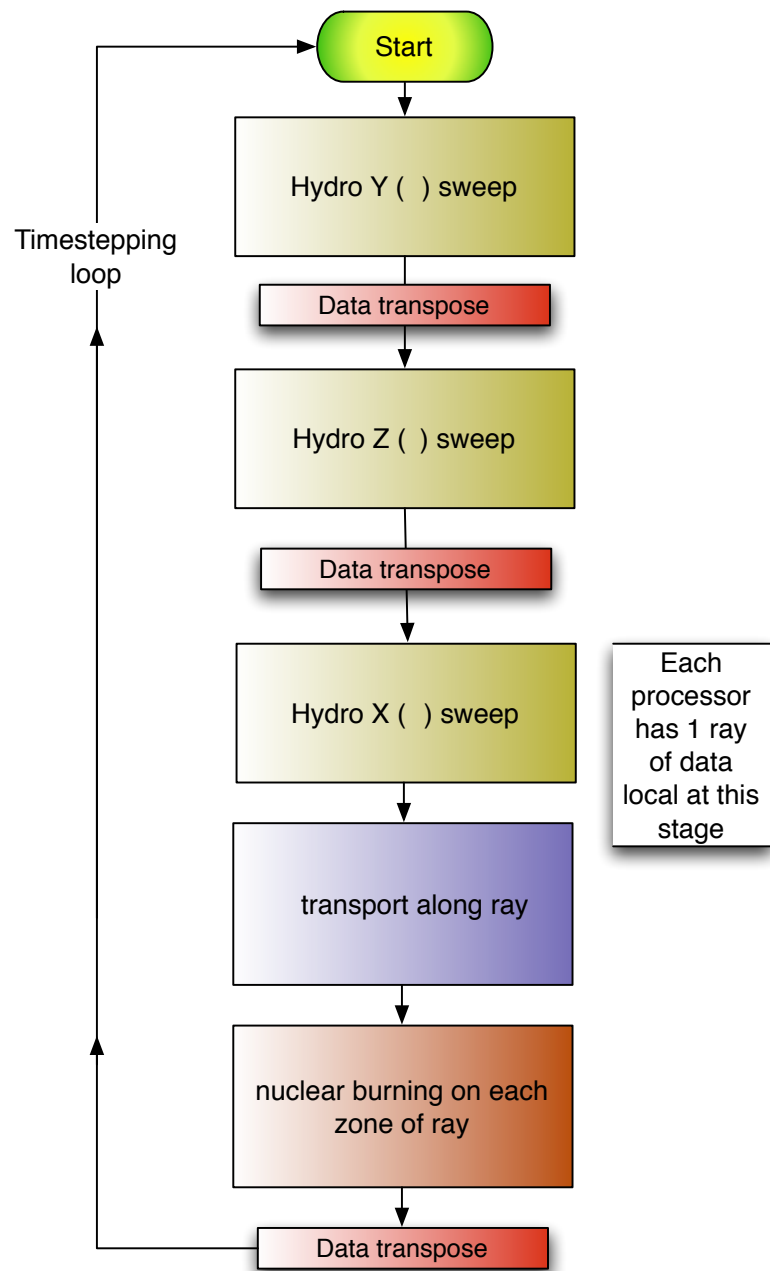


Figure 2.1 Schematic CHIMERA flowchart.

each hydrodynamic directional sweep, the position of a tracer particle at timestep $t^{(n)}$, $(r^{(n)}, \theta^{(n)})$, is advanced to $t^{(n+1)}$ according the simple Euler method, assuming constant velocity $(v_r^{(n)}, v_\theta^{(n)})$ through the time interval $\Delta t^{(n)} = t^{(n+1)} - t^{(n)}$:

$$r^{(n+1)} = r^{(n)} + v_r^{(n)} \Delta t^{(n)} (\text{following the radial sweep}), \quad (2.2)$$

$$\theta^{(n+1)} = \theta^{(n)} + v_\theta^{(n)} \Delta t^{(n)} (\text{following the latitudinal sweep}). \quad (2.3)$$

Physical quantities are linearly interpolated to tracer particle positions from the zone-center (cell-averaged) values of the computational grid; the lone exception being the interpolation of differential neutrino number fluxes, which are defined at zone edges.

The tracer particles are initially distributed into *rows*, radial shells uniformly-spaced in mass, beginning $0.1 M_\odot$ inside the edge of the progenitor’s iron core. Thus, no tracers are placed in the inner iron core, conserving the tracers for matter more likely to be ejected. The particles within each row are placed into *columns* in latitude that represent uniform volume (and hence uniform mass): $\Delta(\cos \theta) = 2/N$, where $N = 40$ particles per row for B-Series models. For B12-WH07, $N_{\text{tp}} = 4,000$ tracer particles are used, translating to 40 columns and 100 rows. Each tracer represents $\Delta m = 1.87 \times 10^{-4} M_\odot$, initially extending from ≈ 890 km to the carbon-enriched oxygen-shell at $\approx 15,000$ km. This degree of tracer resolution is common among prior nucleosynthesis studies employing the TPM (Nagataki et al., 1997; Pruet et al., 2005; Nishimura et al., 2006) and is similar to the “medium” resolution case of Nishimura et al. (2015). For more massive progenitors, more tracers are employed. However, the number of tracers grows more slowly than the mass in the silicon and oxygen shells, resulting in lower mass resolution in the more massive models. A description of the initial tracer particle distribution and representative mass of each tracer particle for each of the B-Series models is given in detail in Table 2.1.

Table 2.1. Initial distributions of Lagrangian tracer particles

Initial distribution	Models			
	B12-WH07	B15-WH07	B20-WH07	B25-WH07
Number of particles (N_{tp})	4000	5000	6000	8000
Number of mass shells (rows)	100	125	150	200
Particles per mass shell (columns)	40	40	40	40
Mass per shell [$M_{\odot} \times 10^{-3}$]	7.472	11.46	14.18	13.94
Mass per particle (Δm) [$M_{\odot} \times 10^{-4}$]	1.868	2.864	3.545	3.486
Inner boundary				
Inner row radius [km]	890.8	1,131	1,385	1,472
Inner edge mass [$M_{\odot}$]	1.203	1.321	1.424	1.480
Average mean mass number ($\bar{A}$)	37.77	42.42	43.05	42.17
Outer boundary				
Outer row radius [km]	15,000	19,456	19,751	19,751
Outer edge mass [$M_{\odot}$]	3.879	5.476	3.551	4.269
Average mean mass number ($\bar{A}$)	15.16	15.01	16.99	17.05

2.2.5 Nuclear reaction networks

Beyond the α -network described in Section 2.2.2, two additional reactions networks will be utilized in this work. A 150-species network, which we will refer to as the SN150-network, ranging in atomic number from $Z = 0$ to $Z = 30$ and including all isotopes from neutron number $N = Z$ to the most neutron-rich stable isotope for each element, represents a first-order improvement to the α -network. This moderately-sized reaction network encompasses a significant fraction of elemental abundances (see Figure 2.2) and energy-producing reactions important to the core-collapse problem, allowing proper neutronization and, when coupled to the hydrodynamics, a more accurate nuclear energy generation rate. For comparison with all potential nucleosynthetic observables, a larger network consisting of the full REACLIB compilation of 7,852 species (Cyburt et al., 2010) is used. Such a large reaction network is needed to capture more exotic nuclear processes like the νp -process and r -process. Reaction rates are taken from the REACLIB compilation and supplemented/supplanted with β -decay rates and electron capture rates on free nucleons and heavy nuclei (Fuller et al., 1985; Oda et al., 1994; Langanke and Martínez-Pinedo, 2000).

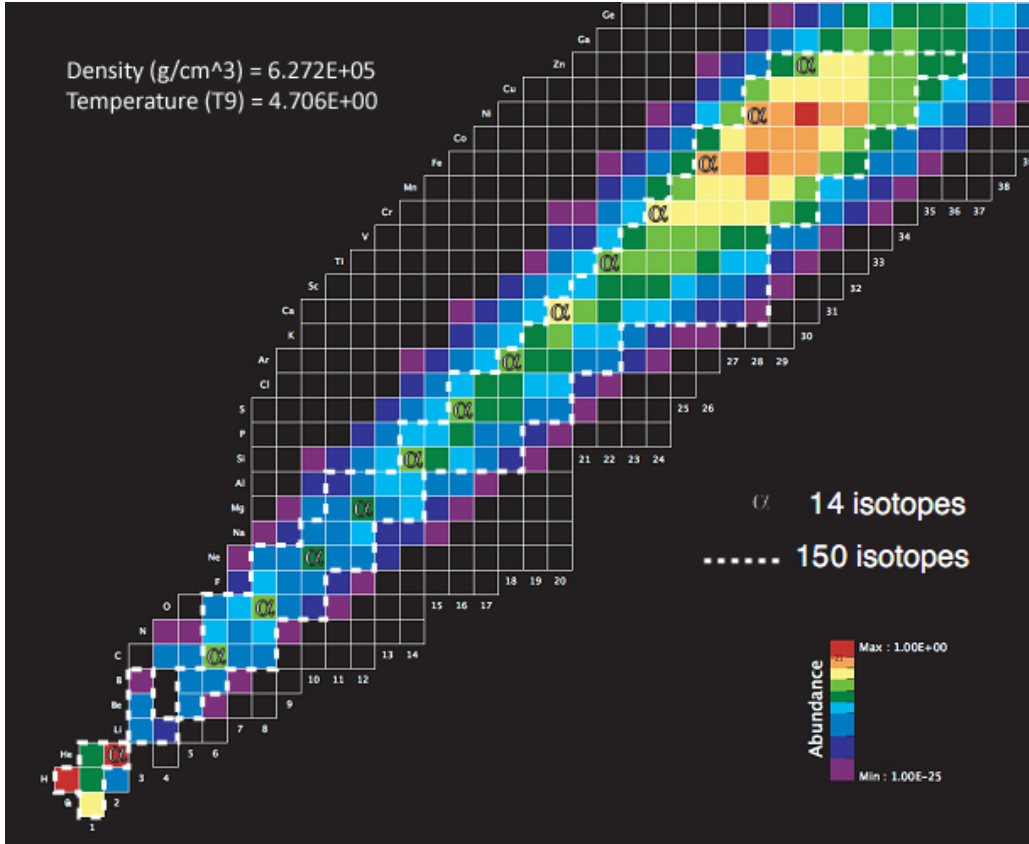


Figure 2.2 α -network isotope abundances and those of the expanded 150-species nuclear network are represented in the figure, calculated from a constant thermodynamic profile. The SN150-network encapsulates a large portion of the more heavily populated species. Of particular note is the exclusion of the three most abundant species (protons, ^{54}Fe , and ^{58}Ni) by the α -network.

Neutrino capture rates on free nucleons corresponding to the reactions

$$\nu_e + n \rightleftharpoons p + e^-, \quad \bar{\nu}_e + p \rightleftharpoons n + e^+ \quad (2.4)$$

are also included in post-processing calculations, for which we also record the integrated number flux of the neutrino distribution, ϕ_ν , with the tracer particles for ν_e and $\bar{\nu}_e$. Fluxes for $\nu_{\mu\tau}$ and $\bar{\nu}_{\mu\tau}$ are also recorded but are not included in the post-processing nucleosynthesis. The neutrino-induced reaction cross-sections also require the neutrino temperatures, T_ν , which we calculate by fitting the numerical neutrino distribution from the radiation-hydrodynamics simulation, $n(\epsilon_\nu)$, to a Fermi-Dirac spectrum of arbitrary degeneracy η :

$$n(\epsilon_\nu) = \frac{1}{F_2(\eta)T_\nu^3} \frac{\epsilon_\nu^2}{\exp((\epsilon_\nu/T_\nu) - \eta) + 1}, \quad (2.5)$$

where $F_2(\eta)$, the second-order Fermi-Dirac integral, is used for normalization to unity.

2.2.6 Post-processing nucleosynthesis

Post-processing calculations for ejected tracer particles which attain NSE begin at a point in time near the transition out of NSE (t_{NSE}), with initial conditions determined by finding the appropriate NSE composition which solves the Saha equation for the selected network and the corresponding thermodynamic conditions: $\rho(t_{\text{NSE}})$, $T(t_{\text{NSE}})$, and $Y_e(t_{\text{NSE}})$ (see, e.g., [Hix and Meyer, 2006](#); [Hartmann et al., 1985](#), and references therein, for more details on the NSE equations and resulting abundances). For tracers that never reach NSE, the initial abundances, temperature, and density are interpolated directly from the composition provided in the stellar progenitor. We then evolve the composition along the TPM-generated thermodynamic trajectories with a standalone implementation of XNet using a fully-implicit integration scheme ([Hix and Thielemann, 1999a](#)). In this way, we are able to generate more detailed nucleosynthetic yields using more realistic nuclear reaction networks.

Parameterized thermodynamic trajectories

Purely parameterized expansion profiles have long been used to study CCSN nucleosynthesis. [Fowler and Hoyle \(1964\)](#) introduced the use of adiabatic expansion following a peak temperature, T_{peak} , and peak density, ρ_{peak} , mimicking the passage of the shock-wave, with a characteristic expansion timescale, τ^* , equal to the free-fall timescale ($446/\sqrt{\rho_{\text{peak}}}$). With this assumption, the thermodynamic trajectory for a single particle may be expressed as

$$T(t) = T_{\text{peak}} \exp\left(-\frac{\Delta t}{3\tau^*}\right), \quad (2.6)$$

$$\rho(t) = \rho_{\text{peak}} \exp\left(-\frac{\Delta t}{\tau^*}\right), \quad (2.7)$$

where $\Delta t = t - t_{\text{peak}}$ is the time since the shock passage.

A number of explorations (see, e.g. [Woosley et al., 1973](#); [Meyer et al., 1998](#); [Hix and Thielemann, 1999b](#)) have used this simple parametrized model for their entire thermodynamic evolution. [Magkotsios et al. \(2010\)](#) utilized both this exponential decline as well as the power-law decline that results from the homologous expansion of a uniform sphere. [Nishimura et al. \(2015\)](#) also employ a power-law description of the expanding matter for simulations of magnetically-driven, rotating CCSNe soon after the early ejecta drops below NSE conditions. [Panov and Janka \(2009\)](#) employed an exponential decrease in temperature and density to describe the first (adiabatic) stage of a homologously expanding neutrino-driven wind before switching to a power-law model at later times, representative of reduced wind acceleration occurring after early homologous expansion. In this case, the density and temperature decline much less steeply during the power-law phase than during exponential expansion and can be calculated from the density (ρ_0) and temperature (T_0) at the time t_0 when the

matter is subjected to the reduced acceleration. For $t > t_0$,

$$T(t) = T_0 \left(\frac{t}{t_0} \right)^{-2/3}, \quad (2.8)$$

$$\rho(t) = \rho_0 \left(\frac{t}{t_0} \right)^{-2}. \quad (2.9)$$

Despite their efforts to account for different phases in the expansion, these purely analytic parameterizations usually begin at peak temperatures and densities and expand smoothly, failing to directly capture thermodynamic variations seen in multi-dimensional models.

Parameterizations like these can also be employed to extrapolate self-consistent thermodynamic trajectories from hydrodynamic simulations to much later times than the original simulations. In that case, *peak* values of temperature and density are replaced, for example in Equation 2.7, by *final* values, T_f and ρ_f , and Δt becomes $t - t_f$, the time since the end of the simulation. With the preceding hydrodynamic evolution in hand, better estimated expansion timescales are possible. For the particle data used herein, the effective expansion timescale, τ^* , is calculated by averaging the instantaneous value, $\tau = -\rho/\dot{\rho}$, during periods of expansion near the end of the simulation. The thermodynamic histories of particles are often quite noisy, so a 25-ms wide, six-degree Savitzky-Golay smoothing filter is applied to the density profile for computation of numerical derivatives (Press et al., 2007). For the epochs we discuss in this paper, we find that the final 150 ms of the simulation provides an adequate time-window for properly sampling the particle behavior. The time-window is also narrowed such that deviations in T^3/ρ from the final value do not exceed 10%. Furthermore, we exclude outliers in the calculation of τ^* by only considering the interquartile range of discrete values of τ over the specified time-window.

The exponential behavior in temperature and density is supplemented with a more slowly declining power-law trajectory (Equation 2.9) after nuclear burning has reached freeze-out conditions ($T \lesssim 0.5$ GK) at time t_{fo} . This prevents the small temperatures

that result from the exponential expansion from producing spurious results below the REACLIB lower temperature limit. The extrapolated thermodynamic trajectory for each tracer particle combines both of these parameterizations:

$$T(t) = \begin{cases} T_f \exp\left(-\frac{t-t_f}{3\tau^*}\right) & \text{if } t_f < t \leq t_{fo}, \\ T_f \exp\left(-\frac{t-t_{fo}}{3\tau^*}\right) \left(\frac{t}{t_{fo}}\right)^{-2/3} & \text{if } t > t_{fo}, \end{cases} \quad (2.10)$$

$$\rho(t) = \begin{cases} \rho_f \exp\left(-\frac{t-t_f}{\tau^*}\right) & \text{if } t_f < t \leq t_{fo}, \\ \rho_f \exp\left(-\frac{t-t_{fo}}{\tau^*}\right) \left(\frac{t}{t_{fo}}\right)^{-2} & \text{if } t > t_{fo}. \end{cases} \quad (2.11)$$

For neutrino-induced reactions, we assume that T_ν remains constant for $t > t_f$ and $\phi_\nu \propto 1/r(t)^2$, where $r(t) = r(t_f) + v_r(t_f)\Delta t$ assumes a constant radial velocity for $t > t_f$.

Chapter 3

Nucleosynthesis Uncertainties

Calculating the nucleosynthesis of neutrino-driven, multi-dimensional CCSN models removes a range of uncertainties related to the various approaches used to generate explosions in parameterized investigations of this nucleosynthesis. Foremost among these are the effects of neutrino-matter interactions and turbulent fluid flow. For fully self-consistent simulations, examination of the nucleosynthesis affords additional observable consequences of the explosion model that can be compared to observations.

However, this progress to greater physical fidelity in our investigations of CCSN nucleosynthesis is not without compromise. Many of the bomb and piston models that have provided the bulk of our understanding of CCSN nucleosynthesis in recent years utilize realistic nuclear reaction networks and continue well after the supernova ejecta reaches the surface of the star, perhaps an hour after the formation of the proto-neutron star (see, e.g., [Woosley and Heger, 2007](#); [Umeda and Nomoto, 2008](#); [Chieffi and Limongi, 2013](#)). To contain computational cost, multi-dimensional studies generally fail to include large nuclear reaction networks within their simulations. As a result, post-processing of Lagrangian thermodynamic histories with a realistic nuclear reaction network is required to generate abundances of all of the isotopes of interest. For Lagrangian methods, like smoothed particle hydrodynamics (SPH), these Lagrangian thermodynamic histories are simply the trajectories of the (active)

particles that represent the fluid in this approach. For Eulerian methods, passive tracer particles must be added to the conventional hydrodynamic evolution, as these grid-based methods are otherwise unable to record the histories of fluid elements, instead evolving (and recording the histories of) fluid quantities at specified locations. Resolution is a limiting factor in any computational simulation. While SPH simulations, by their nature, provide Lagrangian fluid elements that fully sample the hydrodynamic evolution at the intrinsic resolution of the simulation, passive tracers within Eulerian simulations do not necessarily provide similar sampling.

Regardless of the formalism for the hydrodynamic evolution, the use of a realistic network only in post-processing removes the natural feedback between the evolution of the nuclear composition and the thermodynamic conditions. Thus, the accuracy of post-processing nucleosynthesis is only as good as the physical fidelity of the thermonuclear evolution included within the simulations. In most multi-dimensional CCSN studies, for matter at high temperature and density, this role is served by the nuclear equation of state under the assumption of NSE, together with neutrino transport altering the neutronization. At lower temperatures, NSE does not apply; thus, a nuclear reaction network of some type is needed. The simplest approach used in such models is a *flashing* scheme, wherein “Oxygen” is converted directly to “Silicon” at some chosen temperature, and “Silicon” is similarly converted to NSE at another, higher temperature (see, e.g., [Marek and Janka, 2009](#)). Of greater fidelity is an α -network, composed of the 13 (or 14) isotopes with equal and even proton and neutron numbers between ^4He and ^{56}Ni (or ^{60}Zn) and the reactions, predominantly (α, γ) , that link them. While an α -network is nearly complete for carbon burning and a reasonable approximation to oxygen burning, it does not include many of the reaction channels important for the production of iron and nickel ([Timmes et al., 2000](#)), either by silicon burning or by the recombination of dissociated nucleons and α -particles, resulting in misestimation of the rate of nuclear energy release for these processes. A further limitation of an α -network is the inability to track neutronization from electron and neutrino captures, so the neutronization must be monitored separately

or ignored entirely. Even when handled separately, as it is in CHIMERA, it is difficult to evolve the neutronization correctly in the absence of NSE without all relevant species and reaction channels available.

The extreme cost of fully self-consistent simulations commonly limits our most realistic CCSN models to run only several hundred milliseconds after bounce, often aborting the simulations before the nucleosynthesis is complete. These cost-motivated compromises introduce additional sources of uncertainty in the calculation of CCSN nucleosynthesis that must be accounted for if we are to maximize the understanding gained from such studies. Early termination of these simulations requires extrapolation of the thermodynamic history if the thermonuclear evolution is still ongoing when the simulation stops. While a number of past studies have relied on similar extrapolations for their entire thermodynamic evolution, it is nonetheless important to constrain this uncertainty. Early termination also makes it more challenging to determine the mass-cut, which delineates the fates of the matter within the star, and judge the composition of the ejecta. The mass-cut does not impact all isotopes equally, the common perception (see, e.g. [Diehl and Timmes, 1998](#)), based on spherically symmetric models, being that this uncertainty will most strongly impact the products of α -rich freeze-out; however, this question merits re-examination in a multi-dimensional context.

3.1 Quantifying uncertainties

In this section, we quantify the impact of several factors that contribute to uncertainties in multi-dimensional models of CCSN nucleosynthesis. We categorize these uncertainties into those relating to the determination of the multi-dimensional mass-cut (Section [3.1.1](#)), estimation of expansion timescales for use in thermodynamic extrapolation (Section [3.1.2](#)), effects associated with earlier termination of the simulations (Section [3.1.3](#)), and limitations in Lagrangian tracer particle spatial (Section [3.1.4](#)) and temporal (Section [3.1.6](#)) resolution. In Section [3.1.5](#) we discuss

the impact that choices in the transition from NSE has on the composition. We also examine some consequences of the nuclear reaction network size. The full impact of using an α -network must await similar simulations with a large *in situ* nuclear reaction network (see Chapter 5). Some additional sources of uncertainty, for example, those related to the stochasticity inherent in multi-dimensional models, are beyond the scope of this study.

3.1.1 Determination of the multi-dimensional mass-cut

Observations and models agree that core-collapse supernovae are highly asymmetric events driven by complex and/or turbulent fluid flows. The implications of this multi-dimensionality on the nucleosynthesis are lost in 1D simulations, wherein a clear distinction, the mass-cut, is easily made between matter which is ejected to the interstellar medium and that which falls back to the proto-NS (defined hereafter as the region where $\rho > 10^{11} \text{ g cm}^{-3}$). While the placement of the mass-cut varies in time in a spherically symmetric model, for example, as fallback results from matter formerly expanding being decelerated by interactions with the stellar envelope, the mass-cut is nonetheless a unique mass coordinate within the progenitor star. Extending this distinction to 2D and 3D simulations is challenging, as there is no requirement that the ejecta form a contiguous region, an implicit feature of 1D simulations. Further, the ability for accretion and outflow to occur simultaneously makes the determination of even the initial mass-cut a much more gradual process.

Ultimately, this requires evolving a model well beyond the initial development of an explosion until such time that the downflows, which have long been cut-off from the rest of the star at the shock, cease falling onto the proto-NS and accretion dramatically slows. Here, the limitation in our ability to extend the models, due to the computational cost of running simulations with spectral neutrino transport, is a great impediment compared to typical parameterized models. In this study, we have extended four self-consistent models with spectral neutrino transport using CHIMERA

much further than similar models have heretofore been run in order to examine this issue. We find that the initial multi-dimensional mass-cut is not yet fully resolved, despite 1.2–1.4 s of evolution after bounce and ≈ 1 s after the initiation of an explosion.

Examining the mass-cut begins by defining the ejecta. Once the supernova shock breaks through the surface of the star, the ejecta is self-defined as the matter which propagates into the ISM. However, a definition is needed that can be applied at much earlier epochs. The treatment of the explosion energy faces a similar challenge of definition at these early times; thus, we mirror here the treatment of the explosion energy discussed in [Bruenn et al. \(2014\)](#), which is similar to the approach used by several authors in recent years. With contributions from specific kinetic (e_{kin}), thermal (e_{th}), and gravitational binding energy (e_{grav}), the specific total energy,

$$e_{\text{tot}} \equiv e_{\text{kin}} + e_{\text{th}} + e_{\text{grav}}, \quad (3.1)$$

defines the unbound ejecta as particles for which $e_{\text{tot}} > 0$. We label this set of unbound particles as $\mathbb{P}_{\text{unb}}$ and the corresponding mass as M_{unb} . This should not to be confused with the total ejected mass, M_{ej} , which also includes contributions from as yet unshocked matter, both on and above CHIMERA’s computational grid. Likewise, we use $\mathbb{P}_{\text{bound}}$ and M_{bound} to represent the bound matter ($e_{\text{tot}} < 0$) outside of the proto-NS. Ideally, all tracer particles in $\mathbb{P}_{\text{unb}}$ would constitute a portion of the observed ejecta. However, due to the work required to lift the stellar envelope out of the star’s gravitational well, $\mathbb{P}_{\text{unb}}$ is likely an over-estimate of particles that would ultimately be ejected. A further complication is that some particles in $\mathbb{P}_{\text{unb}}$ have negative radial velocities and, thus, increasing temperature and pressure. Therefore, they cannot be reliably extrapolated for post-processing nucleosynthesis. For this reason, it is helpful to categorize $\mathbb{P}_{\text{unb}}$ by radial velocity, which we label as $\mathbb{P}_+$ and $\mathbb{P}_-$ for $v_r > 0$ and $v_r < 0$, respectively. We find that the ultimate fates of particles in $\mathbb{P}_-$ as either ejecta or part of the proto-NS ($\mathbb{P}_{\text{PNS}}$) are often unknowable at the end of the simulation. Consequently, the mass represented by $\mathbb{P}_-$, M_- , is

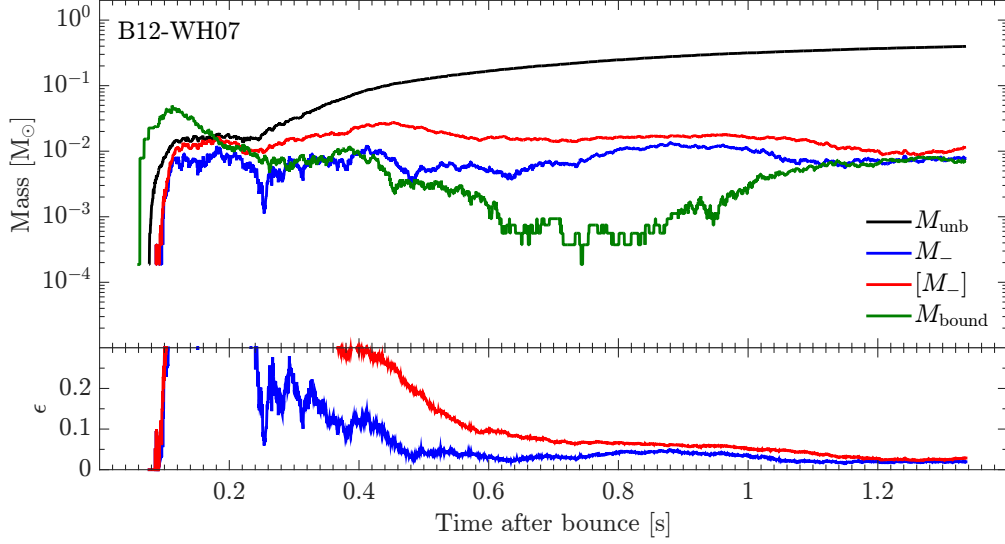


Figure 3.1 Top panel: B12-WH07 total mass represented by particles in $\mathbb{P}_{\text{unb}}$ (black), $\mathbb{P}_{-}$ (blue), $[\mathbb{P}_{-}]$ (red), and $\mathbb{P}_{\text{bound}}$ (green). Bottom panel: Fraction of M_{unb} represented by particles in $\mathbb{P}_{-}$ and $[\mathbb{P}_{-}]$.

one indication of uncertainty in the total ejecta mass. Therefore, trends in $M_{-}(t)$ partially characterize the duration of time we must evolve a model in order to keep this uncertainty manageable. Figures 3.1–3.4 illustrate the temporal behavior of these mass quantities for each model. The black lines illustrate the gradual increase in M_{unb} as the shock gradually lifts the envelope. The green lines illustrate M_{bound} , which remains stubbornly above $0.001 M_{\odot}$ at the end of each model, reflecting the ongoing accretion evident in these models. M_{-} , illustrated by the blue lines, still exhibits significant growth at the end of B20-WH07 and B25-WH07, while B12-WH07 and, possibly, B15-WH07 have leveled out near $0.01 M_{\odot}$. We can attribute this behavior to an immature explosion in B25-WH07 and a weak explosion in B20-WH07. Across all four models, the final values of M_{-} exhibit a monotonic increase with progenitor mass from $0.008 M_{\odot}$ in B12-WH07 to $0.2 M_{\odot}$ in B25-WH07.

For B12-WH07, M_{-} is relatively unchanged in the 100 ms prior to the end of the simulation, defined as $t_{\text{f}-100}$. However, closer inspection reveals that, while the total number of particles in $\mathbb{P}_{-}$ tracks the behavior of M_{-} , the individual particles in $\mathbb{P}_{-}$

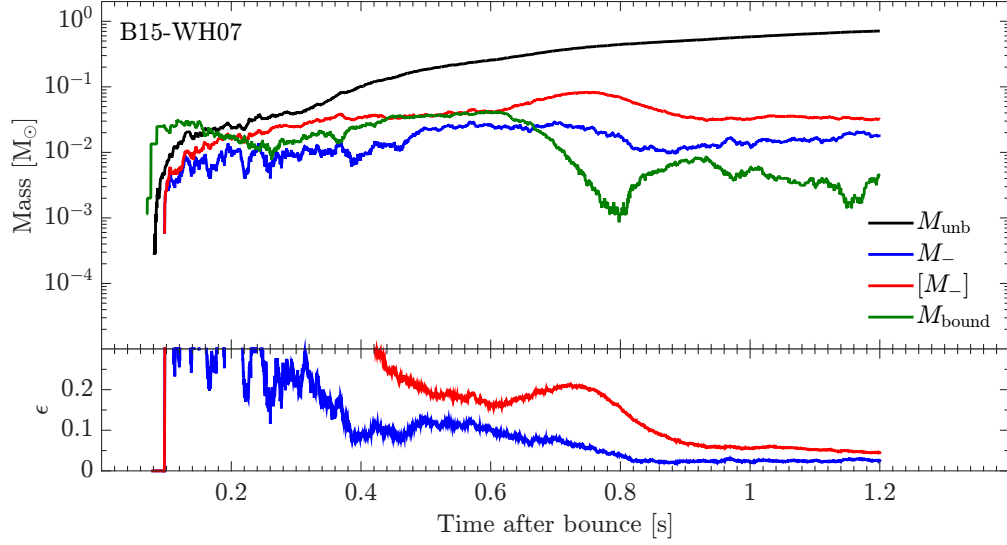


Figure 3.2 Top panel: B15-WH07 total mass represented by particles in $\mathbb{P}_{\text{unb}}$ (black), $\mathbb{P}_-$ (blue), $[\mathbb{P}_-]$ (red), and $\mathbb{P}_{\text{bound}}$ (green). Bottom panel: Fraction of M_{unb} represented by particles in $\mathbb{P}_-$ and $[\mathbb{P}_-]$.

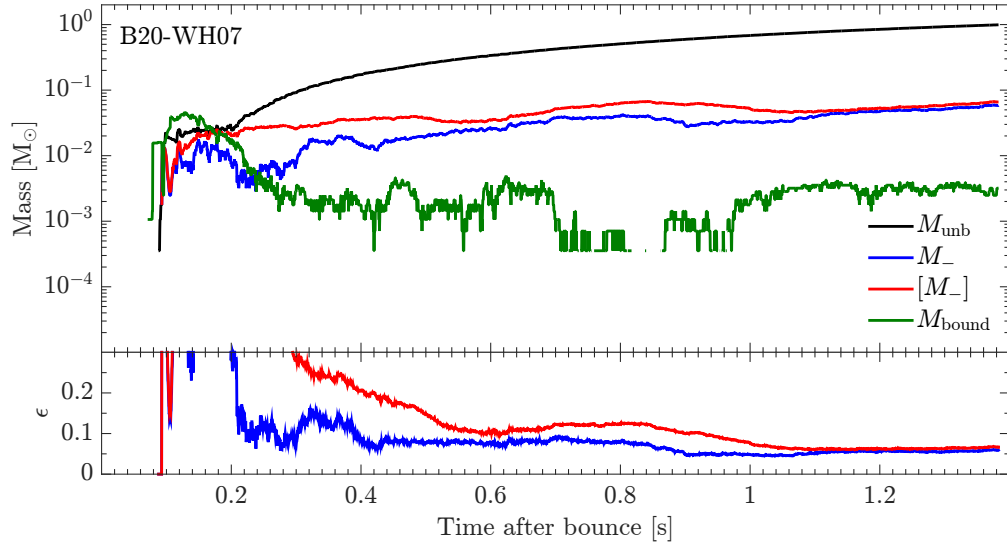


Figure 3.3 Top panel: B20-WH07 total mass represented by particles in $\mathbb{P}_{\text{unb}}$ (black), $\mathbb{P}_-$ (blue), $[\mathbb{P}_-]$ (red), and $\mathbb{P}_{\text{bound}}$ (green). Bottom panel: Fraction of M_{unb} represented by particles in $\mathbb{P}_-$ and $[\mathbb{P}_-]$.

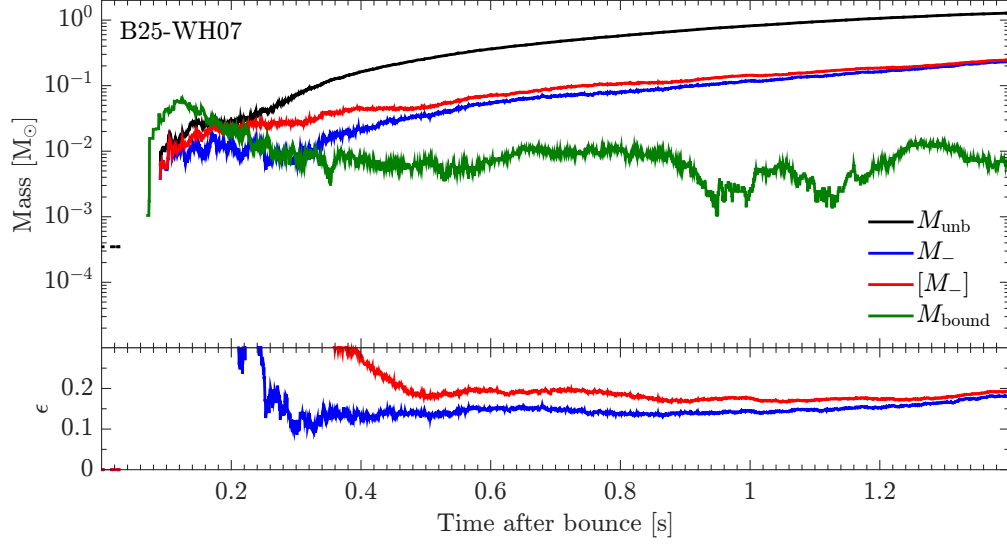


Figure 3.4 Top panel: B25-WH07 total mass represented by particles in $\mathbb{P}_{\text{unb}}$ (black), $\mathbb{P}_{-}$ (blue), $[\mathbb{P}_{-}]$ (red), and $\mathbb{P}_{\text{bound}}$ (green). Bottom panel: Fraction of M_{unb} represented by particles in $\mathbb{P}_{-}$ and $[\mathbb{P}_{-}]$.

are changing as convective flows and shear move particles between $\mathbb{P}_{-}$ and $\mathbb{P}_{+}$. This variability of v_r for $\mathbb{P}_{\text{unb}}$ near the end of the simulation complicates the determination of a particle as being representative of the ejected matter. In Figure 3.5, we illustrate this phenomenon by plotting the various fates of the particles in $\mathbb{P}_{-}(t)$ (black line) at $t - 100$ ms. Ideally, $\mathbb{P}_{-}(t)$ and $\mathbb{P}_{-}(t - 100 \text{ ms})$ would be identical, indicating a consistent determination of the particles' fates. However, since there is a persistent fraction of particles in $\mathbb{P}_{-}(t)$ that are being classified as ejecta only 100 ms in the past ($\mathbb{P}_{+}(t - 100 \text{ ms})$; red line), we identify all particles that were in $\mathbb{P}_{-}$ at any time in the last 100 ms of the simulation, which we label $[\mathbb{P}_{-}]$, as having indeterminate fates and contributing to a better estimated uncertainty in the ejecta mass. We use this type of nomenclature hereafter to refer to quantities derived from $[\mathbb{P}_{-}]$ (e.g. $[M_{-}]$). For B12-WH07, we see that $[M_{-}]$ is $\sim 50\%$ larger than M_{-} , reflecting that a significant portion of $\mathbb{P}_{-}$ is undergoing substantial variations in radial velocity over the past 100 ms. For B15-WH07, $[M_{-}]/M_{-} = 1.78$ is relatively even larger, indicating more exchange of inwardly and outwardly moving particles. Intriguingly, the much larger and still

growing number of particles in $\mathbb{P}_-$ in B20-WH07 and B25-WH07 are not undergoing similar variations, with $[M_-]$ only 13% and 7% larger than M_- , respectively

The fates and peak temperatures, T_{peak} , for shocked particles in the inner 8,000 km of each of the B-Series models are shown at t_f in Figures 3.6–3.9. The shock has generally moved beyond this grid, except in the upper left corners of Figure 3.8 and Figure 3.9, wherein the absence of shocked tracers is visible. Downflows of bound matter ($\mathbb{P}_{\text{bound}}$; open, black circles) are clearly visible, especially in B12-WH07 and B15-WH07, dragging unbound but now infalling particles ($\mathbb{P}_-$; open, colored circles). The much larger mass represented by $\mathbb{P}_-$ particles, M_- , for B20-WH07 and B25-WH07, discussed in Figure 3.3 and Figure 3.4, is plainly visible in the open, colored circles in Figure 3.8 and especially Figure 3.9. Clearly, in both B20-WH07 and B25-WH07, the shock in the equatorial regions has been less successful in pushing the envelope outward, suggesting significant accretion will continue for a considerable time.

Since the tracers are a Lagrangian representation of the matter, we can trace them back in time to their original positions. Figures 3.10–3.13 show the same quantities as Figures 3.6–3.9, but with the tracers positioned at their initial locations, revealing the fate of tracers as a function of their starting point in the progenitor. Arcs reveal features in the progenitor star: red, the outer edge of the iron core; cyan, the transition from silicon to a mix of silicon and oxygen. These same progenitor models were exploded by [Woosley and Heger \(2007\)](#) using a parameterized piston positioned at the $S/N_A k_B = 4.0$ isoentropy contour (solid, magenta line). This represents the mass-cut in the parameterized models and generally lies at the inner boundary of the oxygen-burning shell. The presence of bound particles originating above this mass-cut, and unbound particles below, illustrates the fundamental difference in a multi-dimensional mass-cut. Intriguingly, a significant number of ejected tracers originate in the relatively dense silicon shell, some nearly to the edge of the iron core, which has ramifications for the nucleosynthesis that we will discuss in Chapter 4. Of more immediate interest is the identification of the currently accreting matter.

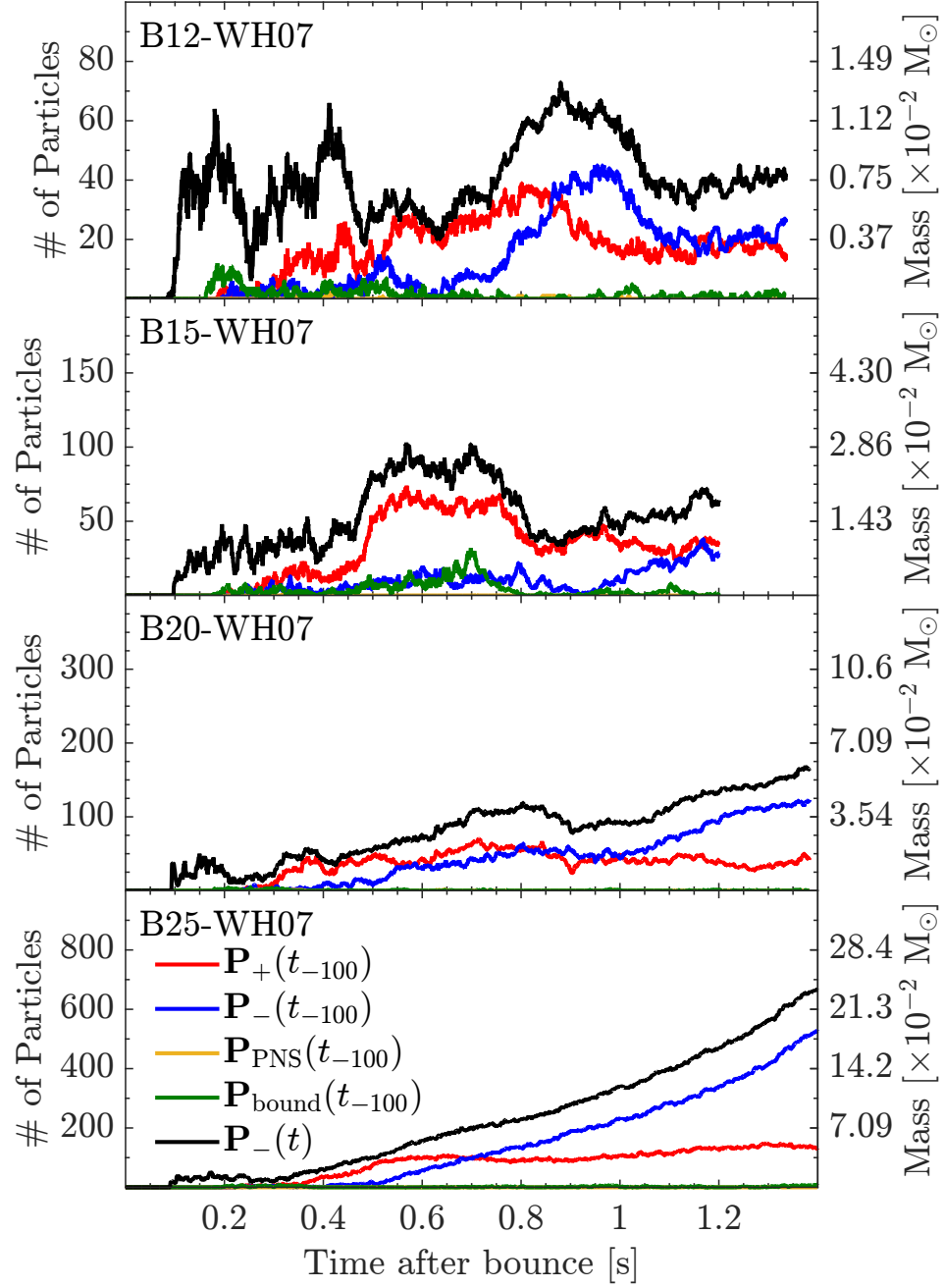


Figure 3.5 Fate classification for particles changes as the simulation progresses. Shown in black are the number of particles in $\mathbb{P}_-(t)$ and the corresponding mass, $M_-(t)$ as a function of time t . Colored lines show the same particles' classifications at an offset time, $t_{-100} = t - 100$ ms.

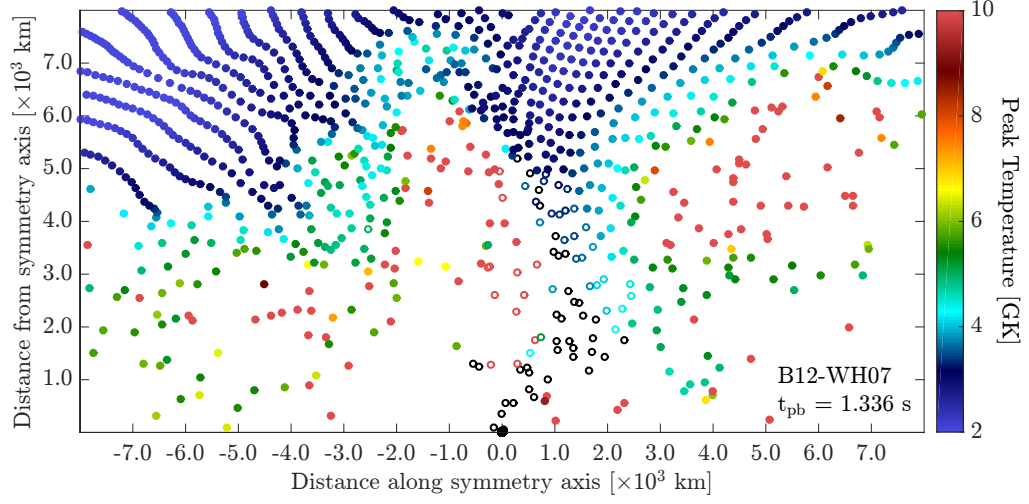


Figure 3.6 B12-WH07 shocked tracer particles in $\mathbb{P}_+(t_f)$ (solid, colored circles), $\mathbb{P}_-(t_f)$ (open, colored circles), $\mathbb{P}_{\text{bound}}(t_f)$ (open, black circles), and those located in the proto-NS (solid, black circles), placed at their locations at t_f and, if unbound, colored by T_{peak} .

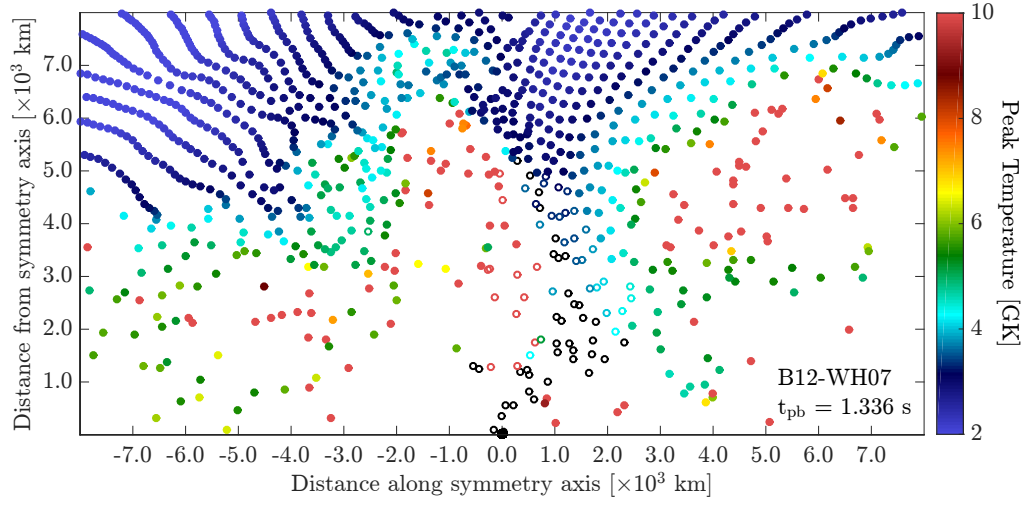


Figure 3.7 B15-WH07 shocked tracer particles in $\mathbb{P}_+(t_f)$ (solid, colored circles), $\mathbb{P}_-(t_f)$ (open, colored circles), $\mathbb{P}_{\text{bound}}(t_f)$ (open, black circles), and those located in the proto-NS (solid, black circles), placed at their locations at t_f and, if unbound, colored by T_{peak} .

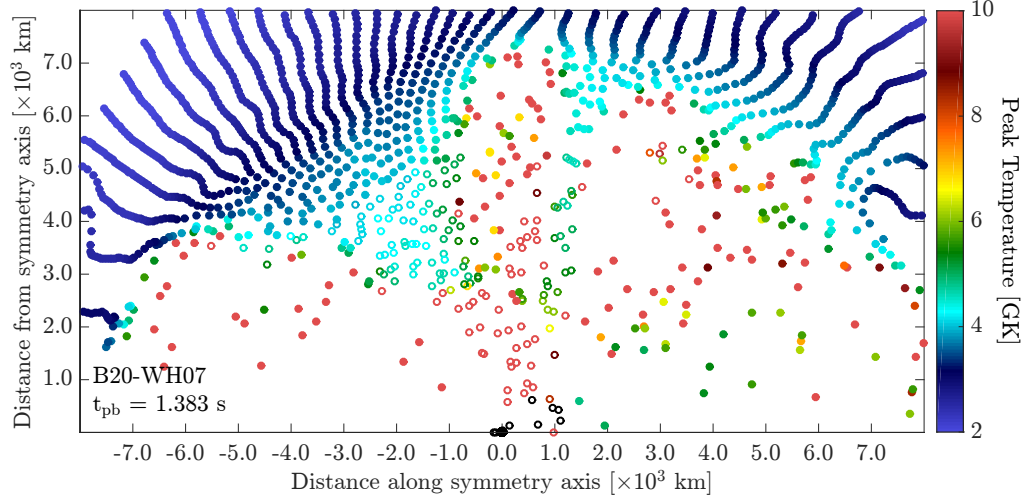


Figure 3.8 B20-WH07 shocked tracer particles in $\mathbb{P}_+(t_f)$ (solid, colored circles), $\mathbb{P}_-(t_f)$ (open, colored circles), $\mathbb{P}_{\text{bound}}(t_f)$ (open, black circles), and those located in the proto-NS (solid, black circles), placed at their locations at t_f and, if unbound, colored by T_{peak} .

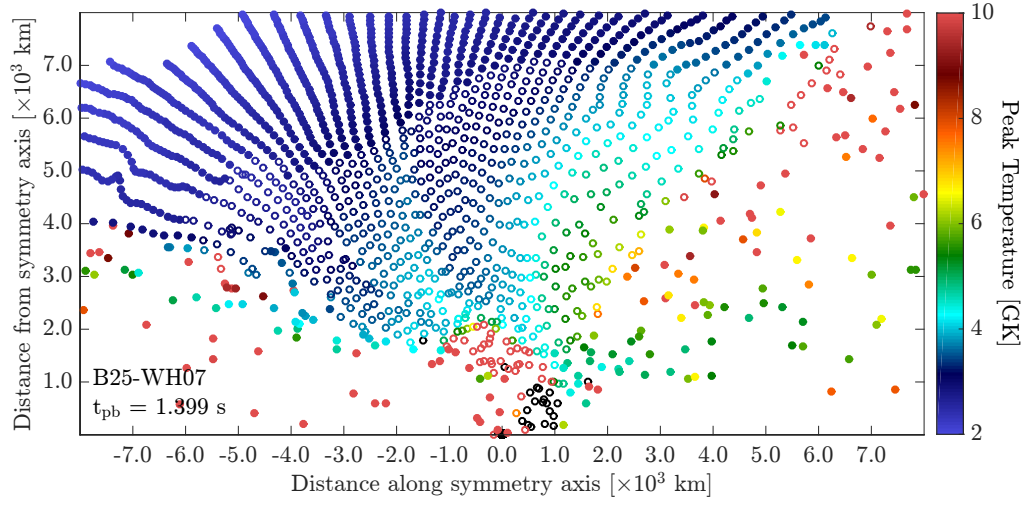


Figure 3.9 B25-WH07 shocked tracer particles in $\mathbb{P}_+(t_f)$ (solid, colored circles), $\mathbb{P}_-(t_f)$ (open, colored circles), $\mathbb{P}_{\text{bound}}(t_f)$ (open, black circles), and those located in the proto-NS (solid, black circles), placed at their locations at t_f and, if unbound, colored by T_{peak} .

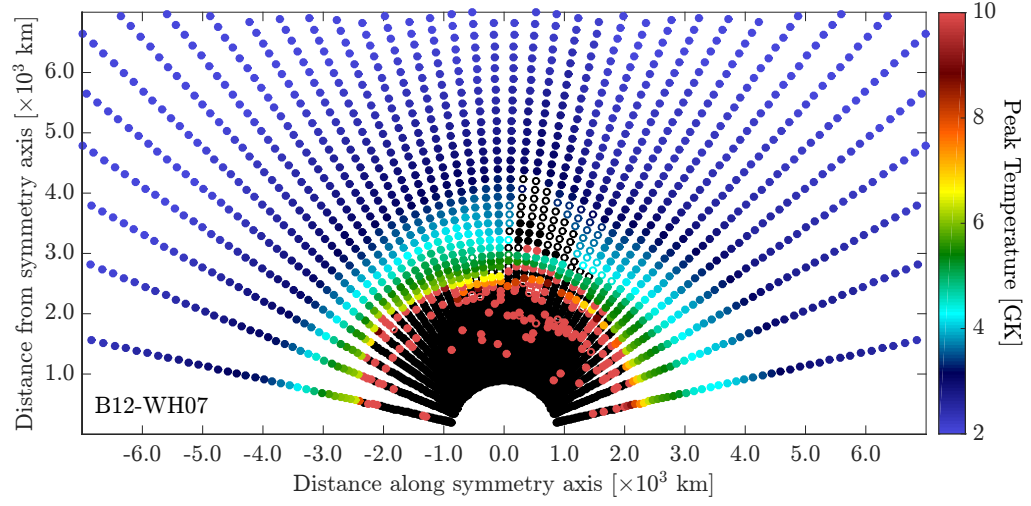


Figure 3.10 B12-WH07 peak temperatures and fates for particles at their initial locations presented as described in Figure 3.6.

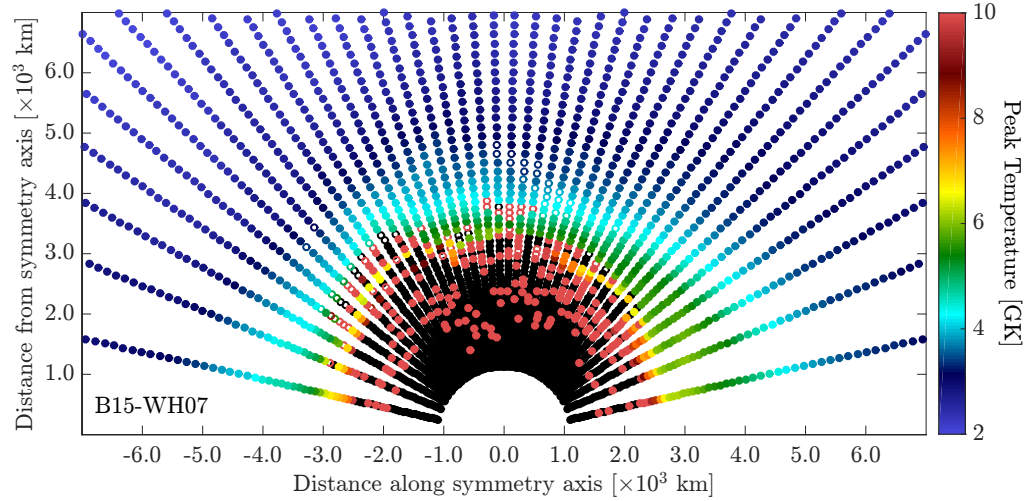


Figure 3.11 B15-WH07 peak temperatures and fates for particles at their initial locations presented as described in Figure 3.7.

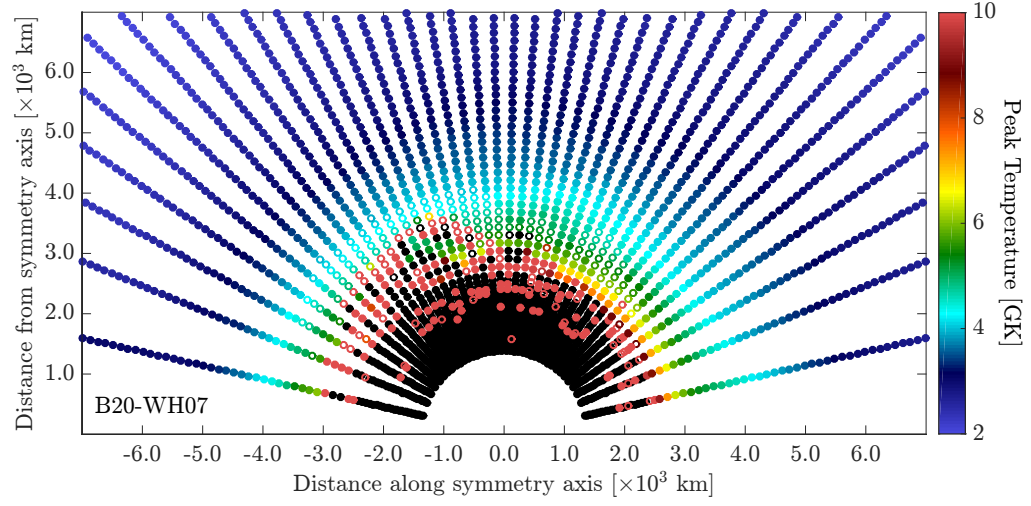


Figure 3.12 B20-WH07 peak temperatures and fates for particles at their initial locations presented as described in Figure 3.8.

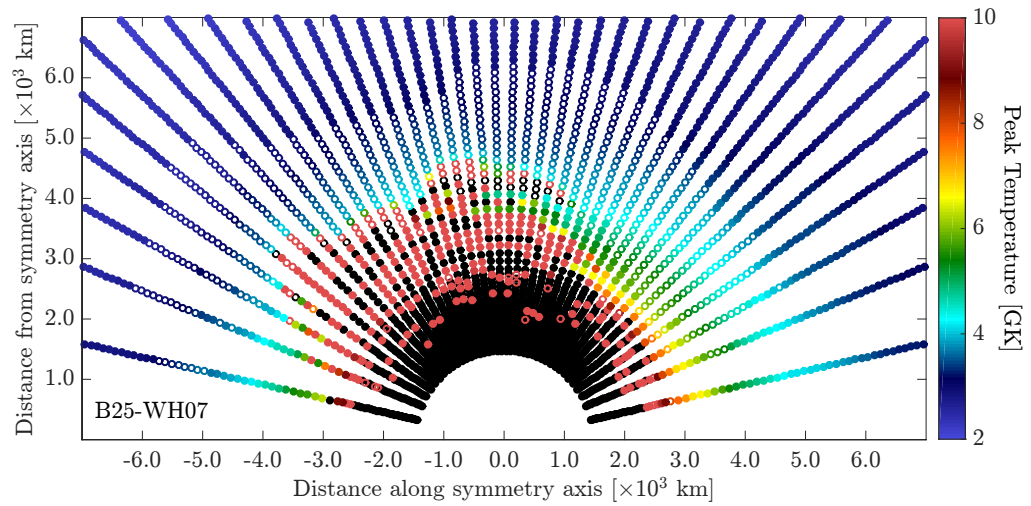


Figure 3.13 B25-WH07 peak temperatures and fates for particles at their initial locations presented as described in Figure 3.9.

In B12-WH07, B15-WH07, and B20-WH07, $\mathbb{P}_-$ (open, colored circles) covers a small, isolated region of the initial particle distribution (see Figures 3.10–3.12), though there is a trend to wider regions in latitude with increasing mass. These particles originate 3,000–4,000 km from the center and have reached peak temperatures of 3–5 GK, which serves as a reasonable proxy for a composition originally consisting of ^{16}O and ^{28}Si and their subsequent explosive burning products as being most susceptible to uncertainty in the identification of the ejecta. This is in contrast to the usual assumption that products of α -rich freeze-out are most susceptible to this determination. The characteristics of $\mathbb{P}_-$ in B25-WH07 are much more extreme than that of the other three models. In the case of the $25 M_\odot$ model, the uncertainty in the identification of the ejecta is not confined to a small region in the initial particle distribution, but nearly extends from pole-to-pole in latitude (see Figure 3.13).

We quantify these uncertainties in all four models in Figures 3.14–3.17 by comparing the total unbound mass of each isotope after post-processing with the SN150-network to that represented by $\mathbb{P}_-$ and $[\mathbb{P}_-]$. The values of $\epsilon \equiv M_-/M_{\text{unb}}$ and $[\epsilon] \equiv [M_-]/M_{\text{unb}}$ for each model, as well as $[\epsilon^i]$ for ^4He , ^{28}Si , ^{44}Ti , and ^{56}Ni , are given in Table 3.1. The larger disagreement of ϵ relative to $[\epsilon]$ in B12-WH07 and B15-WH07 compared to the less evolved B20-WH07 and B25-WH07 models relates to the different behavior of M_- and $[M_-]$ exhibited in B20-WH07 and B25-WH07, and is a testament to the challenge of running simulations sufficiently past bounce such that the multi-dimensional mass-cut is truly resolved.

As illustrated by Figure 3.14, the effect of the indeterminate mass-cut in B12-WH07 is most prevalent for $A \geq 28$, and $[\epsilon^i] \lesssim 0.2$ for any isotope with $M_{\text{unb}}^i(t_f) > 10^{-10} M_\odot$ (connected circles). The impact on the production of these species can be understood by considering the region of the star where the mass-cut has not yet been determined, illustrated by the open, colored circles in Figure 3.6. For B12-WH07, this region is confined to the inner 5,000 km of the star around a cut-off downflow rich in ^{28}Si which continues to accrete onto the proto-NS long after the development of the explosion. This region is similarly confined for both B15-WH07

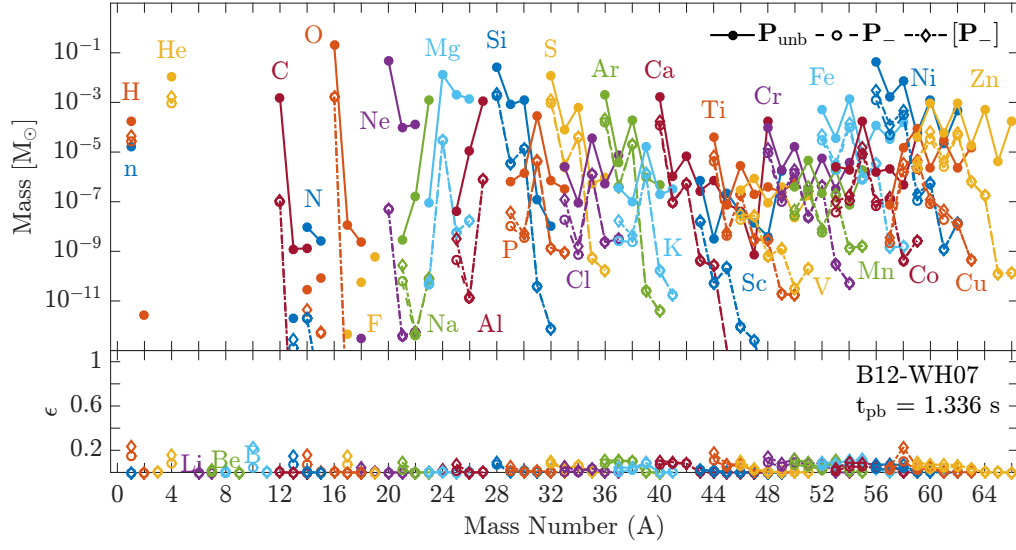


Figure 3.14 B12-WH07 total unbound mass of individual isotopes represented by $\mathbb{P}_{\text{unb}}$ ($M_{\text{unb}}^i(t_f)$; solid lines) and fractions thereof represented by $\mathbb{P}_-$ (ϵ^i ; dashed lines) and $[\mathbb{P}_-]$ ($[\epsilon^i]$; dashed-dotted lines) after post-processing with $T_{\text{NSE}} = 8$ GK. Connected points signify $M_{\text{unb}}^i(t_f) > 10^{-10} M_{\odot}$.

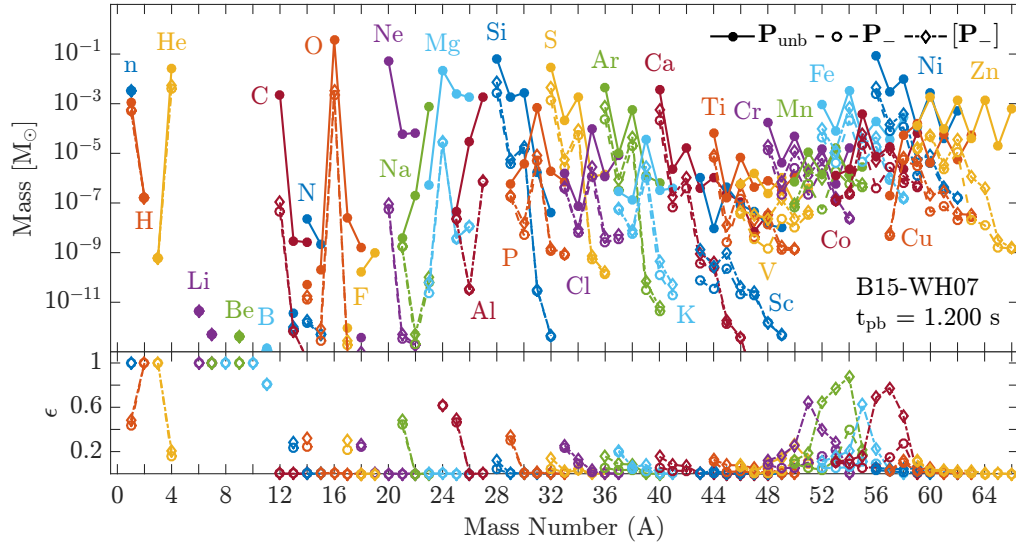


Figure 3.15 B15-WH07 total unbound mass of individual isotopes represented by $\mathbb{P}_{\text{unb}}$ ($M_{\text{unb}}^i(t_f)$; solid lines) and fractions thereof represented by $\mathbb{P}_-$ (ϵ^i ; dashed lines) and $[\mathbb{P}_-]$ ($[\epsilon^i]$; dashed-dotted lines) after post-processing with $T_{\text{NSE}} = 8$ GK. Connected points signify $M_{\text{unb}}^i(t_f) > 10^{-10} M_{\odot}$.

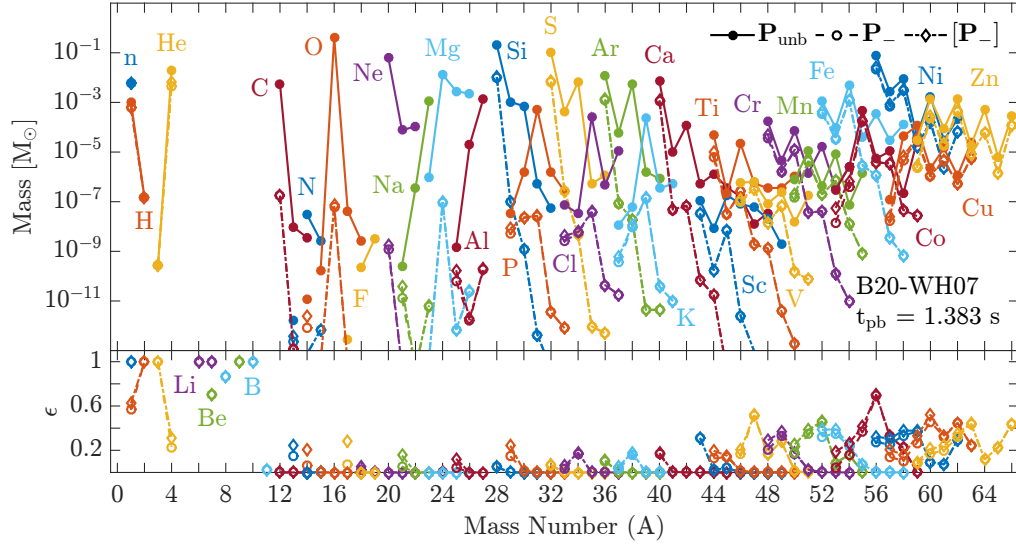


Figure 3.16 B20-WH07 total unbound mass of individual isotopes represented by $\mathbb{P}_{\text{unb}}$ ($M_{\text{unb}}^i(t_f)$; solid lines) and fractions thereof represented by $\mathbb{P}_-$ (ϵ^i ; dashed lines) and $[\mathbb{P}_-]$ ($[\epsilon^i]$; dashed-dotted lines) after post-processing with $T_{\text{NSE}} = 8$ GK. Connected points signify $M_{\text{unb}}^i(t_f) > 10^{-10} M_{\odot}$.

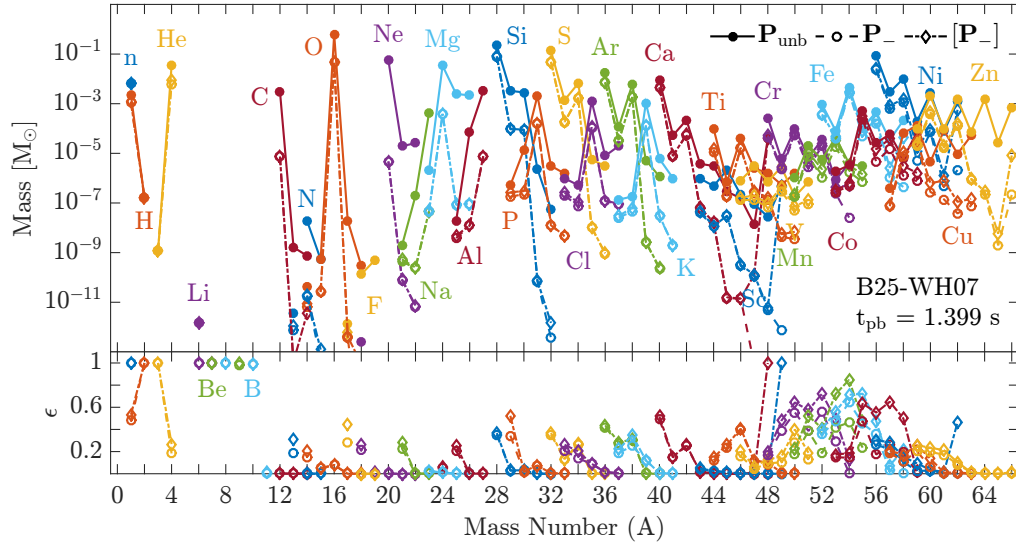


Figure 3.17 B25-WH07 total unbound mass of individual isotopes represented by $\mathbb{P}_{\text{unb}}$ ($M_{\text{unb}}^i(t_f)$; solid lines) and fractions thereof represented by $\mathbb{P}_-$ (ϵ^i ; dashed lines) and $[\mathbb{P}_-]$ ($[\epsilon^i]$; dashed-dotted lines) after post-processing with $T_{\text{NSE}} = 8$ GK. Connected points signify $M_{\text{unb}}^i(t_f) > 10^{-10} M_{\odot}$.

Table 3.1. Nucleosynthesis uncertainties

	Models			
	B12-WH07	B15-WH07	B20-WH07	B25-WH07
t_{pb} at simulation end (t_f) [s]	1.336	1.200	1.383	1.399
Masses at t_f				
Off-grid [$M_\odot$]	8.829	10.04	12.32	11.26
Unshocked [$M_\odot$]	0.1900	0.3600	0.7852	1.368
M_{unb} [$M_\odot$]	0.3964	0.7117	0.9919	1.284
M_+ [$M_\odot$]	0.3893	0.6937	0.9334	1.052
M_- [$M_\odot \times 10^{-2}$]	0.7659	1.804	5.849	23.14
$[M_-]$ [$M_\odot \times 10^{-2}$]	1.139	3.208	6.594	24.71
Combined uncertainties at t_f				
M_-/M_{unb} (Section 3.1.1)	0.0193	0.0254	0.0590	0.1803
$[M_-]/M_{\text{unb}}$ (Section 3.1.1)	0.0287	0.0451	0.0665	0.1926
$ r_{\delta_{\tau^*}} $ (Section 3.1.2)	0.0043	0.0069	0.0101	0.0119
$ r_{\delta_{\Delta\mathbf{r}}} $ (Section 3.1.4)	0.6192	0.7117	0.7767	0.7086
$ r_{\delta_{\text{NSE}}} $ (Section 3.1.5)	0.1083	0.1134	0.0631	0.0770
Individual isotope uncertainties at t_f				
$[\epsilon^i]$ (SN150) (Section 3.1.1)	^4He	0.1607	0.2070	0.3108
	^{28}Si	0.0863	0.1151	0.0502
	^{44}Ti	0.1722	0.1274	0.1956
	^{56}Ni	0.0701	0.0490	0.3239
$\delta_{\tau^*}^i$ (SN150) (Section 3.1.2)	^{44}Ti	0.0272	0.0618	0.1000
$\delta_{\Delta\mathbf{r}}^i$ (α) (Section 3.1.4)	^4He	0.0976	0.1762	0.1176
	^{28}Si	0.0248	0.0059	0.0117
	^{44}Ti	0.9383	0.9345	1.0703
	^{56}Ni	0.0121	0.0130	0.0247
δ_{NSE}^i (SN150) (Section 3.1.5)	^4He	0.2495	0.2682	0.3108
	^{28}Si	0.0000	0.0013	0.0502
	^{44}Ti	0.5531	0.5701	0.4101
	^{56}Ni	0.0350	0.0462	0.0437

and B20-WH07 (Figures 3.7–3.8), though characterized by more matter which has had its initial composition effectively reset by attaining NSE, evidenced by greater uncertainties for iron-group isotopes. This trend also appears in Figures 3.14–3.17, where ϵ^i in B15-WH07, B20-WH07, and B25-WH07 is characteristically different from B12-WH07 for $A > 48$, suggesting that the isotopes of Cr, Mn, Fe, and Co with values of Z/A closest to $Y_e(t_{\text{NSE}})$ of the ejected material are especially susceptible to the partially-resolved, multi-dimensional mass-cut. In Figure 3.9, $\mathbb{P}_-$ in B25-WH07 spans a much larger region of the star, not only the result of a deeper gravitational well, but also a consequence of an explosion that has been less successful in lifting the marginally-unbound, equatorial downflow (see animated Figure 2 in Bruenn et al., 2014).

3.1.2 Thermodynamic extrapolation

The distribution of particle temperatures at t_f in each B-Series simulation, T_f , is shown in Figure 3.18 (red) for $\mathbb{P}_+(t_f)$. In the case of the relatively less-evolved B25-WH07 (see Figure 12 in Bruenn et al., 2014), $\approx 0.11 M_\odot$ of the ejecta continues to experience explosive burning ($T_f \gtrsim 3$ GK), despite 1.4 s of evolution after core-bounce. For the other three models, the nuclear reactions which account for the bulk of the nickel production in CCSN ejecta have ceased. However, secondary nuclear burning processes will continue to alter the abundance distribution until the matter freezes out (Woosley et al., 1994), and proton and neutron captures will continue until the temperature of the ejecta falls below ≈ 0.5 GK (Fröhlich et al., 2006a), particularly in proton-rich ejecta. Short of being able to extend the simulations to this freeze-out temperature, we must extrapolate the thermodynamic conditions using the method described in Section 2.2.6.

In order to determine the collective effect of single-particle extrapolation uncertainties, we post-process thermodynamic profiles generated by extrapolating from points in time in the last 150 ms of the simulation corresponding to the minimum and

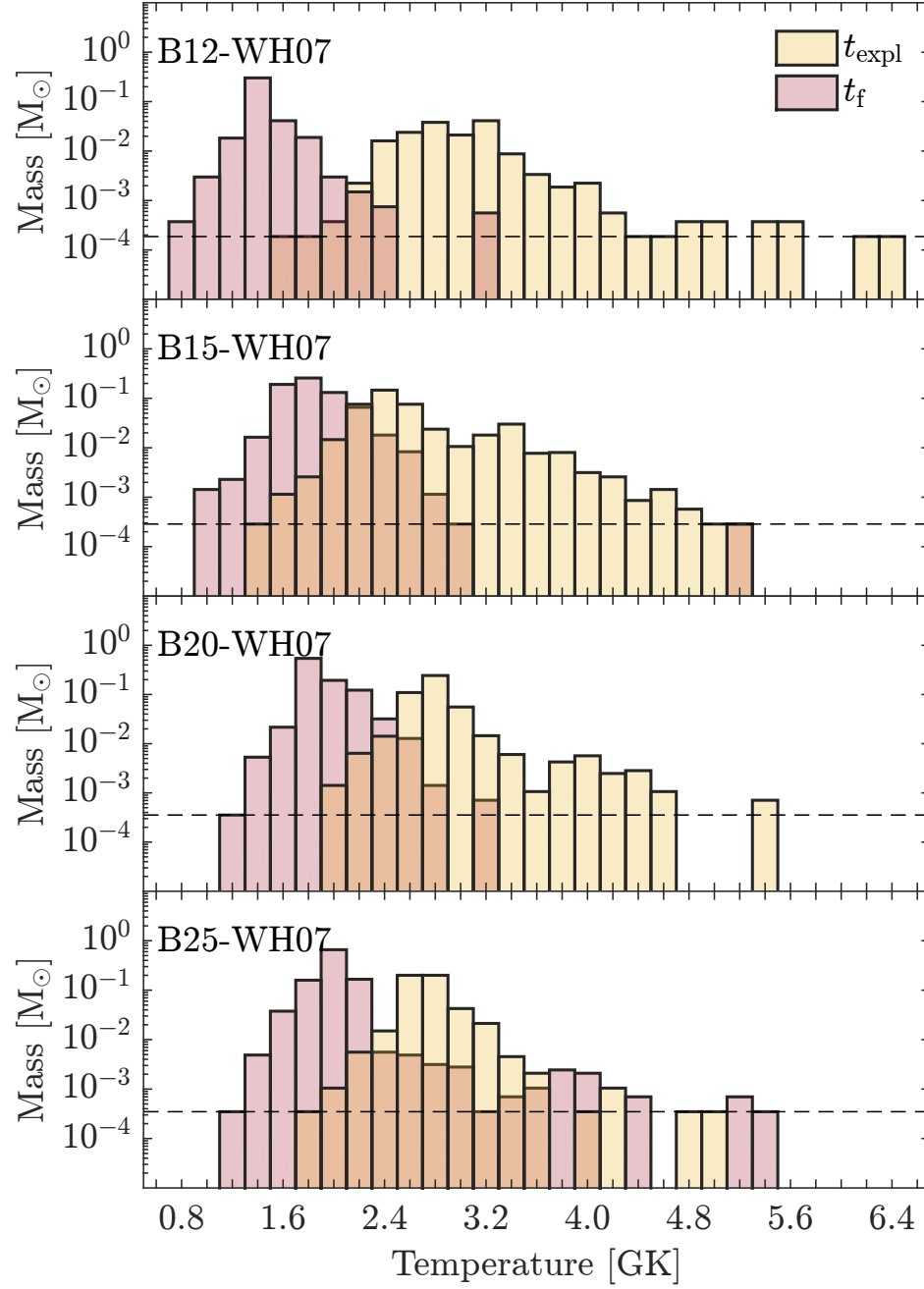


Figure 3.18 B-Series models' distributions of M_+ at t_f (red) and t_{expl} (yellow) in bins of size $\Delta T = 0.2$ GK. The mass represented by one Lagrangian tracer particle is given by the dashed line.

maximum estimates of the expansion timescales, $\tau_{\min}^*$ and $\tau_{\max}^*$, respectively. These changing timescales reflect the effects of ongoing hydrodynamical activity. Of course, any extrapolation will fail to capture future hydrodynamic activity that deviates from true isentropic expansion, but changes over the last 150 ms are a reasonable proxy to estimate this uncertainty. Defining a residual norm for the final composition,

$$||r_{\delta_{\tau^*}}|| \equiv \frac{\sum_i \delta_{\tau^*}^i}{\sum_i |\log_{10}(\sqrt{X_i(\tau_{\max}^*)X_i(\tau_{\min}^*)})|}, \quad (3.2)$$

where $\delta_{\tau^*}^i = |\log_{10}(X_i(\tau_{\max}^*)/X_i(\tau_{\min}^*))|$ and X_i is the mass fraction of species i , we are able to easily identify particles whose nuclear products are particularly susceptible to such activity. Tracer particles with the largest extrapolation uncertainties, as measured by $||r_{\delta_{\tau^*}}||$, typically fall very close to the proto-NS surface and reach peak temperatures in excess of 20 GK before being ejected at high speed (see Figure 3.19). The exposure of such particles to large neutrino fluxes near the neutrino-emitting surface, the *neutrino-sphere*, is consistent with our premise that thermodynamic extrapolations initiated from $T_f \lesssim 2$ GK are necessitated by the ongoing proton and neutron captures that typify neutrino-induced nucleosynthesis. In Figures 3.20–3.23, we show differing estimates of the expansion timescale for four particles from B12-WH07 with the largest values of $||r_{\delta_{\tau^*}}||$. The differences are especially large for particle B12-WH07-P1289, which experiences a brief period of heating just prior to t_f , pushing the temperature above 3 GK and reengaging nuclear reactions that had otherwise ceased. Hydrodynamically, this corresponds to the particle briefly halting its expansion as it retreats back towards the proto-NS before being swept up in the ejecta once more (see Figure 3.24).

However, this specific type of profile is very uncommon. In fact, B12-WH07-P1289 would have been a member of $\mathbb{P}_-$ just 50 ms earlier. For B12-WH07-P1422, B12-WH07-P1616, and B12-WH07-P1737, the differences in the thermodynamic extrapolations are less drastic but not insignificant. In each of these cases, the differing estimates of the expansion timescale can be attributed to hydrodynamical

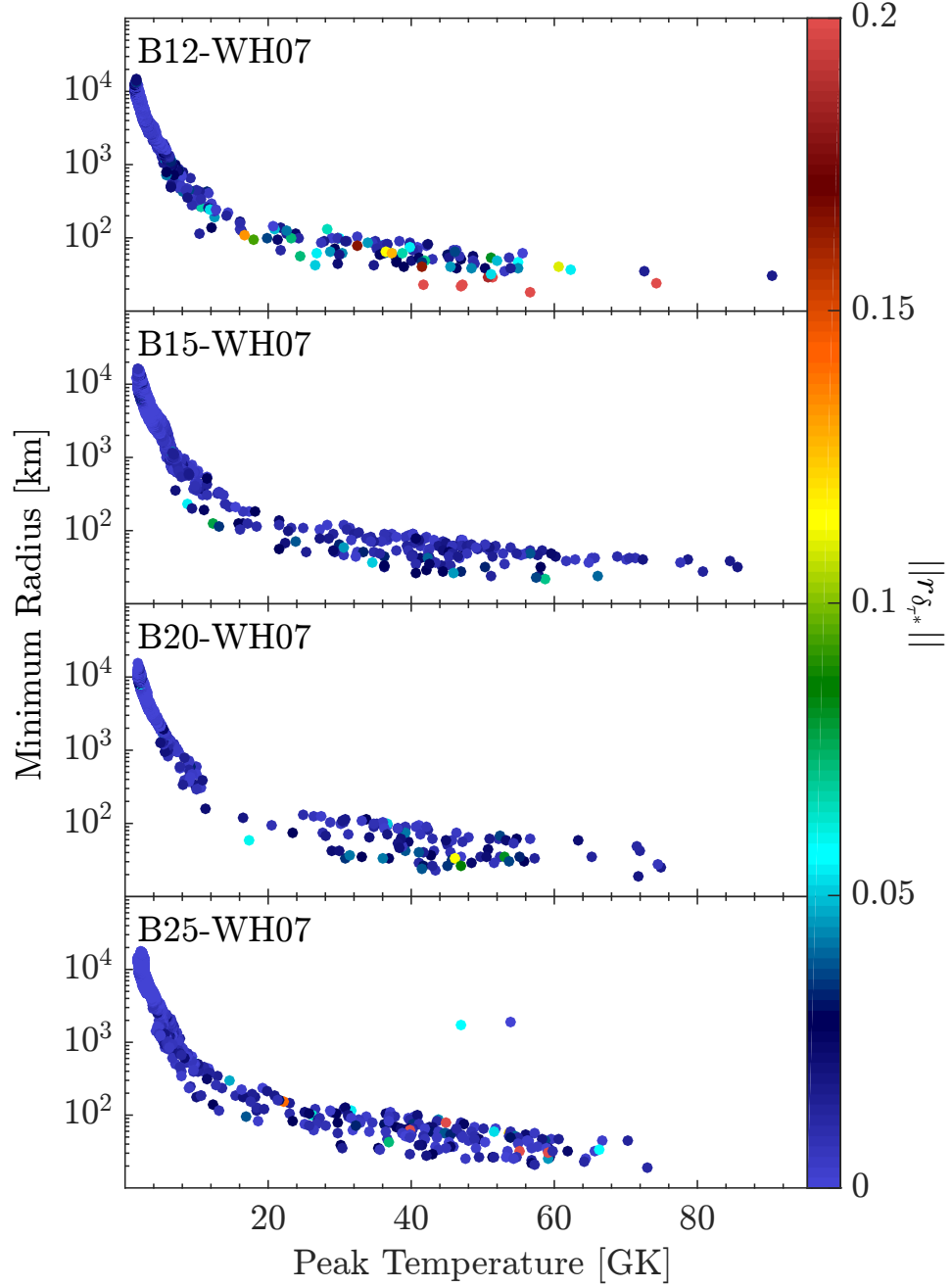


Figure 3.19 Tracer particles in $\mathbb{P}_+(t_f)$ for each B-Series simulation and positioned according to T_{peak} and minimum radius and colored by the residual $||r_{\delta_{\tau*}}||$ (Equation 3.2).

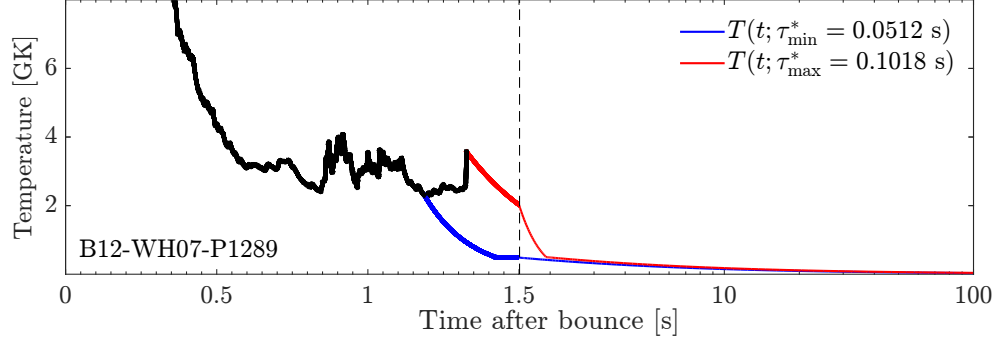


Figure 3.20 B12-WH07-P1289 temperature profile and extrapolation to 100 s, calculated using $\tau_{\max}^*$ (blue line) and $\tau_{\min}^*$ (red line). The dashed line indicates the switch to a logarithmic scale for the time axis.

flows which nudge the particles in question (see Figures 3.25–3.27) and, in so doing, provide a brief period of heating, breaking the assumption of isentropic expansion but not to the extent that expansion ceases outright. For example, B12-WH07-P1422 exhibits significant differences in the final composition as a result of extrapolations that are quite similar but lagged by ≈ 150 ms. Estimates of the expansion timescale in B12-WH07-P1737 differ by a factor of four despite the extrapolations initiating only ≈ 50 ms apart. B12-WH07-P1616 represents a peculiar case; the alteration to its spatial trajectory, evident in Figure 3.26, sends it on a collision course with the persisting equatorial downflow. Though the particle is considered part of the ejecta at t_f , it is now part of a convective eddy and will inevitably soon transition to $\mathbb{P}_-$. Not only does this highlight how nucleosynthesis predictions based on analytic extrapolations can fail to directly capture future hydrodynamic activity, but also elucidates the more subtle effect of different estimates of the expansion timescale.

Figures 3.24–3.27 illustrate the extent to which the spatial trajectories of these tracer particles can differ from those of their immediate neighbors, thus highlighting the highly asymmetric behavior which complicates multi-dimensional nucleosynthesis calculations. As previously mentioned, a shared yet rare characteristic of the selected particles (B12-WH07-P1289, B12-WH07-P1422, B12-WH07-P1616, and B12-WH07-P1737) is their exposure to large neutrino fluxes near the neutrino-sphere. As

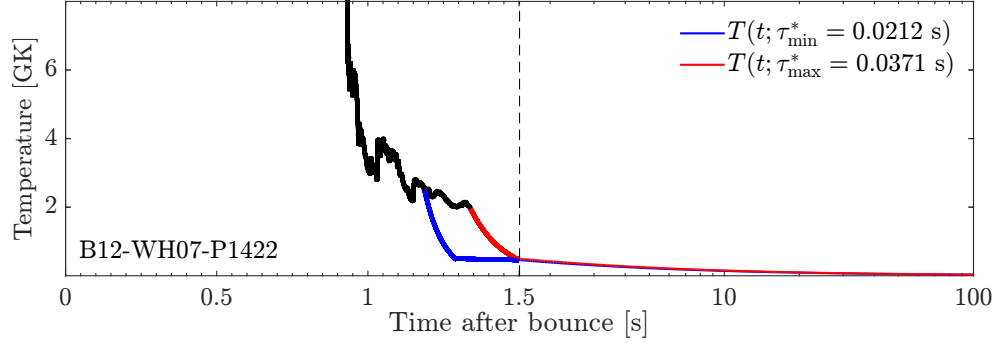


Figure 3.21 B12-WH07-P1422 temperature profile and extrapolation to 100 s, calculated using $\tau_{\max}^*$ (blue line) and $\tau_{\min}^*$ (red line). The dashed line indicates the switch to a logarithmic scale for the time axis.

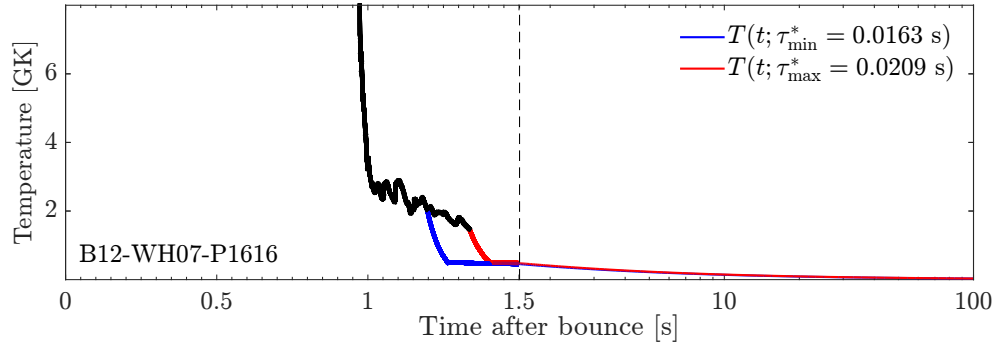


Figure 3.22 B12-WH07-P1616 temperature profile and extrapolation to 100 s, calculated using $\tau_{\max}^*$ (blue line) and $\tau_{\min}^*$ (red line). The dashed line indicates the switch to a logarithmic scale for the time axis.

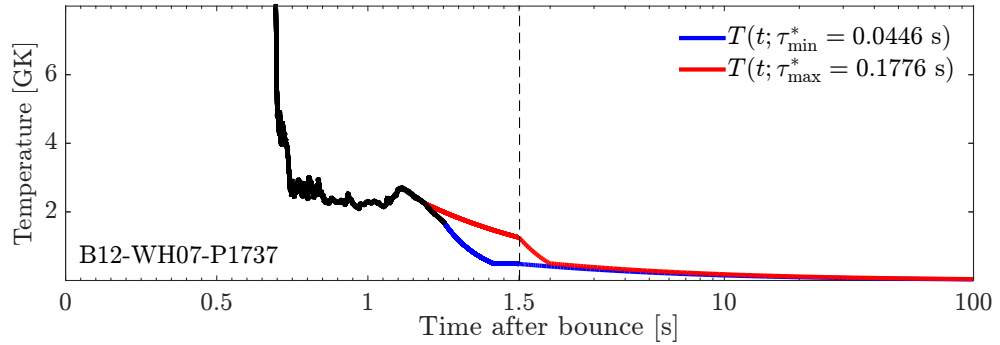


Figure 3.23 B12-WH07-P1737 temperature profile and extrapolation to 100 s, calculated using $\tau_{\max}^*$ (blue line) and $\tau_{\min}^*$ (red line). The dashed line indicates the switch to a logarithmic scale for the time axis.

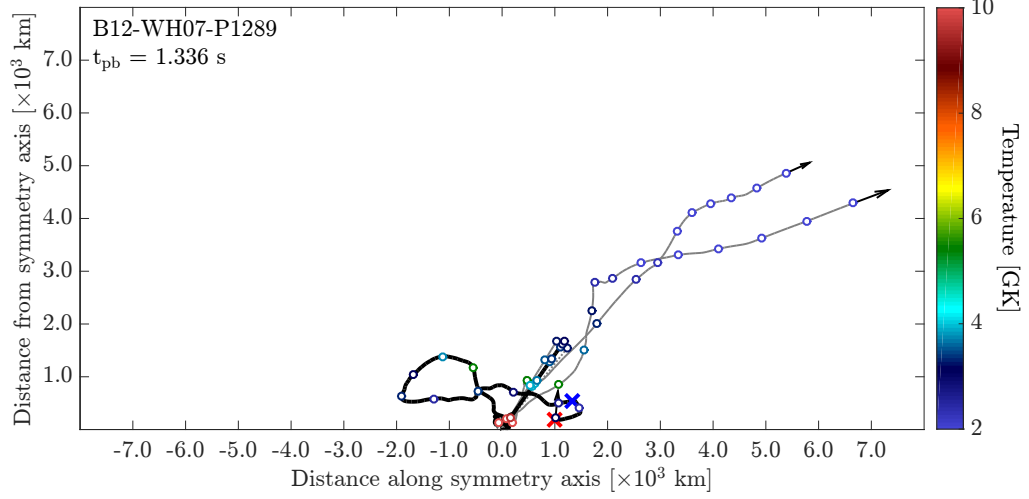


Figure 3.24 B12-WH07-P1289 spatial trajectory (thick, black line), with the initial neighboring tracer particles shown in gray and dotted if the particle does not represent part of the ejecta. Colored circles indicate particle temperatures at 100 ms increments from t_f . Red and blue crosses mark the points corresponding to $\tau_{\max}^*$ and $\tau_{\min}^*$, respectively. The final velocity of each tracer particle, $\vec{v}(t_f)$, is represented by the arrows and scaled accordingly.

evidenced by their immediate neighbors, most tracer particles which descend deep into the gravitational well of the proto-NS become bound and do not represent ejecta matter.

At 100 s after bounce, the composition resulting from these varying extrapolations can be markedly different. As shown in Figure 3.28–3.31, deviations from predicted trajectories after t_f can lead to non-trivial uncertainties in the composition for individual particles.

The tracers discussed in the previous paragraphs were selected by their extreme uncertainties. For most tracers, and therefore the total ensemble, the impact of the uncertainties is much less pronounced. The extent to which this impacts the total ejecta mass for each nuclear species i , M_+^i , represented by $\mathbb{P}_+$ (the particles for which we perform extrapolations) is shown for each B-Series model in Figures 3.32–3.35. The relatively low temperatures of particles in $\mathbb{P}_+(t_f)$ (see Figure 3.18) helps to limit the overall impact of extrapolation uncertainties to only a few nuclear

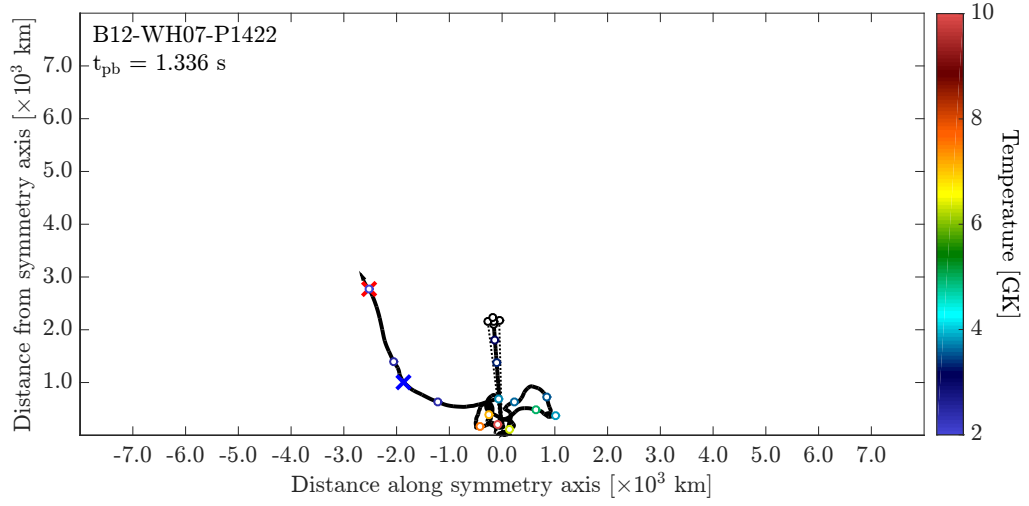


Figure 3.25 B12-WH07-P1422 spatial trajectory (thick, black line), with the initial neighboring tracer particles shown in gray and dotted if the particle does not represent part of the ejecta. Colored circles indicate particle temperatures at 100 ms increments from t_f . Red and blue crosses mark the points corresponding to $\tau_{\max}^*$ and $\tau_{\min}^*$, respectively. The final velocity of each tracer particle, $\vec{v}(t_f)$, is represented by the arrows and scaled accordingly.

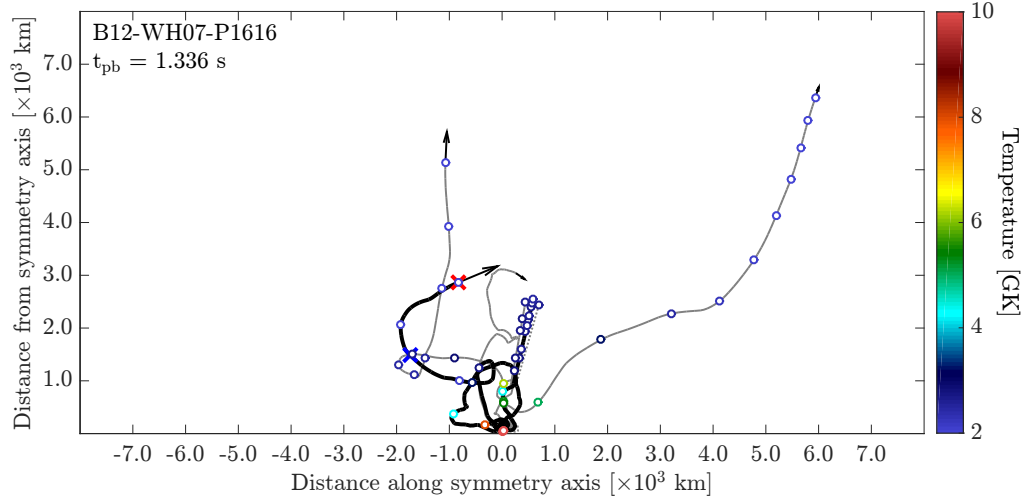


Figure 3.26 B12-WH07-P1616 spatial trajectory (thick, black line), with the initial neighboring tracer particles shown in gray and dotted if the particle does not represent part of the ejecta. Colored circles indicate particle temperatures at 100 ms increments from t_f . Red and blue crosses mark the points corresponding to $\tau_{\max}^*$ and $\tau_{\min}^*$, respectively. The final velocity of each tracer particle, $\vec{v}(t_f)$, is represented by the arrows and scaled accordingly.

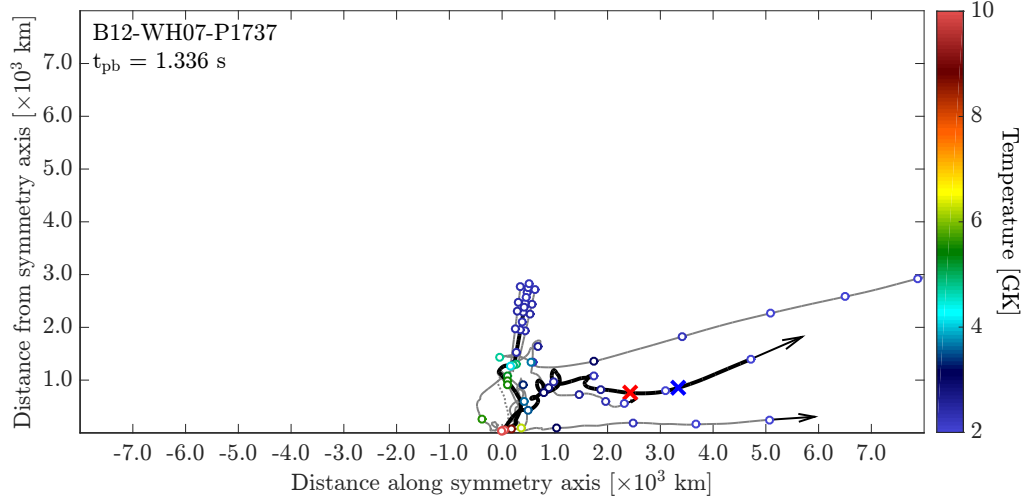


Figure 3.27 B12-WH07-P1737 spatial trajectory (thick, black line), with the initial neighboring tracer particles shown in gray and dotted if the particle does not represent part of the ejecta. Colored circles indicate particle temperatures at 100 ms increments from t_f . Red and blue crosses mark the points corresponding to $\tau_{\max}^*$ and $\tau_{\min}^*$, respectively. The final velocity of each tracer particle, $\vec{v}(t_f)$, is represented by the arrows and scaled accordingly.

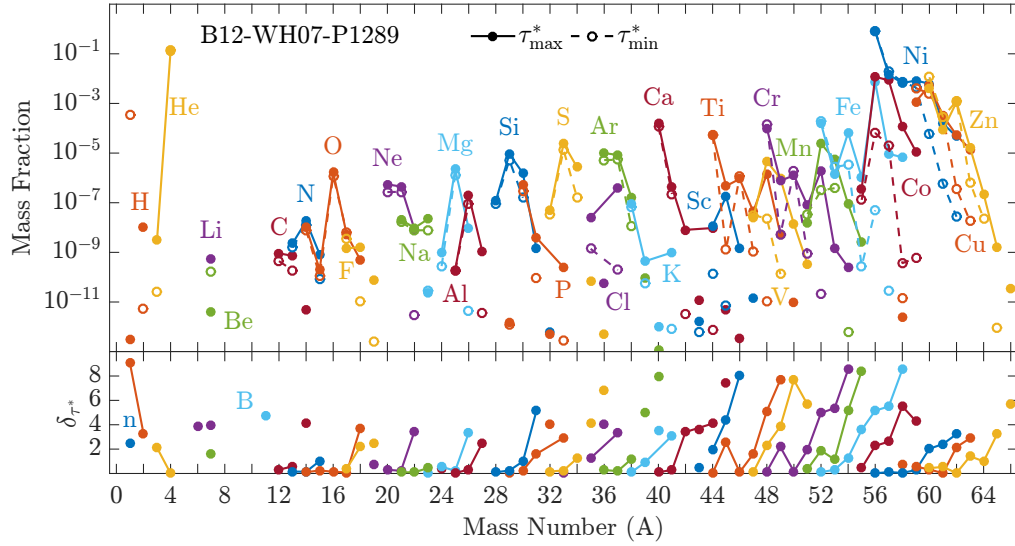


Figure 3.28 Top panel: B12-WH07-P1289 predicted ejecta mass fractions from post-processing the two different extrapolations shown in Figure 3.20. Bottom panel: Relative deviation of the composition between the two extrapolations plotted for each species i as $\delta_{\tau^*}^i \equiv |\log_{10}(X_i(\tau_{\max}^*)/X_i(\tau_{\min}^*))|$. Connected points signify $X_i(t_f) > 10^{-10}$.

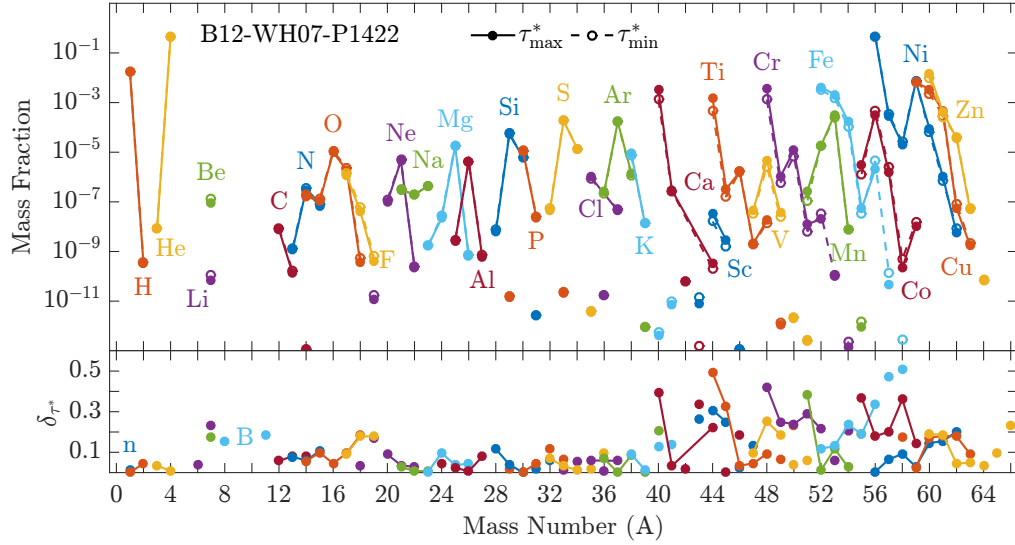


Figure 3.29 Top panel: B12-WH07-P1422 predicted ejecta mass fractions from post-processing the two different extrapolations shown in Figure 3.21. Bottom panel: Relative deviation of the composition between the two extrapolations plotted for each species i as $\delta_{\tau^*}^i \equiv |\log_{10}(X_i(\tau_{\max}^*)/X_i(\tau_{\min}^*))|$. Connected points signify $X_i(t_f) > 10^{-10}$.

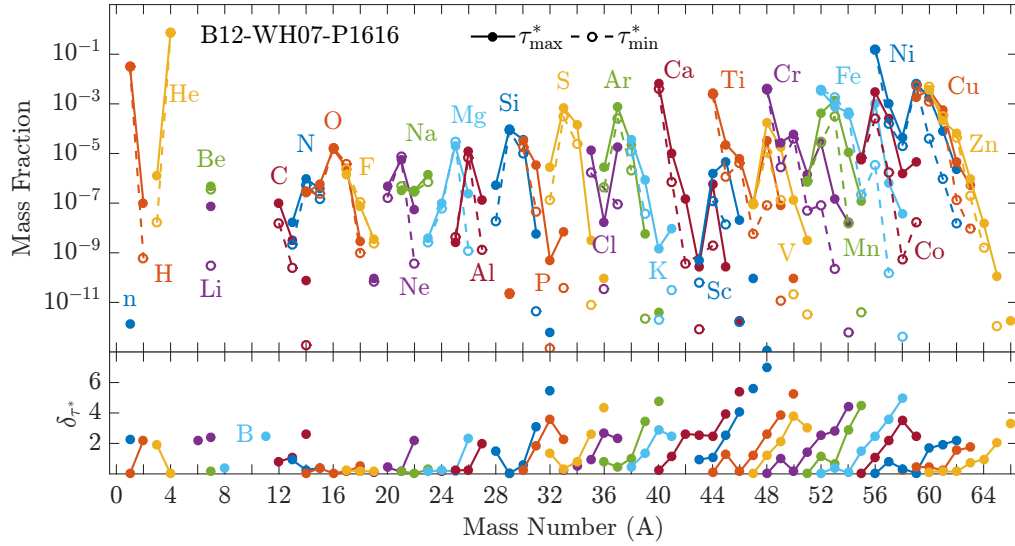


Figure 3.30 Top panel: B12-WH07-P1616 predicted ejecta mass fractions from post-processing the two different extrapolations shown in Figure 3.22. Bottom panel: Relative deviation of the composition between the two extrapolations plotted for each species i as $\delta_{\tau^*}^i \equiv |\log_{10}(X_i(\tau_{\max}^*)/X_i(\tau_{\min}^*))|$. Connected points signify $X_i(t_f) > 10^{-10}$.

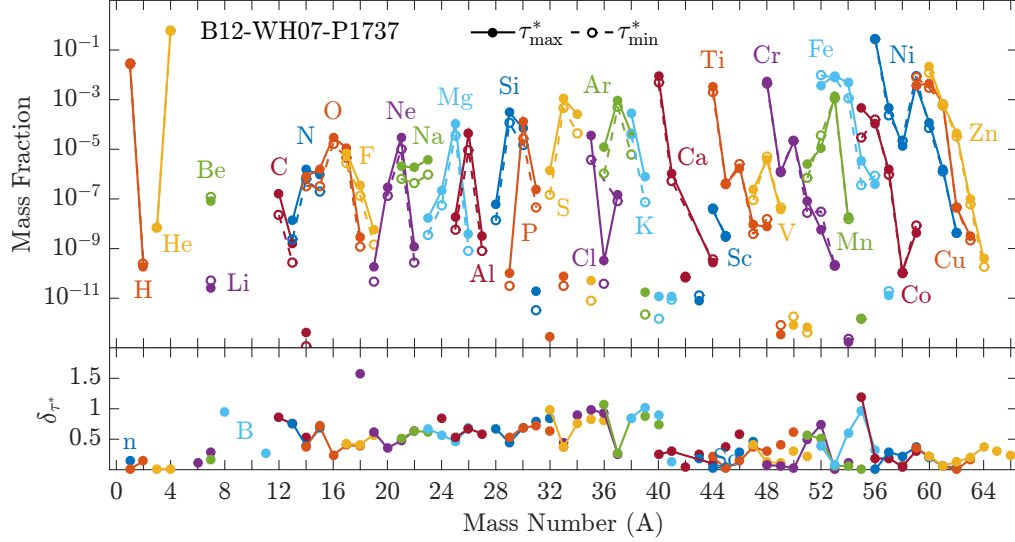


Figure 3.31 Top panel: B12-WH07-P1737 predicted ejecta mass fractions from post-processing the two different extrapolations shown in Figure 3.23. Bottom panel: Relative deviation of the composition between the two extrapolations plotted for each species i as $\delta_{\tau^*}^i \equiv |\log_{10}(X_i(\tau_{\max}^*)/X_i(\tau_{\min}^*))|$. Connected points signify $X_i(t_f) > 10^{-10}$.

products. In general, $\delta_{\tau^*}^i \equiv |\log_{10}(M_+^i(\tau_{\max}^*)/M_+^i(\tau_{\min}^*))|$ is larger for low-yield isotopes (e.g. ^3He , ^{13}C , ^{18}O , ...), wherein the extrapolation uncertainties for a small subset of tracer particles can have a greater effect. We also identify trends of larger uncertainties for some isotopes that can't be entirely attributed to a small number of tracer particles (e.g. ^{38}K , ^{43}Sc , ^{56}Co , and ^{57}Co). Uncertainties in ^{44}Ti production, important to supernova remnant observations, are small, but non-negligible ($0.79 \lesssim M_+^i(\tau_{\max}^*)/M_+^i(\tau_{\min}^*) \lesssim 0.95$; see Table 3.1 for values).

Other isotopes are affected by variations in τ^* , but their identities vary between models. B20-WH07, for example, is uniquely characterized by a noticeable increase in $\delta_{\tau^*}^i$ for $12 \leq A \leq 30$. B25-WH07 is also unique among the B-Series simulations in that the extrapolation error can be larger than 20% for several of the most neutron-rich isotopes of elements for which $Z \geq 14$, including ^{32}Si , ^{36}S , ^{40}Ar , ^{49}Sc , ^{50}Ti , ^{51}V , ^{53}Cr , ^{54}Mn , ^{58}Fe , and ^{59}Co .

As a single measure of extrapolation uncertainties for a given model, we define a global residual using Equation 3.2 but replacing the mass fraction, X_i , with M_+^i . Not

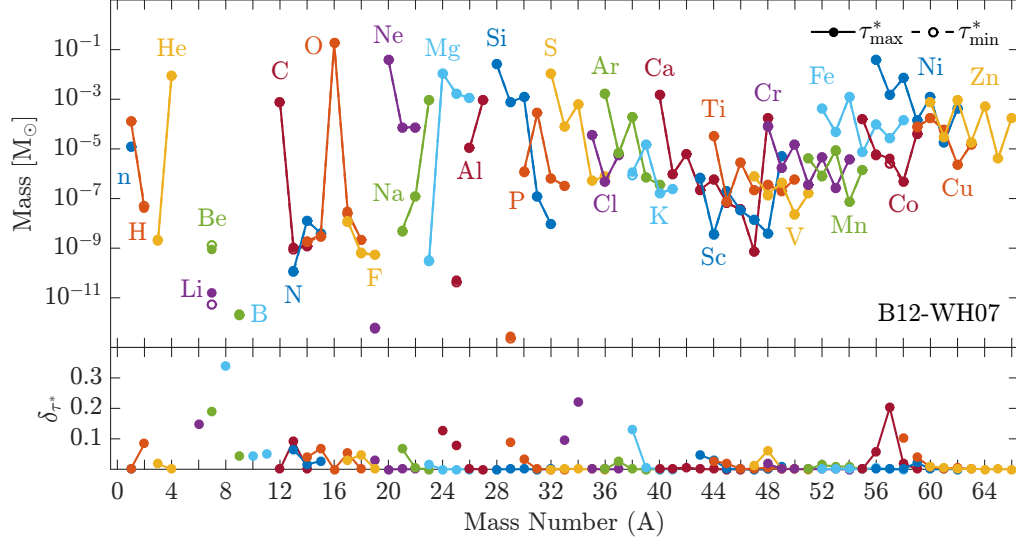


Figure 3.32 Top panel: M_+^i at 100 s after bounce and calculated for expansion timescales $\tau_{\max}^*$ (solid line) and $\tau_{\min}^*$ (dashed line) for particles in $\mathbb{P}_+$ for the B12-WH07 model. Bottom panel: relative deviation of the composition between the two extrapolations plotted for each isotope i as $\delta_{\tau^*}^i \equiv |\log_{10}(M_+^i(\tau_{\max}^*)/M_+^i(\tau_{\min}^*))|$. Connected points signify $M_+^i(t_f) > 10^{-10} M_\odot$.

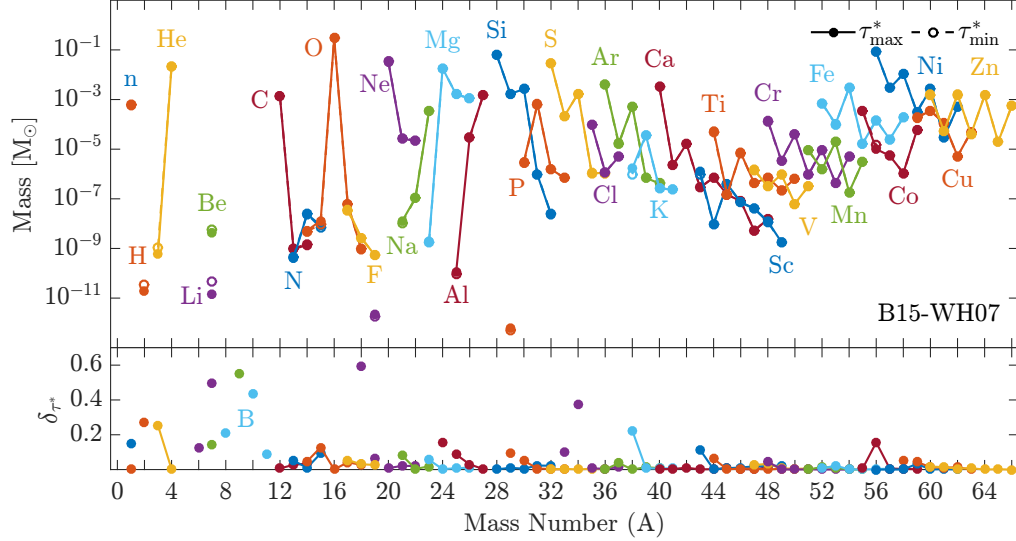


Figure 3.33 Top panel: M_+^i at 100 s after bounce and calculated for expansion timescales $\tau_{\max}^*$ (solid line) and $\tau_{\min}^*$ (dashed line) for particles in $\mathbb{P}_+$ for the B15-WH07 model. Bottom panel: relative deviation of the composition between the two extrapolations plotted for each isotope i as $\delta_{\tau^*}^i \equiv |\log_{10}(M_+^i(\tau_{\max}^*)/M_+^i(\tau_{\min}^*))|$. Connected points signify $M_+^i(t_f) > 10^{-10} M_\odot$.

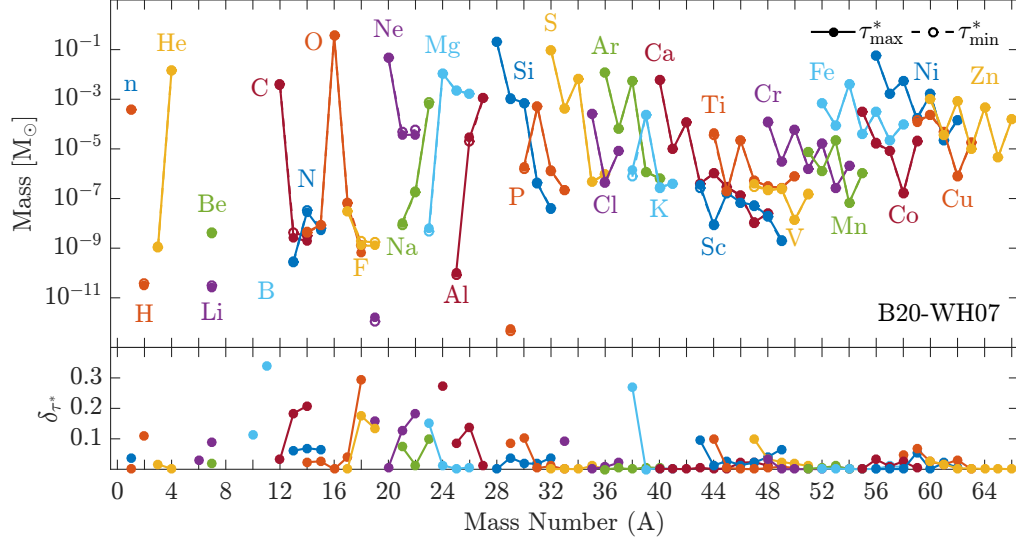


Figure 3.34 Top panel: M_+^i at 100 s after bounce and calculated for expansion timescales $\tau_{\max}^*$ (solid line) and $\tau_{\min}^*$ (dashed line) for particles in $\mathbb{P}_+$ for the B20-WH07 model. Bottom panel: relative deviation of the composition between the two extrapolations plotted for each isotope i as $\delta_{\tau^*}^i \equiv |\log_{10}(M_+^i(\tau_{\max}^*)/M_+^i(\tau_{\min}^*))|$. Connected points signify $M_+^i(t_f) > 10^{-10} M_\odot$.

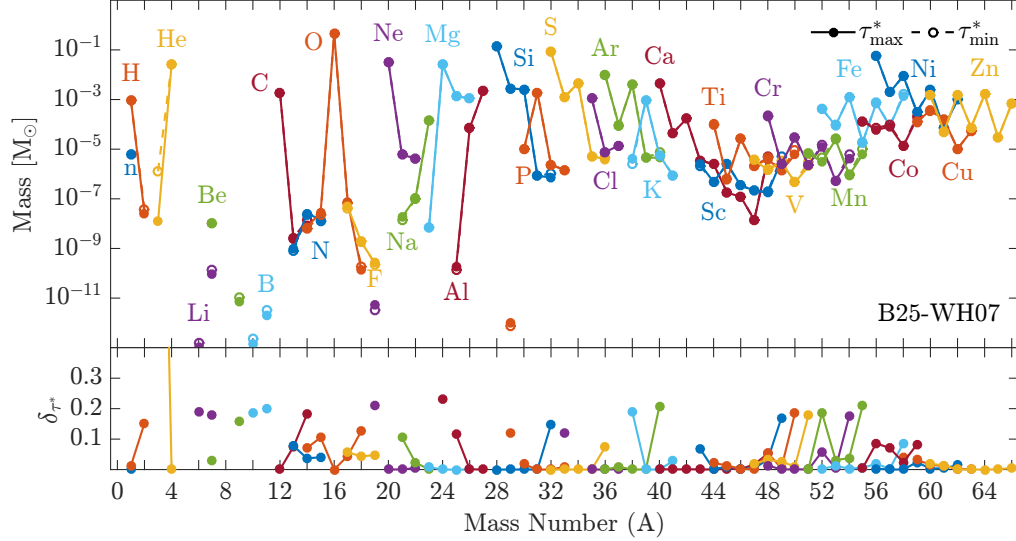


Figure 3.35 Top panel: M_+^i at 100 s after bounce and calculated for expansion timescales $\tau_{\max}^*$ (solid line) and $\tau_{\min}^*$ (dashed line) for particles in $\mathbb{P}_+$ for the B25-WH07 model. Bottom panel: relative deviation of the composition between the two extrapolations plotted for each isotope i as $\delta_{\tau^*}^i \equiv |\log_{10}(M_+^i(\tau_{\max}^*)/M_+^i(\tau_{\min}^*))|$. Connected points signify $M_+^i(t_f) > 10^{-10} M_\odot$.

surprisingly, $\|r_{\delta_{\tau*}}\|$ increases with progenitor mass but is small relative to the other uncertainties (see Table 3.1).

3.1.3 Uncertainties at early times

The goal of any calculation of CCSN nucleosynthesis is the final distribution of the ejecta in composition and velocity. The evolution to this final state can be divided into several stages. The first, notionally, is the development of the explosion, followed by 2) the development of the mass-cut, separating the ejecta from the neutron star, 3) the completion of the nucleosynthesis, as all of the matter expands and cools sufficiently for nuclear reactions to cease, and 4) the final development of the velocity distribution as the outgoing ejecta passes through the stellar envelope. These four stages are not, in practice, as separate as this list implies and the mixing of these stages is exacerbated in multi-dimensions.

For investigations primarily focused on the development of the explosion, the temptation is strong to conserve computational resources by stopping the simulation once the successful revival of the supernova shock seems guaranteed or, at the latest, as the growth of the explosion energy levels off. We define this time as t_{expl} and estimate $t_{\text{expl}} = 600$ ms for B12-WH07 and $t_{\text{expl}} = 800$ ms for the other B-Series simulations (see Figure 12a in Bruenn et al., 2014). The decline in the growth of the explosion energy is concurrent with a similar decrease in the growth of the unbound mass (M_{unb} ; see Figures 3.1–3.4); however, using $\epsilon(t)$ in these figures as a proxy for the evolution of the multi-dimensional mass-cut, we see that the models at t_{expl} are much less mature than at t_{f} . The disparity between $\epsilon(t_{\text{expl}})$ and $[\epsilon](t_{\text{expl}})$ clearly demonstrates the particles representative of ejecta are in flux, further supported by the growth in M_{bound} seen after t_{expl} in each model as the shock moves outward before leveling off near t_{f} .

Such early truncation of the simulation often occurs with much of the ejecta at final temperatures above 3 GK (see Figure 3.18; yellow) and fails to capture all stages

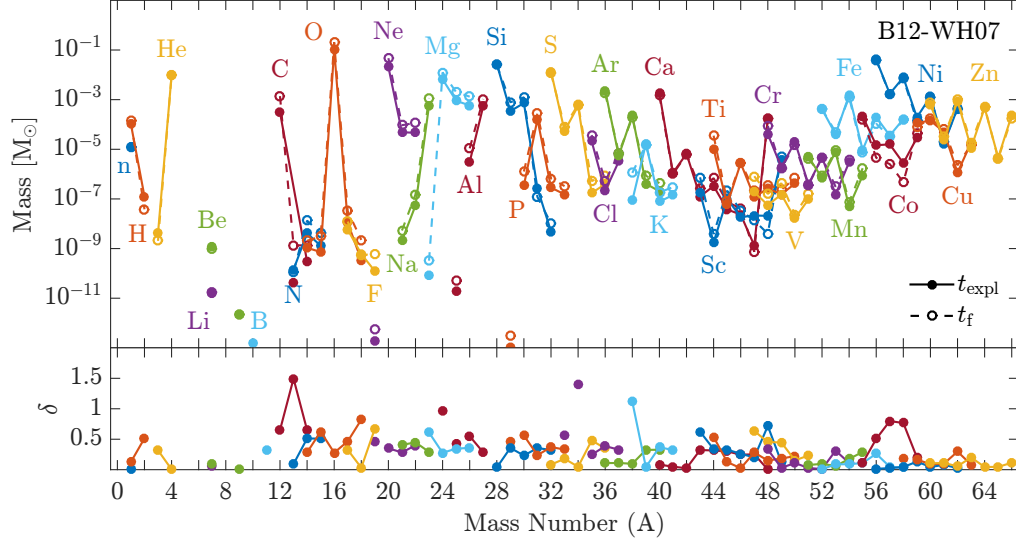


Figure 3.36 Top panel: M_+^i of B12-WH07 at 100 s after bounce, calculated from t_{expl} (solid lines) and t_f (dashed lines). Bottom panel: Relative deviation of the composition between the different end times plotted for each isotope i as $\delta^i \equiv |\log_{10}(M_+^i(t_{\text{expl}})/M_+^i(t_f))|$. Connected points signify $M_+^i(t_{\text{expl}}) > 10^{-10} M_\odot$.

of explosive nucleosynthesis *in situ* when coupling to the hydrodynamics is important. In this case, investigation of the nucleosynthesis will much more heavily rely on extrapolations of the thermodynamic history, described in detail in Section 2.2.6. Coming, as it does, at a point the supernova’s evolution where hydrodynamics remains very active, this extrapolation is fraught with uncertainty. As a measure of this, we compare predictions of the nucleosynthetic yields determined from t_{expl} and t_f at 100 s in Figure 3.36. Whereas uncertainties relating to thermodynamic extrapolation at t_f (see Section 3.1.2) are small relative to other uncertainties, the magnitude of variations between $M_+^i(t_{\text{expl}})$ and $M_+^i(t_f)$ for $A \geq 12$, which includes the effects of both a different multi-dimensional mass-cut and contrasting expansion timescales, can exceed an order of magnitude, with a factor of three being quite common. Interestingly, the α -nuclei from silicon to nickel are relatively unaffected (e.g. $M_+^{56\text{Ni}(t_{\text{expl}})}/M_+^{56\text{Ni}(t_f)} = 1.033$)

3.1.4 Spatial resolution

Any simulation, by its nature, replaces continuous thermodynamic variables with a discrete number of elements, either in space (Eulerian) or in mass (Lagrangian). This discretization adds an uncertainty that is magnified if the number of elements is too small to capture the important features in sufficient detail. For post-processing nucleosynthesis, the resolution in question is the number and distribution of the Lagrangian tracer particles used to gather the thermodynamic histories.

The initial distribution of tracer particles in our simulations guarantees that we are sampling the ejecta uniformly in mass. Consequently, there are density-dependent variations in the spatial resolution, $\Delta \mathbf{r}$, of the ejecta. If sufficiently large, these variations may limit the ability of Lagrangian tracer particles to sample the ejecta at resolutions which reproduce the nuclear burning conditions initially encountered in the simulation. In particular, tracer particles tend to under-resolve regions of relatively low-density. While we could adjust the initial tracer mass to better sample low-density regions in the progenitor, our ability to do this for dynamically developing low-density regions is limited. Past studies of the convergence properties of tracer particles in supernova nucleosynthesis (see, e.g., [Seitenzahl et al., 2010](#)) have been limited to Type Ia supernovae, which exhibit a narrower entropy range.

We introduce here a novel way to explore the limitations of tracer post-processing by post-processing with a network identical to that used *in situ* within CHIMERA. Care is taken to also generate initial abundances, both for particles that reach NSE and those that do not, that are identical to the methods used within CHIMERA. Thus, we have two representations of the nuclear composition that differ only in their effective resolution and the inability of the Lagrangian tracer particles to mix their composition. The total ejected mass of each nuclear species i from *in situ* nucleosynthesis, M_C^i , is calculated by integrating over all zones where $e_{\text{tot}} > 0$. The ejected mass from the equivalent post-processing calculation, M_{PP}^i , is calculated with the $e_{\text{tot}} > 0$ criterion applied to particles instead of zones. The relative

difference between *in situ* and post-processing calculations for individual isotopes, $\delta_{\Delta\mathbf{r}}^i \equiv |\log_{10}(M_{\text{PP}}^i/M_C^i)|$, $M_C^i(t)$, and $M_{\text{PP}}^i(t)$ are shown throughout each B-Series simulation in Figures 3.37–3.40. There is general agreement between $M_C^i(t)$ and $M_{\text{PP}}^i(t)$ for most species. ^{28}Si and ^{56}Ni , which can be taken as representation of their neighbors, show some variations early. However, by t_f and, in fact, even by t_{expl} , these differences are only a few percent. There is a consistent, stark discrepancy in the total mass of ^{44}Ti (yellow lines) and, to a lesser extent, ^4He , across all four models. In B12-WH07, for example, the value from the *in situ* calculation, $M_C^{44\text{Ti}}(t_f) \approx 1.08 \times 10^{-3} M_\odot$, is greater than that from post-processing, $M_{\text{PP}}^{44\text{Ti}}(t_f) \approx 1.24 \times 10^{-4} M_\odot$, by nearly an order of magnitude. To understand the origin of these inconsistencies, consider that the nuclei most affected are products of α -rich freeze-out occurring in low-density, expanding ejecta and are, therefore, most susceptible to inadequate tracer particle spatial resolution. The deficit of α -rich freeze-out products in the post-processing results cannot be attributed to a lack of mixing therein, as mixing would dilute the α -richness of this ejecta and, therefore, further reduce the production of these nuclei. As we will discuss in Chapter 4, the poor resolution in the low-density ejecta also has implications for the neutron-rich products of α -poor freeze-out, as well as νp -process and r -process products in the immature neutrino-driven wind, but we are unable to quantify this effect as we’ve done for the α -network species.

To provide context regarding the magnitude of this disagreement, we compare $M_C^i(t_f)$ and $M_{\text{PP}}^i(t_f)$ to post-processing calculations performed with a more realistic 150-species network in Figure 3.41. In each model, the unbound ^{56}Ni mass is relatively unaffected, but there are significant differences in the total unbound mass for ^{44}Ti , ^{48}Cr , ^{52}Fe , and ^{60}Zn . These differences can be largely attributed to the availability of additional reaction pathways during explosive burning, particularly those involving (n, γ) and (p, γ) reactions (Hix and Thielemann, 1996; Timmes et al., 2000; Magkotsios et al., 2010). The effect of spatial resolution on the production of ^{44}Ti is of roughly the same order, but in the opposing direction, as that seen

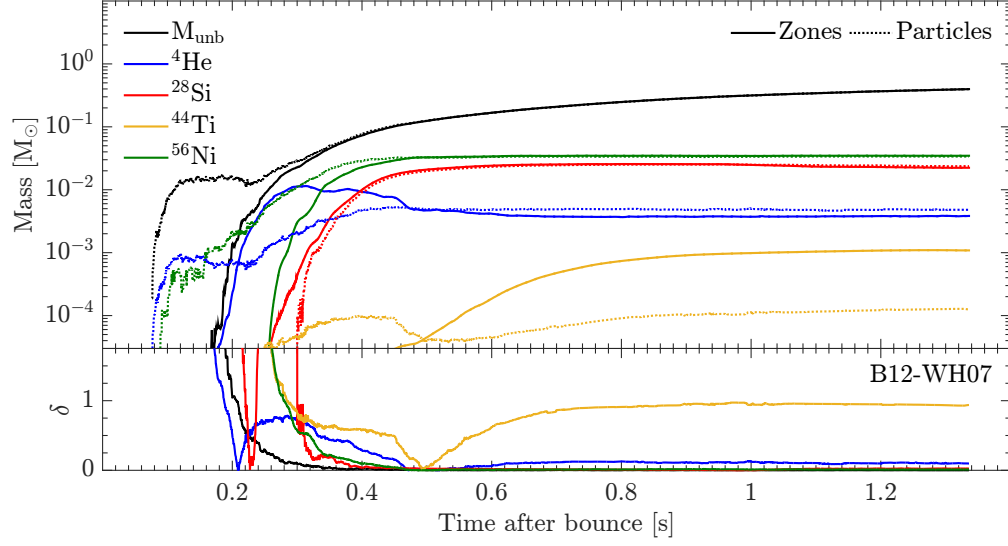


Figure 3.37 Top panel: B12-WH07 Total unbound mass of several α -network species as determined from the original simulation ($M_C^i(t)$; solid lines) and post-processed using identical thermodynamic histories from Lagrangian tracer particles ($M_{\text{PP}}^i(t)$; dotted lines). Bottom panel: Relative deviation from the original *in situ* nucleosynthesis plotted as $\delta_{\Delta\mathbf{r}}^i \equiv |\log_{10}(M_{\text{PP}}^i/M_C^i)|$.

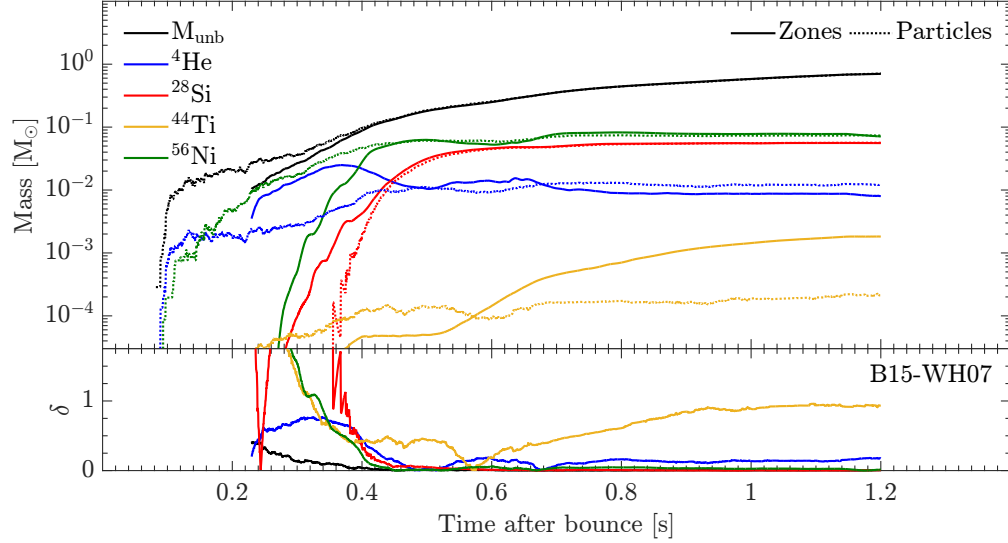


Figure 3.38 Top panel: B15-WH07 Total unbound mass of several α -network species as determined from the original simulation ($M_C^i(t)$; solid lines) and post-processed using identical thermodynamic histories from Lagrangian tracer particles ($M_{\text{PP}}^i(t)$; dotted lines). Bottom panel: Relative deviation from the original *in situ* nucleosynthesis plotted as $\delta_{\Delta\mathbf{r}}^i \equiv |\log_{10}(M_{\text{PP}}^i/M_C^i)|$.

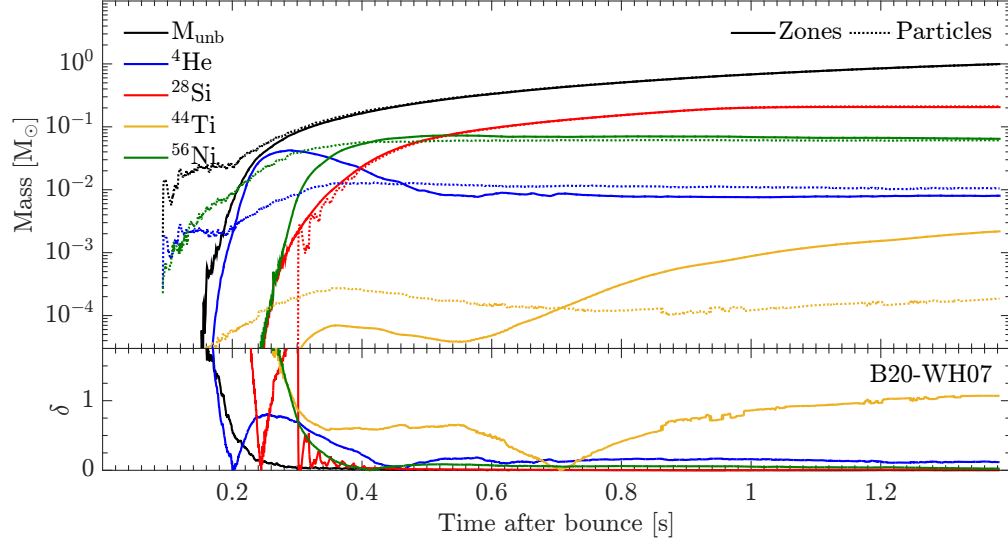


Figure 3.39 Top panel: B20-WH07 Total unbound mass of several α -network species as determined from the original simulation ($M_C^i(t)$; solid lines) and post-processed using identical thermodynamic histories from Lagrangian tracer particles ($M_{PP}^i(t)$; dotted lines). Bottom panel: Relative deviation from the original *in situ* nucleosynthesis plotted as $\delta_{\Delta\mathbf{r}}^i \equiv |\log_{10}(M_{PP}^i/M_C^i)|$.

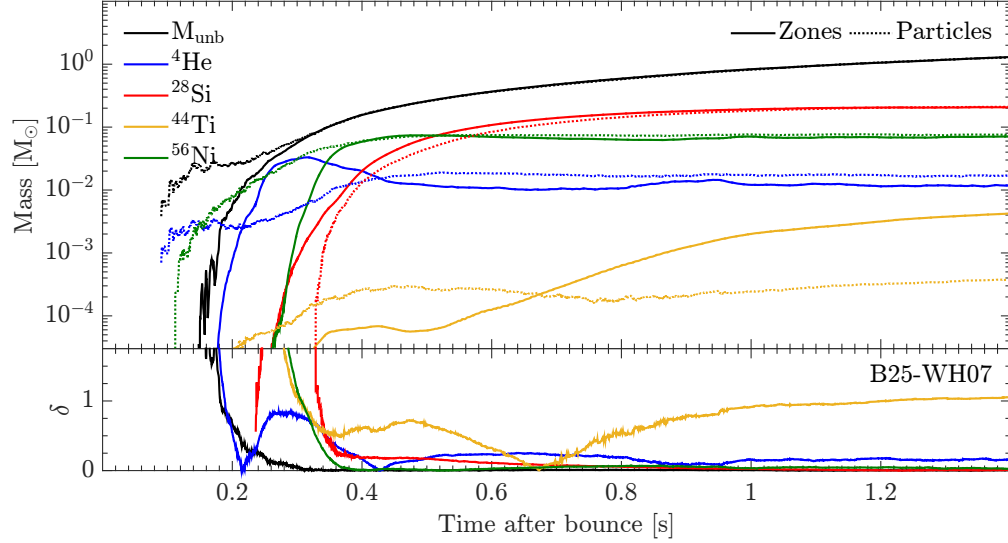


Figure 3.40 Top panel: B25-WH07 Total unbound mass of several α -network species as determined from the original simulation ($M_C^i(t)$; solid lines) and post-processed using identical thermodynamic histories from Lagrangian tracer particles ($M_{PP}^i(t)$; dotted lines). Bottom panel: Relative deviation from the original *in situ* nucleosynthesis plotted as $\delta_{\Delta\mathbf{r}}^i \equiv |\log_{10}(M_{PP}^i/M_C^i)|$.

when switching from the α -network to the SN150-network. Without an *in situ* large network simulation, we are unable to fully quantify how spatial resolution of the tracer particles may impact nucleosynthesis with realistic nuclear networks. However, this work suggests that much higher tracer particle spatial resolution, and ultimately, large, *in situ* nuclear networks are needed to correctly calculate α -rich freeze-out.

The susceptibility of post-processing to inadequate spatial resolution can also be broadly characterized by the mass distribution of $Y_e(t_f)$ for unbound matter (see Figure 3.42). In these mass histograms, calculated from both individual zone data (white) and tracer particle data (blue), it becomes clear that the masses represented by a single tracer particle (dashed line) in the B-Series models fail to adequately resolve ejecta outside of $0.49 < Y_e(t_f) < 0.51$. While this constitutes by far the majority of the matter, it neglects some of the most interesting nucleosynthesis. For B12-WH07 and, to a large extent, B15-WH07, increasing the number of tracer particles by an order of magnitude would serve to capture much more of the Y_e mass distribution and is a relatively easy solution to implement. Applying a similar approach to B20-WH07 and B25-WH07 would require an untenable number of particles to effectively capture the long tails of the distribution.

As in Equation 3.2, we define

$$\|r_{\delta_{\Delta\mathbf{r}}}\| \equiv \frac{\sum_i \delta_{\Delta\mathbf{r}}^i}{\sum_i |\log_{10}(\sqrt{M_C^i(t_f)M_{PP}^i(t_f)})|}. \quad (3.3)$$

From this measure, it becomes clear that uncertainties stemming from spatial resolution, even though they apply to only a small subset of species, are the largest, single source of error in the B-Series models (see Table 3.1).

3.1.5 NSE transition and network size

Compositional evolution via the nuclear reaction network, both within the simulation and as a post-processing calculation, is an initial-value problem, with the initial values provided by one of two different methods (Section 2.2.5). For particles which have

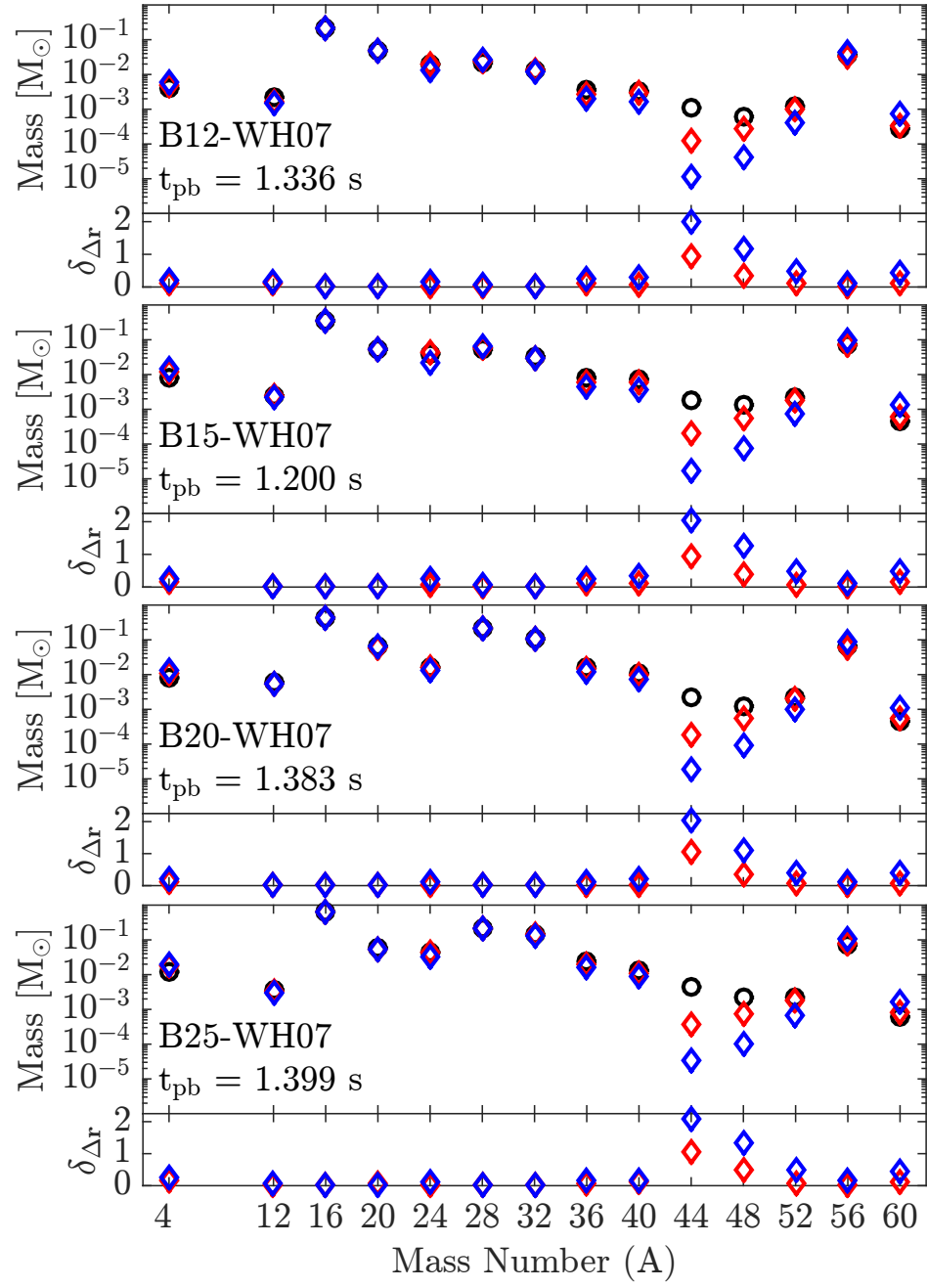


Figure 3.41 Top panels: M_C^i (black circles) and M_{PP}^i (diamonds) at the end of each simulation and transitioned out of NSE using $T_{NSE}(\rho)$ from Equation 2.1. The post-processed nucleosynthesis results are shown for two different networks: the α -network used in the simulation (red) and a 150-species network (blue). Bottom panels: Deviations from the original *in situ* nucleosynthesis plotted for each α -network isotope i as $\delta_{\Delta r}^i \equiv |\log_{10}(M_{PP}^i/M_C^i)|$.

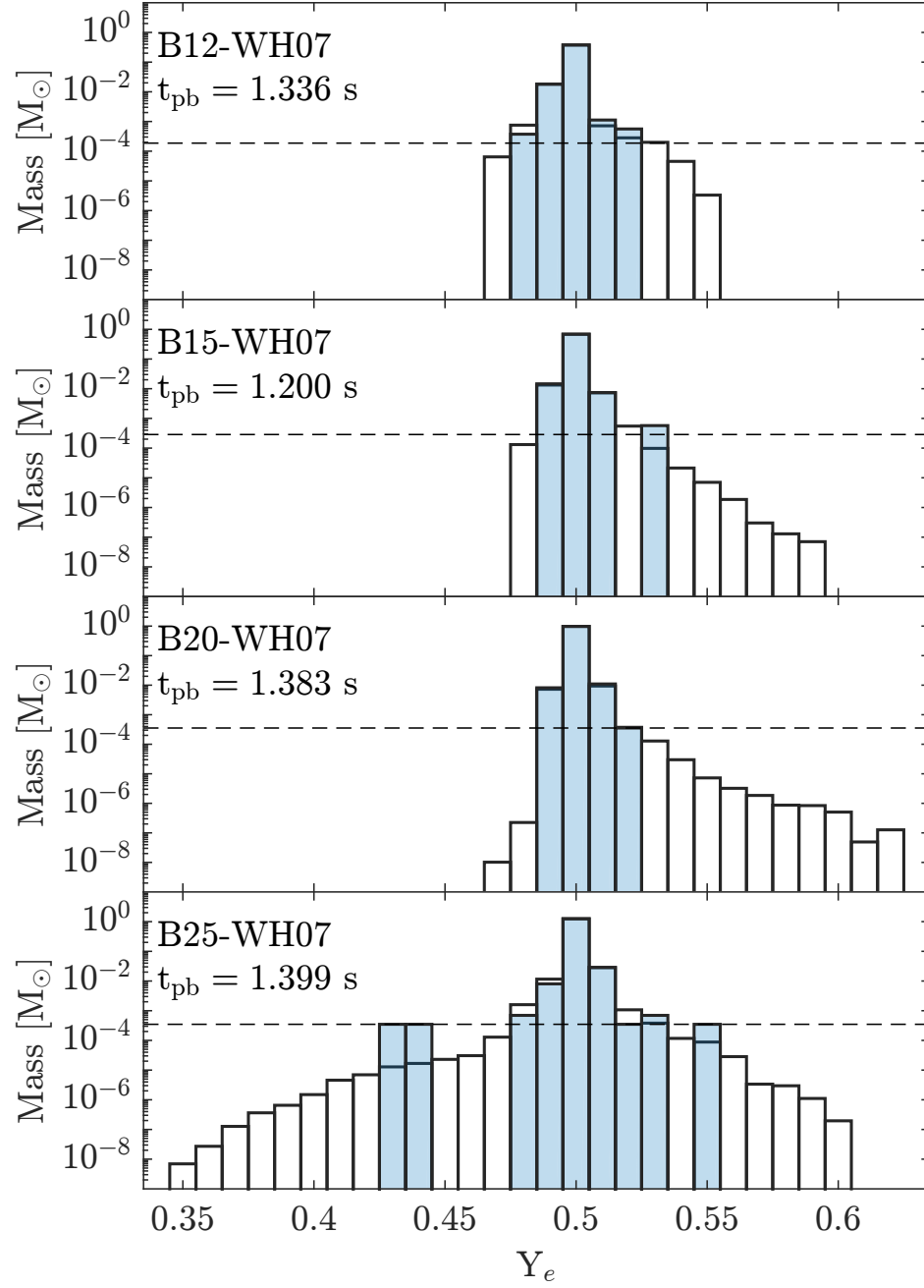


Figure 3.42 Mass histograms of $M_{\text{unb}}(t_f)$, with bin sizes of $\Delta Y_e(t_f) = 0.1$ for B-Series models and calculated using both unbound particle data (blue) and grid data (white). The mass represented by one Lagrangian tracer particle is given by the dashed line.

never reached NSE, the initial composition of the progenitor is mapped onto the nuclear network used for the nuclear evolution, providing the initial abundances. For particles which have reached NSE, the initial abundances from a NSE calculation can be mapped onto the network. CHIMERA’s treatment of the transition of matter into NSE (Section 2.2.1) is comparable to (or in some cases, better than) that used in other CCSN codes of similar capability—e.g., CASTRO (Almgren et al., 2010; Zhang et al., 2011, 2013), PROMETHEUS-VERTEX (Buras et al., 2006b; Marek and Janka, 2009), CoCoNuT-VERTEX (Müller et al., 2012b), ZELMANI (Ott et al., 2011, 2013), and Zeus+IDSA (Suwa et al., 2010, 2013). The transition condition is motivated by the temperatures and densities at which complete silicon burning would occur within the current global timestep. For temperatures above this threshold, the use of the nuclear network is superfluous, as the network will achieve NSE every timestep. For simplicity, the transition out of NSE occurs when the temperature drops below this NSE condition (Equation 2.1 for CHIMERA). However, for the rapidly changing conditions in expanding CCSN matter, the assumption of NSE has been shown to break down when the temperature falls below 6 GK (Meyer et al., 1998).

This leaves a dilemma for this or any similar post-processing study. Is it better to be consistent with the NSE-to-network transition used within the supernova simulation, or should an earlier (higher temperature) transition out of NSE be adopted for the network? As a test of the NSE transition criteria in the B-Series simulations, we post-process the nucleosynthesis using the same α -network used with the simulations and vary the conditions at which the transition to nuclear burning from the NSE composition occurs. In Figure 3.43, we compare the unbound masses of individual isotopes, transitioned out of NSE using either $T_{\text{NSE}}(\rho)$, as defined in Equation 2.1, or $T_{\text{NSE}} = 8$ GK and show the relative deviation for each species i as $\delta_{\text{NSE}}^i \equiv |\log_{10}(M_{\text{PP}}^i(T_{\text{NSE}}(\rho))/M_{\text{PP}}^i(T_{\text{NSE}} = 8 \text{ GK}))|$. The *in situ* calculation transitions out of NSE at a temperature $\approx 2\text{--}3$ GK lower than the tested value of 8 GK. This reduces the α -richness of the eventual freeze-out by maintaining NSE longer than it would physically. As a result, we see a significant shift in the masses of ^4He ,

^{44}Ti , ^{48}Cr , and ^{60}Zn in each model (e.g., $M_{\text{PP}}^{44\text{Ti}}(T_{\text{NSE}} = 8 \text{ GK})/M_{\text{PP}}^{44\text{Ti}}(T_{\text{NSE}}(\rho)) \approx 3.0$), highlighting the failure of $T_{\text{NSE}}(\rho)$ to fully capture α -rich freeze-out in the ejecta. This argues that for a stricter set of criteria for the breakdown of NSE should be adopted for use in post-processing than the $\approx 5\text{--}6 \text{ GK}$ commonly used within models of the CCSN mechanism so that one may properly achieve α -rich freeze-out. Furthermore, the transition used within the models themselves should be investigated if direct nucleosynthesis results are to be used to constrain models. We define

$$||r_{\delta_{\text{NSE}}}|| \equiv \frac{\sum_i \delta_{\text{NSE}}^i}{\sum_i |\log_{10}(\sqrt{M_{\text{PP}}^i(T_{\text{NSE}}(\rho))M_{\text{PP}}^i(T_{\text{NSE}} = 8 \text{ GK})})|} \quad (3.4)$$

for direct comparison with the uncertainties defined by Equation 3.2 and Equation 3.3 (see Table 3.1).

The same post-processing calculations using CHIMERA’s α -network also provide insight into the limitations of this network on the nucleosynthesis in the simulation. Limitations in tracer particle spatial resolution significantly constrain our ability to capture α -rich freeze-out in post-processing calculations (Section 3.1.4), but this uncertainty is mildly abated by improved treatment of the NSE transition, which enhances production of α -rich freeze-out species (see Figure 3.43). This effect is visible for both the SN150- and α -network, and $\delta_{\text{NSE}}^i(\alpha)$ is nearly identical to $\delta_{\text{NSE}}^i(\text{SN150})$. Differences in ejected mass of individual isotopes incurred from nuclear network size can vary (compare blue diamonds to red diamonds in Figures 3.43); the extent of which can be as high as an order of magnitude for ^{44}Ti . However, for species like ^{56}Ni , the effect is smaller ($\approx 20\%$). With this uncertainty in mind, we have reasonable confidence quoting the production of Ni and species from O–Ca from the *in situ* α -network, but the values for the products of α -rich freeze-out require the use of a larger *in situ* network.

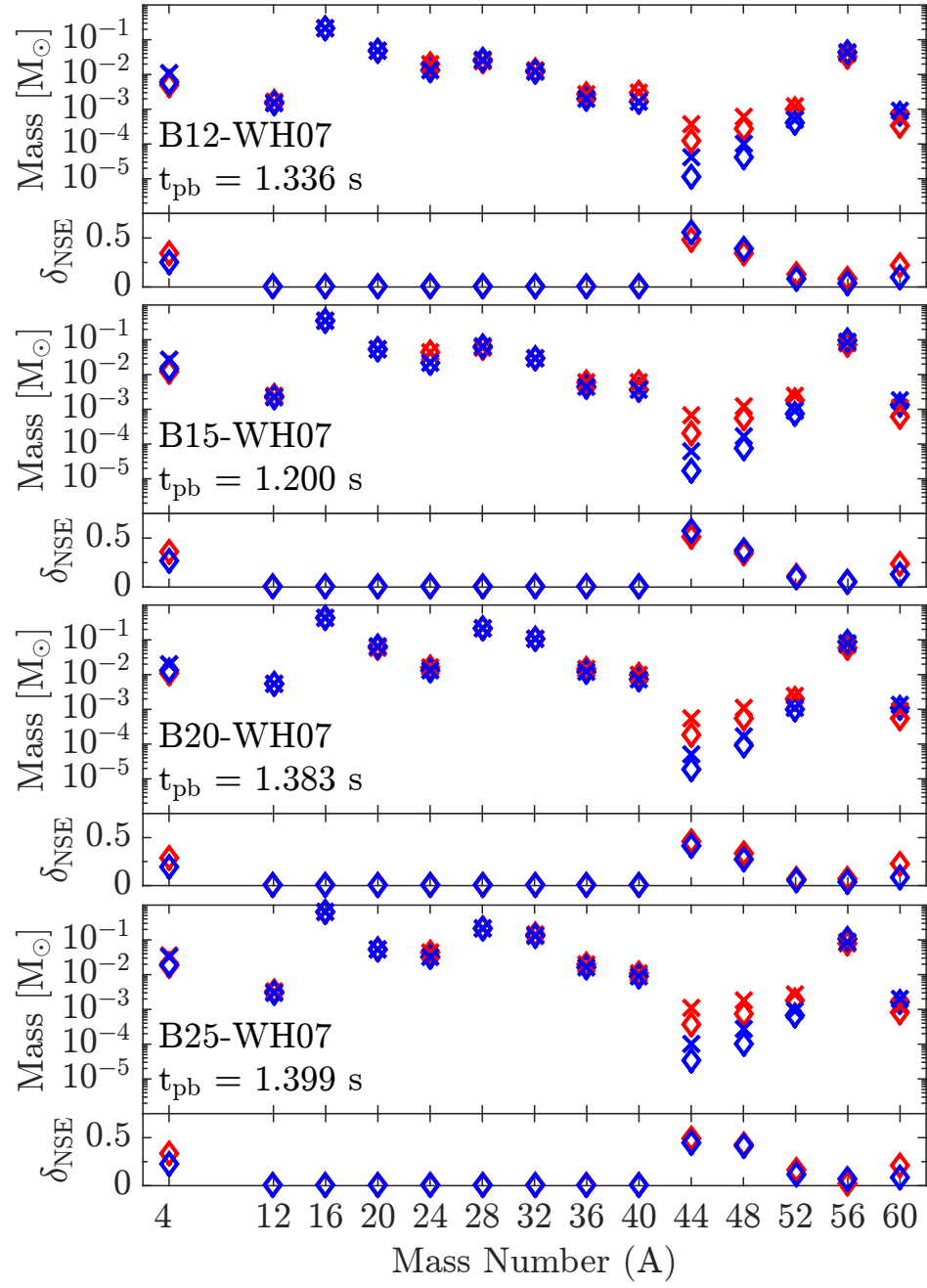


Figure 3.43 Top panels: $M_{\text{PP}}^i(t_f)$ transitioned out of NSE using $T_{\text{NSE}}(\rho)$ (diamonds) and $T_{\text{NSE}} = 8$ GK (crosses). The post-processed nucleosynthesis results are shown in the top panels for two different networks: the α -network used in the simulation (red) and a 150-species network (blue). Bottom panels: Relative deviation of composition between different values of T_{NSE} plotted for each species i as $\delta_{\text{NSE}}^i = |\log_{10}(M_{\text{PP}}^i(T_{\text{NSE}}(\rho))/M_{\text{PP}}^i(T_{\text{NSE}} = 8 \text{ GK}))|$.

3.1.6 Time resolution

The convective and turbulent nature of CCSNe make it highly probable for tracer particle thermodynamic states to change very rapidly. To capture this detail, CHIMERA records the temporal history of each particle independently whenever the temperature changes by 0.1% from the last record and, likewise, limits changes in density and integrated neutrino number flux, ϕ_ν , to 1%. These sampling criteria ensure that all significant features in the temporal histories of the tracer particles are captured. However, this high temporal cadence limits the number of tracers that can be evolved if the total cost of the simulation is not to be limited by tracer I/O. Independent sampling of individual tracers for the hundreds-of-thousands of tracer particles necessary to adequately sample a 3D simulation poses an even heavier and perhaps untenable load on I/O. One alternative to this approach is to record the thermodynamic states of all tracer particles at fixed time intervals along with the typical checkpoint data of the simulation. While this addresses the logistical concerns of managing a large amount of data, it runs the risk of insufficiently sampling the histories of individual particles. The biggest danger of less frequent sampling is the underestimate of local maxima in temperature and density in the thermodynamic history. The exponential temperature dependence of thermonuclear reactions can potentially greatly magnify the impact of under-sampling in the local peak conditions. The balanced reactions which maintain NSE, particularly those linking ^4He to ^{12}C , are especially susceptible to peak temperature and density conditions (Meyer et al., 1998). Thermodynamic histories which fail to capture this peak behavior due to inadequate time resolution can thereby misestimate the conditions of α -rich freeze-out.

We quantify this effect and other sampling-related concerns in tracer particle histories by post-processing thermodynamic profiles down-sampled to fixed time intervals. We compare the resulting composition profile to that from the dynamic time interval criteria described above for ^4He , ^{28}Si , ^{44}Ti , and ^{56}Ni for both the α -network and SN150-network in Figure 3.44 for B12-WH07.

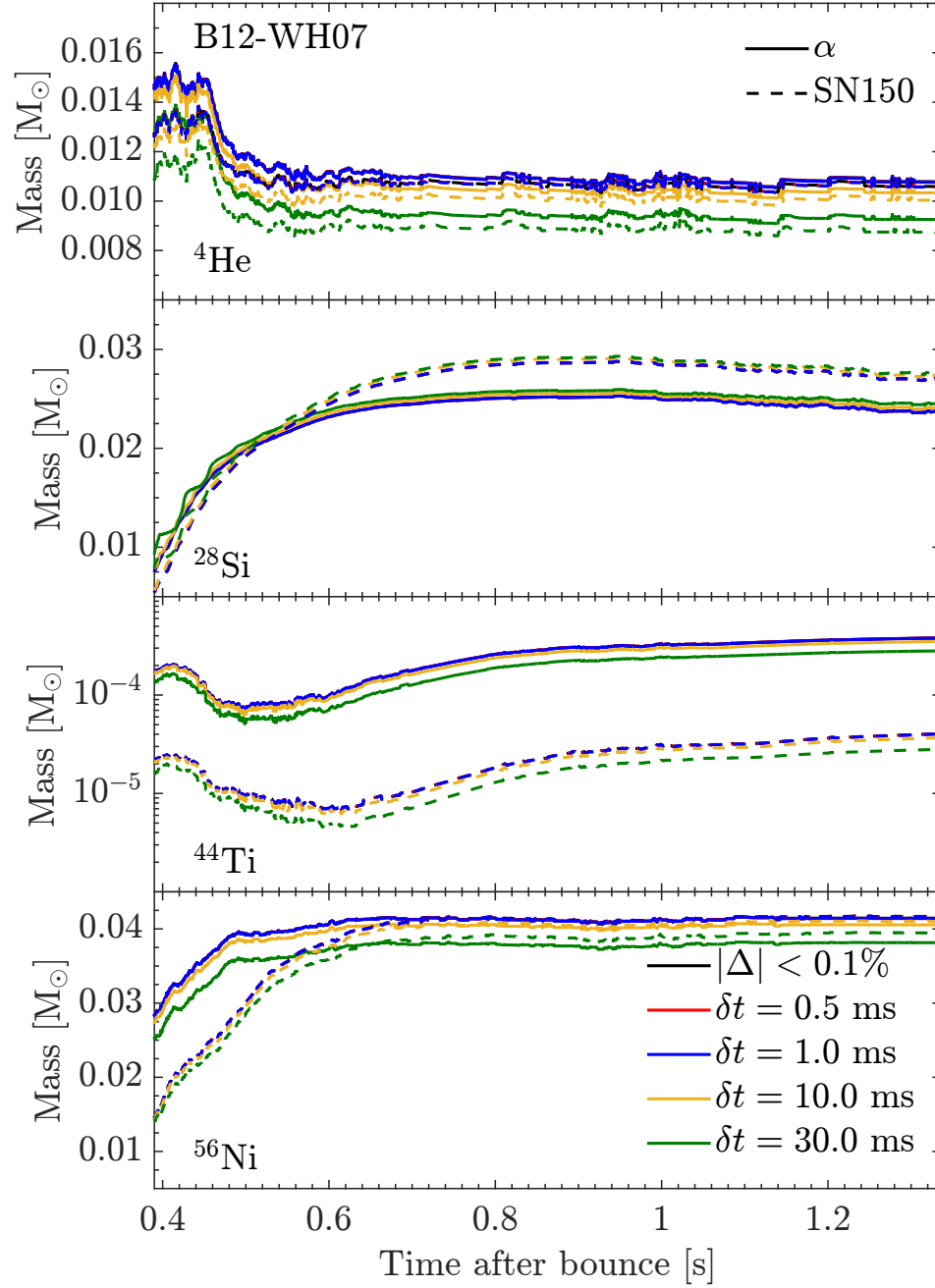


Figure 3.44 B12-WH07 total unbound mass, M_{unb} , for ${}^4\text{He}$, ${}^{28}\text{Si}$, ${}^{44}\text{Ti}$, and ${}^{56}\text{Ni}$ from post-processing calculations using both the α -network (solid lines) and SN150-network (dashed lines) and performed with thermodynamic profiles generated using different fixed sampling intervals, δt , and a dynamic time interval chosen such that $|\Delta| < 0.1\%$, where $\Delta = \max(|\Delta T|, |\Delta\rho|/10, |\Delta\phi_\nu|/10)$.

We find that a fixed rate of sampling the thermodynamic state reproduces post-processed abundances from the dynamic time interval criteria to within 0.5% so long as the fixed interval, δt , does not exceed 1 ms. For $\delta t > 1$ ms, post-processing calculations fail to capture the important fluctuations in density and temperature, particularly those that define the conditions of α -rich freeze-out. The subsequent errors incurred in the total unbound mass is independent of the reaction network size, and ^{44}Ti is most affected by poor time resolution ($\approx 10\%$ error for $\delta t = 10$ ms and $\approx 30\%$ error for $\delta t = 30$ ms).

3.2 Summary

In this chapter, we have discussed some of the uncertainties which complicate post-processing nucleosynthesis calculations from *ab initio* multi-dimensional CCSN simulations evolved beyond the initial stages of explosive nuclear burning but not yet to conditions for nuclear reactions to cease. We provide specific examples of how these uncertainties impact nucleosynthesis predictions for the four axisymmetric models of [Bruenn et al. \(2014\)](#). A broader discussion of nucleosynthesis in these models is presented in Chapter 4.

Our results can be summarized as follows:

1. Even after 1.2–1.4 s of post-bounce evolution and asymptotic explosion energies, the multi-dimensional mass-cut remains unresolved in each model, impacting the production of nuclear species in borderline ejecta near ongoing accretion flows. The consequences of this are particularly pronounced in B25-WH07, wherein the ultimate fate of $\approx 0.2 M_{\odot}$ of a total $\approx 1.3 M_{\odot}$ of gravitationally-unbound matter is indeterminate. The state of the multi-dimensional mass-cut is even more dire if the simulations are truncated at 600–800 ms after bounce, after the explosion energy has leveled off but before explosive nucleosynthesis has completed.

2. Despite temperatures below the threshold for explosive nuclear burning, a result of the extended running times, local hydrodynamic deviations from isentropic expansion continue to play a non-trivial role on secondary nuclear processes and neutrino-induced nucleosynthesis by altering the expansion timescale estimate necessary for extrapolation to freeze-out at $T \approx 0.5$ GK.
3. The ability of Lagrangian tracer particles to effectively reproduce the *in situ* nuclear burning conditions of the B-Series simulations is significantly reduced in regions of α -rich freeze-out. In each of the four models, ^{44}Ti is consistently under-produced. The magnitude of this effect is similar, but in the opposing direction, to that of replacing the α -network used in the post-processing calculation with a more realistic 150-species network. While this effect targets only those species that result from α -rich freeze-out, it has the largest global effect of the uncertainties tested. Ideally, large *in situ* networks are the best method to address this issue. Failing that, much higher numbers of tracer particles are needed.
4. Furthermore, we argue for a stricter set of criteria for transitioning out of NSE than the commonly used $T_{\text{NSE}} \approx 5\text{--}6$ GK within models of the CCSN mechanism. While sufficient for the transition of matter into NSE, this criteria fails to capture the process of α -rich freeze-out crucial to the production of ^{44}Ti .
5. We find that recording the thermodynamic conditions of all tracer particles at a fixed time interval $\delta t \leq 1$ ms to be a viable alternative to independently tracking the detailed history of each particle, wherein deviations in the nuclear burning inputs (i.e. ρ , T , and ϕ_ν) are limited explicitly.

In light of these findings, we have modified CHIMERA, when possible, in an attempt to reduce these uncertainties for future models. With regard to [3](#), ongoing models have improved the spatial resolution of tracer particle sampling by increasing the number of tracer particles by roughly one order of magnitude. The larger burden this

would place on the file system is sufficiently alleviated with fixed time interval I/O for tracer particles. Our results in 5 give us confidence in this approach. Lastly, taking our own advice in 4, we have implemented a framework in CHIMERA to use arbitrary criteria for the NSE transition. When combined with quasi-statistical equilibrium methods (Hix et al., 2007; Parete-Koon et al., 2008), CHIMERA will be capable of seamlessly evolving nuclear burning networks through the NSE transition.

In theory, both the indeterminate mass-cut and expansion timescale uncertainties could be reduced by extending the simulation to freeze-out. However, given the inadequate spatial resolution of the tracer particles and an inherent limitation in the accuracy of the rate of nuclear energy released by the smaller network within the hydrodynamics, we cannot rely entirely on post-processing methods to obtain an accurate representation of the nucleosynthesis. Since the nucleosynthesis depends on the thermodynamic conditions and, consequently, nuclear energy generation, a feedback exists that cannot be captured with post-processing, significantly affecting the abundances of species such as ^{44}Ti , ^{57}Fe , ^{58}Ni , and ^{60}Zn (Woosley and Weaver, 1995). As a result of this feedback, Magkotsios et al. (2010) find strong differences in the α -richness between supernova models, fundamentally altering the conditions of α -rich freeze-out which are also subject to neutronization in the bath of neutrinos near the core. Calculations which cannot track neutronization in the composition (e.g. α -network) are intrinsically limited in their ability to calculate realistic nucleosynthesis. This deficiency cannot be completely ameliorated via post-processing with larger networks. Improving upon the existing *in situ* α -network with a more realistic 150-species nuclear network capable of properly tracking neutronization and energy release via particle captures is an important step towards resolving this problem and is the subject of ongoing work.

Chapter 4

Nucleosynthesis in Axisymmetric Ab Initio Core-Collapse Supernova Simulations of 12–25 $M_{\odot}$ Stars

In Chapter 3, I discussed how multi-dimensional effects complicate nucleosynthesis calculations. In spite of these uncertainties, our models represent a significant step towards calculating self-consistent nucleosynthesis. Unfortunately, the computational burden of *ab initio* CCSN models, combined with the vast parameter space characterizing massive stars prior to their collapse, will likely demand that the larger community continue to rely on parameterized 1D models as inputs to galactic chemical evolution studies for some time. However, self-consistent models like the B-Series simulations provide the best available constraints to guide parameterized models.

In order to produce successful explosions, it is necessary for 1D models to parameterize the mass-cut and explosion energy. This has obvious consequences on nucleosynthesis processes that are dependent on the passing asymmetric shock and anisotropic explosion mechanism. This may include products of explosive oxygen and silicon burning, α -rich or normal freeze-out from NSE, and other species made during the neutrino-driven wind via the r -process and/or νp -process. In this chapter,

I compare nucleosynthesis results from the B-Series models with those of [Woosley and Heger \(2007\)](#), hereafter referred to as the WH07 models, which were obtained from parameterized, spherically symmetric explosion models and tuned to reproduce observations by setting the explosion energy to 1.2×10^{51} ergs (equivalently 1.2 B) and the initial location of the mass-cut at the point where the dimensionless entropy $S/N_A k_B = 4.0$.

4.1 Comparing self-consistent 2D to parameterized 1D models

Beyond the direct study of the nucleosynthesis products, supernova models, be they 1D or multi-D, parameterized or self-consistent, provide input for calculations of galactic chemical evolution and comparison to observations. Typically, these take the form of the total mass of each ejected isotope as a function of stellar mass. Thus, total isotopic yields are a good place to start the comparison between the nucleosynthesis predictions from the CHIMERA B-Series models and the parameterized WH07 models. In [Section 4.1.1](#), we will define these yields. Two critical differences between the CHIMERA simulations and those of [Woosley and Heger \(2007\)](#) play central roles in understanding the differences in the nucleosynthesis: the multi-dimensional nature of the explosion and the impact of self-consistent neutrino fluxes. These will be discussed in [Section 4.1.2](#) and [Section 4.1.3](#), respectively. In [Section 4.2](#), we will conclude with a detailed analysis of the differences between our self-consistent models and the parameterized models.

4.1.1 Calculating total yields

The total mass fraction of ejecta for each isotope i ,

$$X_{\text{ej}}^i = \frac{M_{\text{ej}}^i}{\sum_i M_{\text{ej}}^i}, \quad (4.1)$$

is calculated by combining contributions from post-processed, shocked ejecta, M_+^i , with unshocked material both on- and off-grid (including the stellar wind), M_{unsh}^i and M_{off}^i , respectively, from the [Woosley and Heger \(2007\)](#) models' nucleosynthetic yields:

$$M_{\text{ej}}^i = M_+^i + M_{\text{unsh}}^i + M_{\text{off}}^i. \quad (4.2)$$

M_{unsh}^i , the unshocked, on-grid contribution, is calculated by linearly interpolating the discrete mass fractions from the WH07 post-explosion model, $X_{\text{WH07}}^{(k),i}$, of the appropriate mass shell, $\delta M_{\text{WH07}}^{(k)} = M_{\text{WH07}}^{(k)} - M_{\text{WH07}}^{(k-1)}$, to the initial mass coordinate, M_j , for each tracer particle in $\mathbb{P}_{\text{unsh}}$. X_j^i , the resulting mass fractions for each tracer particle j , are then integrated over the mass of the unshocked tracer particles, for the total mass of each isotope:

$$X_j^i = X_{\text{WH07}}^{(k),i} \frac{M_j - M_{\text{WH07}}^{(k-1)}}{\delta M_{\text{WH07}}^{(k)}} - X_{\text{WH07}}^{(k-1),i} \frac{M_j - M_{\text{WH07}}^{(k)}}{\delta M_{\text{WH07}}^{(k)}} \quad (4.3)$$

$$M_{\text{unsh}}^i = \sum_{j \in \mathbb{P}_{\text{unsh}}} X_j^i \Delta m. \quad (4.4)$$

The contribution from unshocked material that is outside of the computational grid in CHIMERA, M_{off}^i , does not require this interpolation procedure, since it is not sampled by tracer particles. It is M_+^i that contains the important contributions to the nucleosynthesis yields from the CHIMERA models. Differentiating M_{ej}^i from the parameterized WH07 simulations, M_+^i is determined by post-processing the extrapolated thermodynamic trajectories of the shocked ejecta, $\mathbb{P}_+$, with the full REACLIB compilation described in [Section 2.2.5](#).

4.1.2 Multi-dimensional mass-cut

In nearly spherical explosions, as those commonly seen in ECSN models ([Wanajo et al., 2011, 2013a,b](#)), it is not unreasonable to consider a single column of tracer particles as a representative sample of the total tracer particle population and not

wholly dissimilar from 1D Lagrangian simulations. However, typical Fe-core collapse SNe exhibit large scale asymmetries in the explosion mechanism (e.g. accretion streams, SASI, convective instabilities, ...). As such, the evolution of one column of tracer particles poorly samples the explosion dynamics and nucleosynthesis. Qualitative differences from 1D models are clearly evident in the radii of tracer particles in different columns.

In Figure 4.1, we show the evolution of the column of particles (B12-WH07-C1) initially distributed nearest to the north pole ($\theta = 12.8^\circ$). These particles behave in a spherically symmetric manner prior to encountering the shock ($R_{\text{shock}}(\theta)$; solid, magenta line), at which point several of the trajectories become scattered in radius. For the first 200 ms after core-bounce, before the shock has been revived and is still roughly spherical, small lateral velocities do not disrupt this 1D perspective. Soon after the shock is reenergized by neutrino-heating and convective instabilities, the asphericities in the shock become clearly evident in the deviations between $R_{\text{shock}}(\theta)$ and the angle-averaged shock radius $\langle R_{\text{shock}} \rangle$ (dashed, magenta line). The resulting increase in lateral velocities behind the shock quickly distorts any prior resemblance to spherically symmetric models, yet it is not clear from B12-WH07-C1 that the idea of a traditional mass-cut is entirely without merit, since beyond 400 ms after bounce, there is a clear distinction between tracers that are part of the ejecta and those that reside in the proto-NS (dashed, blue line). However, this seemingly spherical behavior is somewhat misleading, as some of the ejected particles “pass” neighboring particles from initially larger radii. Furthermore, there are strong variations in behavior as a function of latitude, especially closer to the equator. In Figure 4.2, we show the same evolution, but for a tracer particle column (B12-WH07-C18) initially located along the equatorial plane ($\theta = 82.8^\circ$). In combination with convective flows, accretion streams that persist long after the development of the explosion serve to aid the proto-NS in capturing tracer particles at late times ($t_{\text{pb}} \gtrsim 1$ s) while simultaneously ejecting matter exposed to large neutrino fluxes and thermodynamic conditions unique to the inner regions of the shocked cavity that tend to be omitted from the ejecta in 1D

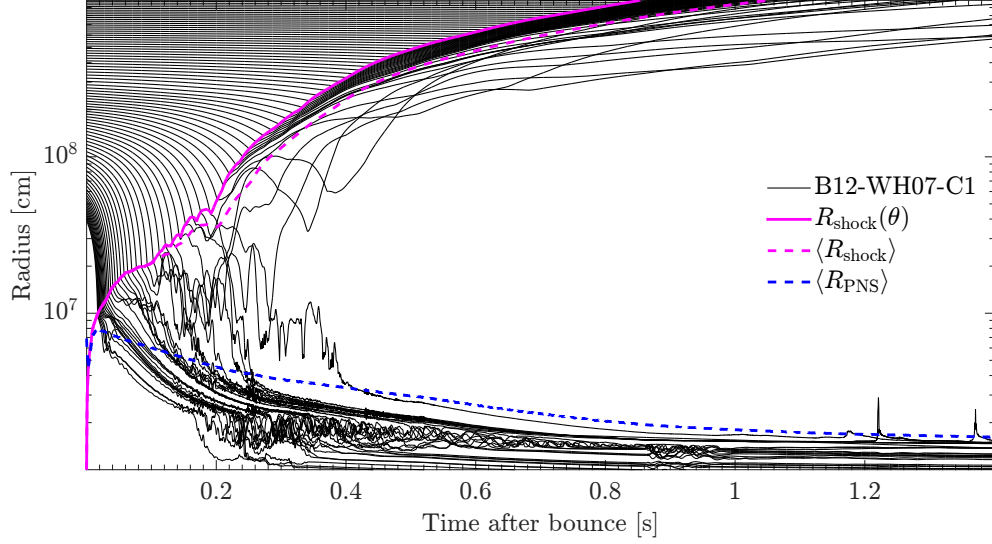


Figure 4.1 Radii evolution of tracer particles in a column initially near the north pole of the $12 M_{\odot}$ model (B12-WH07-C1), representing mass elements initially distributed in radius along $\theta = 12.8^{\circ}$. The solid, magenta line tracks the shock radius for this latitude, $R_{\text{shock}}(\theta)$, and the dashed, magenta line shows the angle-averaged shock radius $\langle R_{\text{shock}} \rangle$. The dashed, blue line represents the surface of the proto-NS $\langle R_{\text{PNS}} \rangle$, as determined by the angle-averaged outer boundary of the region where $\rho > 10^{11} \text{ g cm}^{-3}$.

simulations. The ejection of a tracer particle from the surface of the proto-NS at $t_{\text{pb}} \approx 1 \text{ s}$ in Figure 4.2 suggests a nascent neutrino-driven wind, another feature not captured by 1D explosion models. However, note that accretion continues after this wind particle and others like it are ejected, an indication that the full development of the wind is delayed.

The wealth of observational data for ^{44}Ti and ^{56}Ni makes the extent to which simulations can reproduce the total production and spatial distribution of these isotopes an excellent metric by which to gage models of the nucleosynthesis. Produced in the innermost regions of the shock-heated cavity and with a half-life of 58.9 yr (Ahmad et al., 2006), the production of ^{44}Ti and its subsequent radioactive decay in the high-energy X-ray spectrum is an unparalleled tracer for asymmetries in the explosion mechanism itself. The fraction of ejected ^{44}Ti at 100 s after bounce for the

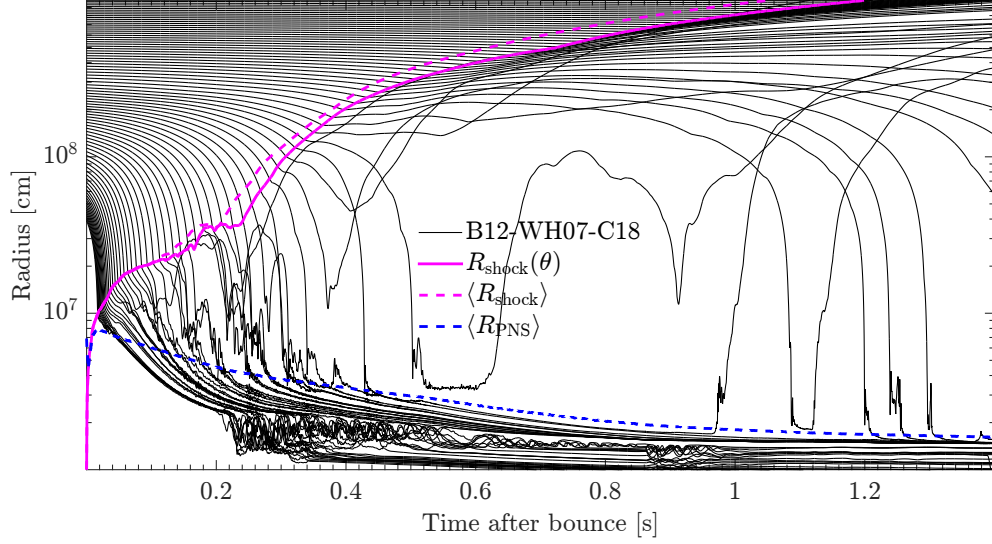


Figure 4.2 Same as Figure 4.1, except now for tracer particles in a column near the equatorial plane of the $12 M_{\odot}$ model (B12-WH07-C18), representing mass elements initially distributed in radius along $\theta = 82.8^{\circ}$.

B-Series models is shown for each tracer particle at its initial location in Figures 4.3–4.6. The enclosed mass at the 1D mass-cut of the WH07 models (solid, magenta line) is usually located at the inner boundary of the oxygen-burning shell (solid, cyan line). For the B-Series models, the location of this 1D mass-cut typically lies farther from the iron-core (solid, red line) than its 2D counterpart (dashed, magenta line), calculated as the combined mass of proto-NS material (solid, black circles) and bound material (open, black circles) at t_f . As a result, the 1D calculation could fail to capture large regions of ejecta critical to ^{44}Ti production while also ejecting material in the oxygen-rich silicon-shell which might not have otherwise been ejected. Examination of Figures 4.3–4.6 highlights that, while a spherical mass-cut can be constructed, it is not a good representation of the fate of individual mass elements. Some of the tracer particles that started above this spherical mass-cut become part of the proto-NS, while some that started below become part of the ejecta. The multi-dimensional fluid flows do not just alter the gross quantities of the ejecta but have a chaotic effect on the fates of individual mass elements.

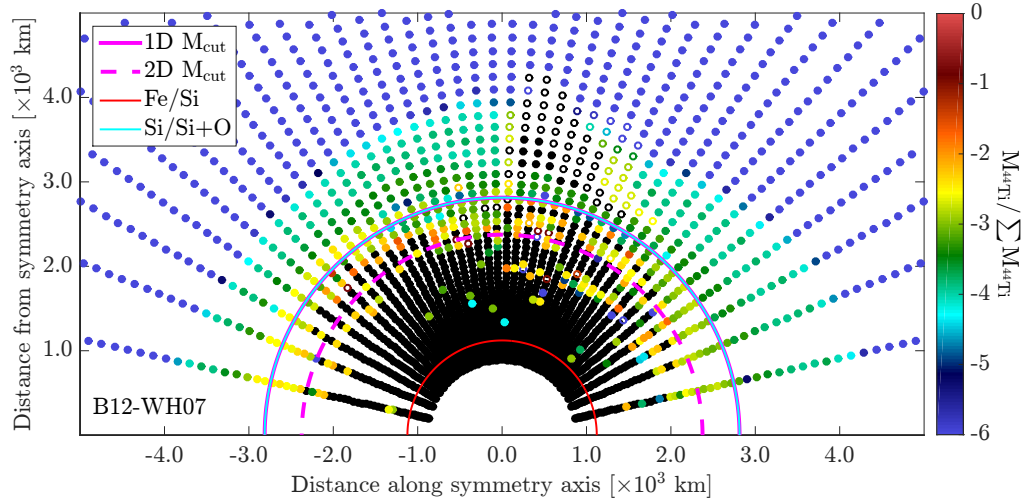


Figure 4.3 B12-WH07 shocked tracer particles in $\mathbb{P}_+(t_f)$ (solid, colored circles), $\mathbb{P}_-(t_f)$ (open, colored circles), $\mathbb{P}_{\text{bound}}(t_f)$ (open, black circles), and those located in the proto-NS (solid, black circles) at t_f , placed at their initial locations in the progenitor star. Particles in $\mathbb{P}_{\text{unb}}$ are colored by ^{44}Ti mass as a fraction of the total ejected ^{44}Ti mass at $t_{\text{pb}} = 100$ s on a log-scale. The Fe-core/Si-shell interface (solid, red line) and Si-shell/(Si+O)-shell interface (solid, cyan line) of the progenitor star are also shown. The initial location of the mass-cut, (M_{cut}), is plotted for the 1D WH07 model as a solid, magenta line. The dashed, magenta line signifies an initial enclosed mass equal to the sum of the proto-NS mass and bound mass from the 2D simulation at t_f .

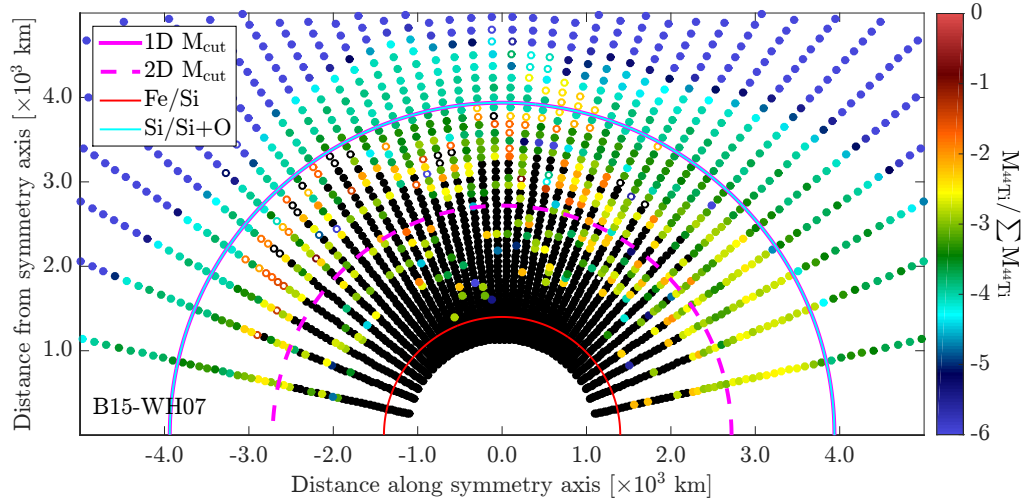


Figure 4.4 B15-WH07 shocked tracer particles in $\mathbb{P}_+(t_f)$ (solid, colored circles), $\mathbb{P}_-(t_f)$ (open, colored circles), $\mathbb{P}_{\text{bound}}(t_f)$ (open, black circles), and those located in the proto-NS (solid, black circles) at t_f , placed at their initial locations in the progenitor star. Particles in $\mathbb{P}_{\text{unb}}$ are colored by ^{44}Ti mass as a fraction of the total ejected ^{44}Ti mass at $t_{\text{pb}} = 100$ s on a log-scale. The Fe-core/Si-shell interface (solid, red line) and Si-shell/(Si+O)-shell interface (solid, cyan line) of the progenitor star are also shown. The initial location of the mass-cut, (M_{cut}), is plotted for the 1D WH07 model as a solid, magenta line. The dashed, magenta line signifies an initial enclosed mass equal to the sum of the proto-NS mass and bound mass from the 2D simulation at t_f .

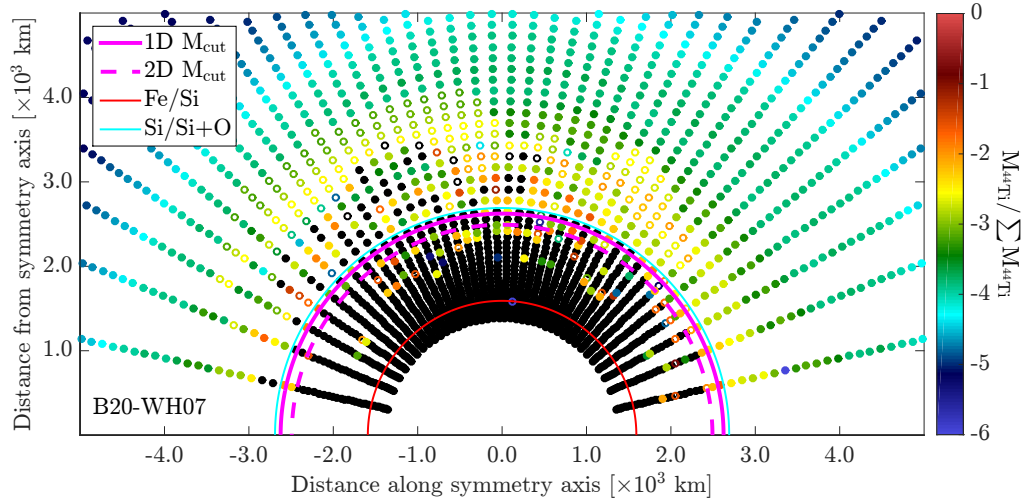


Figure 4.5 B20-WH07 shocked tracer particles in $\mathbb{P}_+(t_f)$ (solid, colored circles), $\mathbb{P}_-(t_f)$ (open, colored circles), $\mathbb{P}_{\text{bound}}(t_f)$ (open, black circles), and those located in the proto-NS (solid, black circles) at t_f , placed at their initial locations in the progenitor star. Particles in $\mathbb{P}_{\text{unb}}$ are colored by ^{44}Ti mass as a fraction of the total ejected ^{44}Ti mass at $t_{\text{pb}} = 100$ s on a log-scale. The Fe-core/Si-shell interface (solid, red line) and Si-shell/(Si+O)-shell interface (solid, cyan line) of the progenitor star are also shown. The initial location of the mass-cut, (M_{cut}), is plotted for the 1D WH07 model as a solid, magenta line. The dashed, magenta line signifies an initial enclosed mass equal to the sum of the proto-NS mass and bound mass from the 2D simulation at t_f .

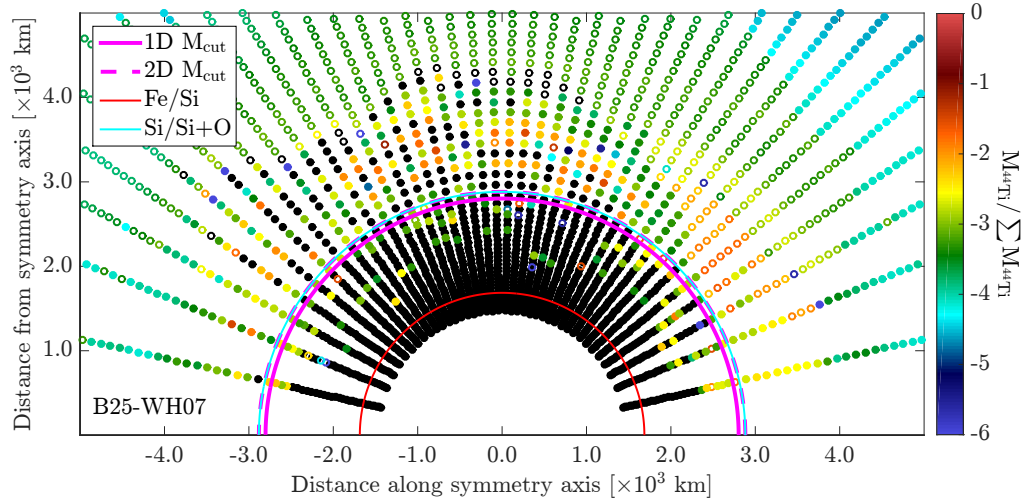


Figure 4.6 B25-WH07 shocked tracer particles in $\mathbb{P}_+(t_f)$ (solid, colored circles), $\mathbb{P}_-(t_f)$ (open, colored circles), $\mathbb{P}_{\text{bound}}(t_f)$ (open, black circles), and those located in the proto-NS (solid, black circles) at t_f , placed at their initial locations in the progenitor star. Particles in $\mathbb{P}_{\text{unb}}$ are colored by ^{44}Ti mass as a fraction of the total ejected ^{44}Ti mass at $t_{\text{pb}} = 100$ s on a log-scale. The Fe-core/Si-shell interface (solid, red line) and Si-shell/(Si+O)-shell interface (solid, cyan line) of the progenitor star are also shown. The initial location of the mass-cut, (M_{cut}), is plotted for the 1D WH07 model as a solid, magenta line. The dashed, magenta line signifies an initial enclosed mass equal to the sum of the proto-NS mass and bound mass from the 2D simulation at t_f .

4.1.3 Neutrino-induced nucleosynthesis

In addition to multi-dimensional effects, the parameterized 1D explosion models of [Woosley and Heger \(2007\)](#) also cannot include self-consistent neutrino interactions, which have been shown to qualitatively affect the ejecta composition through the possibility of neutrino-driven, proton-rich outflows contributing to the production of isotopes with $A > 64$ ([Pruet et al., 2005](#); [Fröhlich et al., 2006a](#)). The sensitivity of these products to the explosion mechanism make them excellent tools for probing the CCSN central engine. The impact of the neutrinos on the composition is strongest when the matter is closest to the neutrino source. However, the matter at such times is generally in NSE; thus, the total effect of the neutrino interactions is to change the global Y_e . At later times, once NSE has frozen out ($T \lesssim 6$ GK), and especially once photo-disintegrations have ceased ($T \lesssim 3$ GK), neutrinos play a more intimate role in altering the composition via individual neutrino capture reactions manifest in the nuclear reaction network. In [Section 4.2](#), we will discuss some of the interesting effects that the alteration of the electron fraction can produce, but in this section, we are focused on the later epoch and the effect of neutrino captures after the breakdown of NSE.

For some tracer particles, for example B12-WH07-P1616, a significant impact from the neutrino-induced reactions can be seen, with the abundances of species like ^{64}Zn boosted by approximately three orders of magnitude (see [Figure 4.7](#)). Following the approach in [Chapter 3](#), we define a residual norm for the final composition,

$$\|r_{\delta_\nu}\| \equiv \frac{\sum_i \delta_\nu^i}{\sum_i |\log_{10}(\sqrt{X_i(\nu\text{-rateson})X_i(\nu\text{-ratesoff})})|}, \quad (4.5)$$

as a means to easily compare the impact of neutrino-induced nucleosynthesis between individual tracer particles, where $\delta_\nu^i = |\log_{10}(X_i(\nu\text{-rates on})/X_i(\nu\text{-rates off}))|$. Using $\|r_{\delta_\nu}\|$ as a proxy, it is clear that particles with thermodynamic and neutrino exposure histories like B12-WH07-P1616, for which $\|r_{\delta_\nu}\| = 0.339$, are relatively rare in the sample from the four B-Series models (see [Figure 4.8](#)). Particles which exhibit the

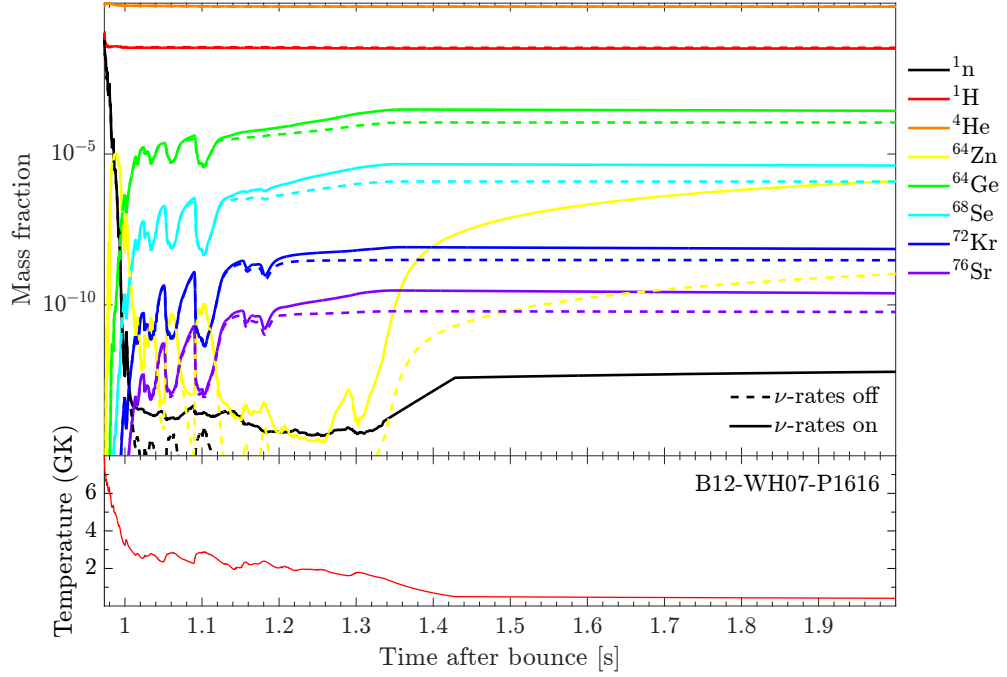


Figure 4.7 Evolution of composition (top) and temperature (bottom) with (solid lines) and without (dashed lines) neutrino reactions for B12-WH07-P1616, a particle with a significant contributions from the neutrino-induced reactions which are critical to the production of isotopes such as ^{64}Zn (yellow lines), ^{64}Ge (green lines), ^{68}Se (cyan lines), ^{72}Kr (blue lines), and ^{76}Sr (purple lines).

νp -process, like B12-WH07-P1616, may become more common as the neutrino-driven wind develops. However, ongoing accretion continues to inhibit the wind more than 1.2–1.4 seconds after bounce.

In fact, the delay in the development of the wind is a noteworthy feature of the B-Series models. The total effect of neutrino-induced reactions for free nucleons on the nucleosynthesis is demonstrated for each B-Series model by performing two post-processing calculations to 1 yr after bounce, one with neutrino-induced reactions (Equation 2.4) and the other excluding such reactions. The abundances of each species relative to solar (i.e. production factor, $P^i = X_{\text{ej}}^i/X_{\odot}^i$; Lodders, 2003) for each calculation are normalized to the production factor of ^{16}O . The production

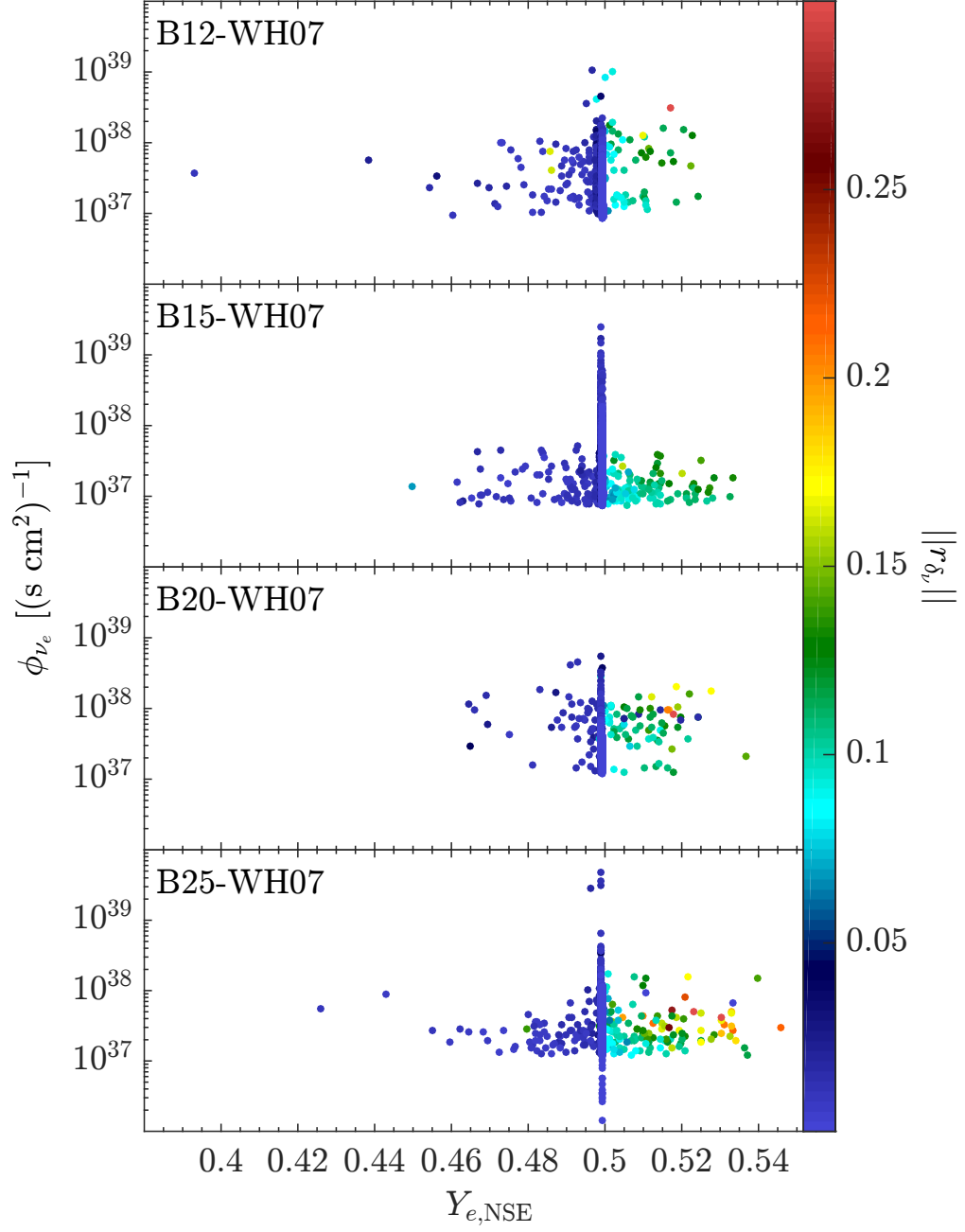


Figure 4.8 Tracer particles in $\mathbb{P}_+(t_f)$ for each B-Series simulation and positioned according to $Y_{e,\text{NSE}}$ and integrated ν_e number flux at t_f and colored by the total compositional effect of neutrino interactions after NSE freeze-out ($\|r_{\delta_\nu}\|$; Equation 4.5).

factors for mass number A_i , P_A^i , and atomic number Z_i , P_Z^i , where

$$P_A^i = \frac{\sum_{A_k=A_i} X_{\text{ej}}^k}{\sum_{A_k=A_i} X_{\odot}^k} / P^{16\text{O}} \quad (4.6)$$

$$P_Z^i = \frac{\sum_{Z_k=Z_i} X_{\text{ej}}^k}{\sum_{Z_k=Z_i} X_{\odot}^k} / P^{16\text{O}}, \quad (4.7)$$

are shown in Figure 4.9 and Figure 4.10, respectively. Plotted as solid lines with filled circles are results for calculations which include neutrino and anti-neutrino captures and emissions from free nucleons. Results from calculations which exclude these neutrino reactions are plotted as dashed lines with open diamonds. The effect of neutrino-induced reactions is weak in the B-Series models, and we do not see a robust νp -process. This situation may change with the development of a neutrino-driven wind at later times, though such later development will probably result in a weaker wind. Still, neutrino-induced reactions do have a modest quantitative impact on the nucleosynthetic yields for $43 \lesssim A \lesssim 90$ and $21 \lesssim Z \lesssim 40$, particularly in the slightly more proton-rich ejecta of B25-WH07 (see Figure 3.42).

4.2 A detailed look at nucleosynthesis differences

Beyond the effects of multi-dimensionality discussed in Section 4.1.2 and neutrino-induced nucleosynthesis discussed in Section 4.1.3, detailed comparison of 2D and 1D models reveals a number of interesting features unique to multi-D CCSN models. To reveal those features, we compare the production factors P_A^i and P_Z^i (Equation 4.6 and Equation 4.7) from the B-Series models (solid lines, filled circles) with those from the WH07 explosion models (dashed lines, open circles) in Figure 4.11 and Figure 4.12. In addition to quantitative differences for most values of Z , the B-Series nucleosynthetic yields for $30 \lesssim Z \lesssim 42$ and $60 \lesssim A \lesssim 90$ are qualitatively different from the WH07 results. The bulk of these differences can be attributed to large, distinct peaks in P_A^i and P_Z^i .

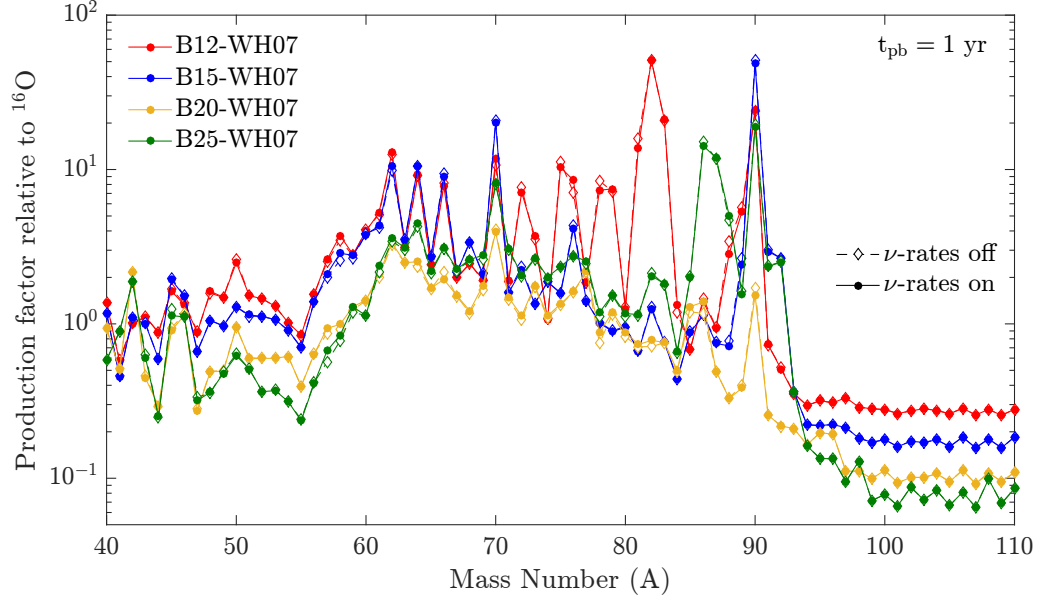


Figure 4.9 B-Series production factors 1 yr after bounce normalized to that of ^{16}O as a function of mass number A for post-processing calculations performed with (solid lines, filled circles) and without (dashed lines, open diamonds) neutrino-induced reactions.

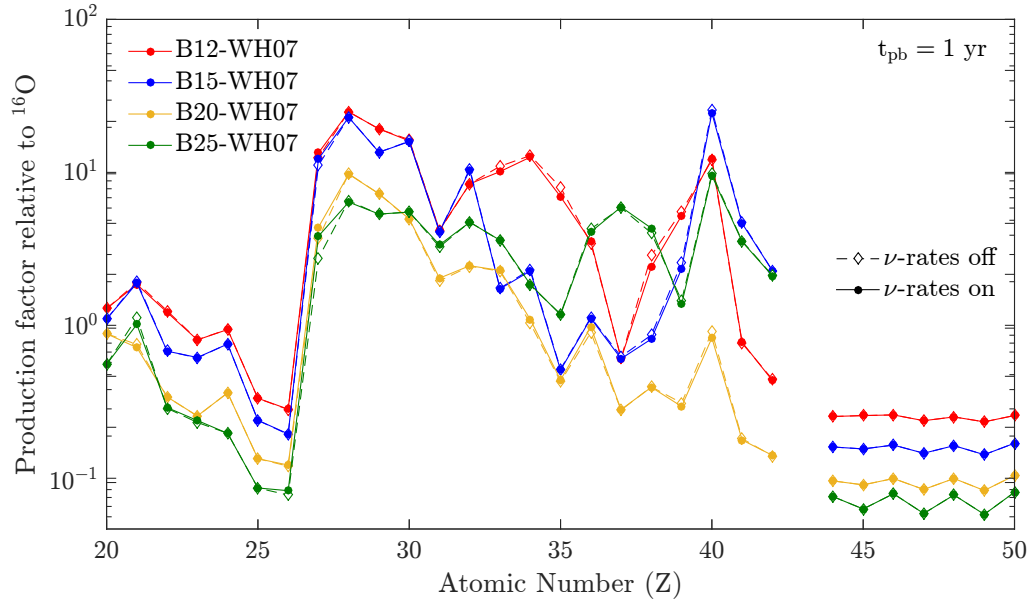


Figure 4.10 B-Series production factors 1 yr after bounce normalized to that of ^{16}O as a function of atomic number Z for post-processing calculations performed with (solid lines, filled circles) and without (dashed lines, open diamonds) neutrino-induced reactions.

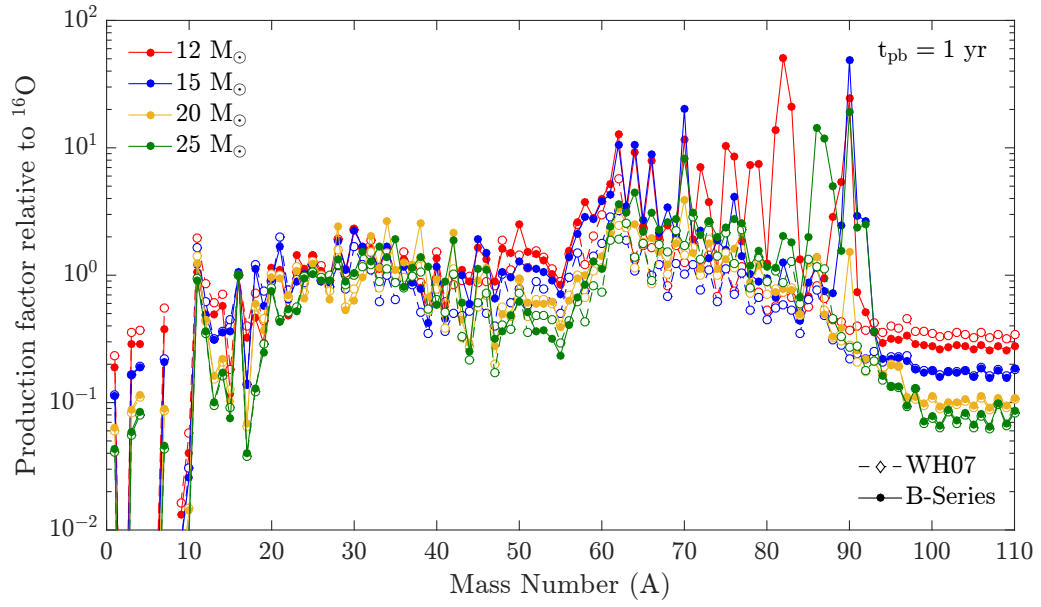


Figure 4.11 Production factors 1 yr after bounce normalized to that of ^{16}O as a function of mass number A for B-Series models (solid lines, filled circles) and WH07 models (dashed lines, open circles).

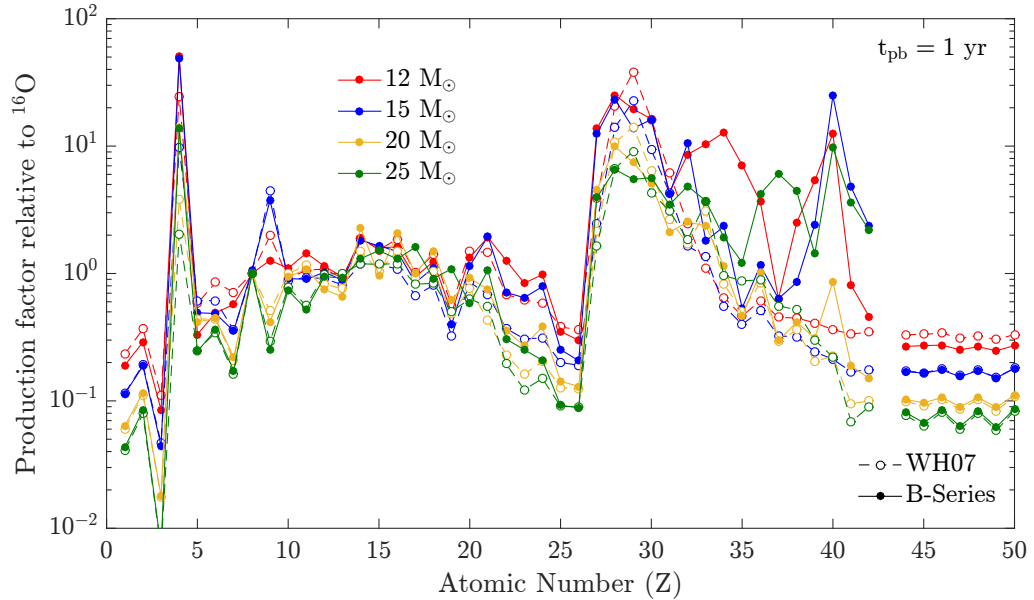


Figure 4.12 Production factors 1 yr after bounce normalized to that of ^{16}O as a function of atomic number Z for B-Series models (solid lines, filled circles) and WH07 models (dashed lines, open circles).

Figures 4.13–4.16 illustrate these differences in greater detail. These figures show production factors, P^i , for each isotope resulting from CHIMERA simulations (solid lines, filled circles) and WH07 explosion models (dashed lines, open circles). Normalization bands are plotted for $P^{16\text{O}}$ (dashed line) within a factor of two (dotted lines). Isotopes of the same element are plotted as the same color and connected by lines.

Many of the larger differences for $A \leq 90$ are attributed to a more robust α -rich freeze-out—a direct consequence of convective instabilities which persist late into the multi-dimensional simulations. Particular isotopes affected by this enhanced α -rich freeze-out include $^{43,44}\text{Ca}$, ^{45}Sc , $^{50,52}\text{Cr}$, ^{59}Co , and $^{58,60,61,62}\text{Ni}$ (Table III in Woosley et al., 2002). For several of these isotopes, this alone directly addresses an underproduction in WH07 models relative to solar values. It can also lead to an overproduction of the Ni isotopes in the B-Series models, particularly in B12-WH07. In the case of ^{44}Ca , the seeming underproduction in both the B-Series and WH07 models is simply the consequence of a long half-life of ≈ 60 yr for its parent isotope (^{44}Ti).

The processes of dispersion of the products of hydrostatic carbon-, oxygen-, neon-, and silicon-burning as well as those of explosive oxygen-, neon-, and silicon-burning are also sensitive to the asymmetric shock and the details of the convective behavior (i.e. mass-cut). These are the other primary processes responsible for notable differences in the yields of intermediate-mass elements. The details of which products are affected is highly-dependent on the initial composition of matter which encounters the shock after it has weakened sufficiently to allow explosive burning, as opposed to dissociation ($T_{\text{post-shock}} \lesssim 6$ GK), but before it has weakened to the point where nuclear burning ceases altogether ($T_{\text{post-shock}} \lesssim 2$ GK). Consider the following examples of how this sensitivity may vary between models. In B12-WH07, the differences from WH07 are most prevalent for the explosive silicon-burning products $^{46,47,48,49}\text{Ti}$ and ^{52}Cr , though the differences in ^{52}Cr could be driven by α -rich freeze-out. In B15-WH07, the largest differences are confined to ^{28}Si , $^{32,33,34}\text{S}$,

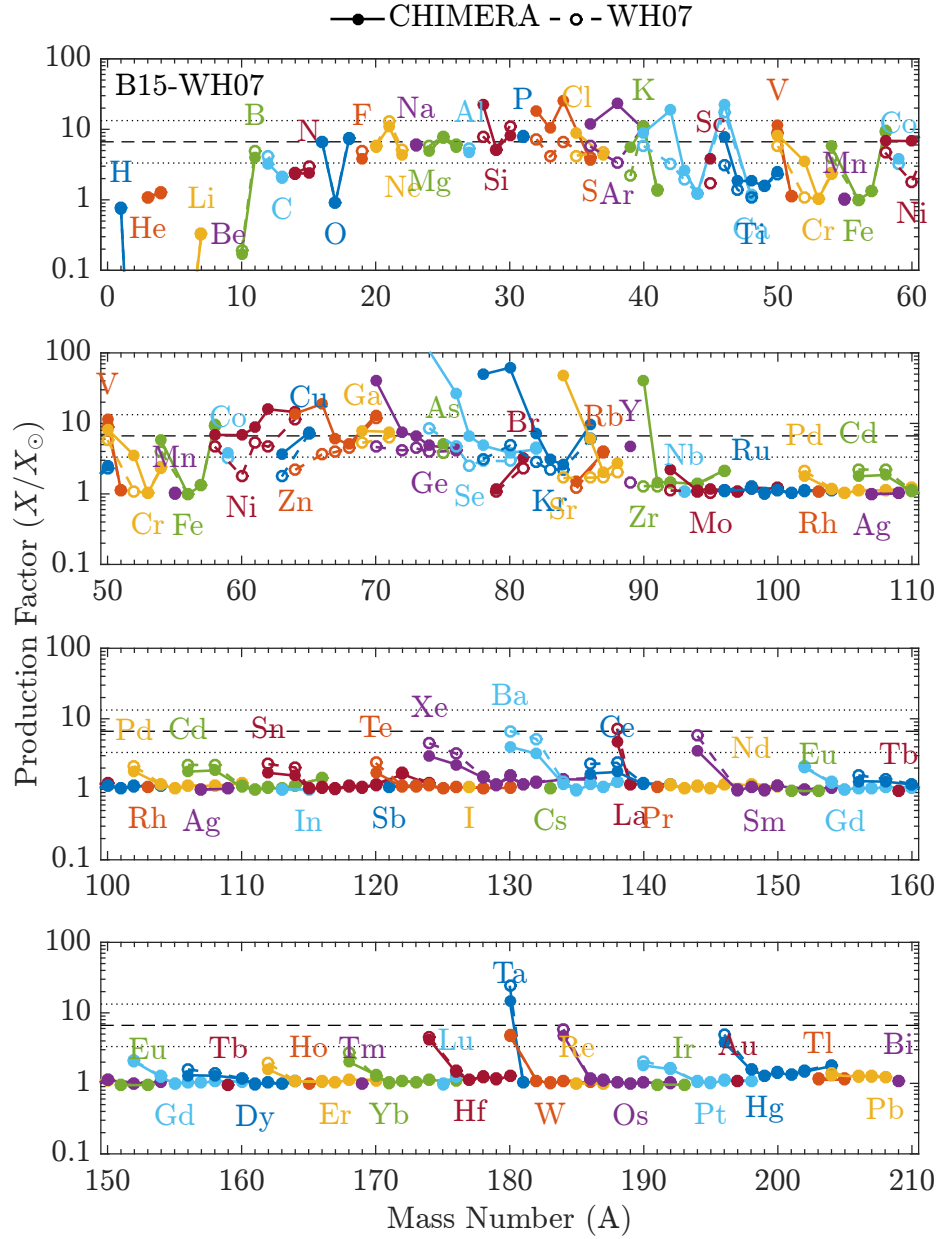


Figure 4.14 Final nucleosynthesis production factors (abundances relative to solar abundances) as a function of mass number at 1 yr after bounce for B15-WH07 (solid lines) and the parameterized 1D explosion model (dashed lines; Woosley and Heger, 2007). Isotopes of a given element are all the same color and connected by lines. Normalization bands (dotted lines) are provided using a factor of two difference in the production factor of ^{16}O .

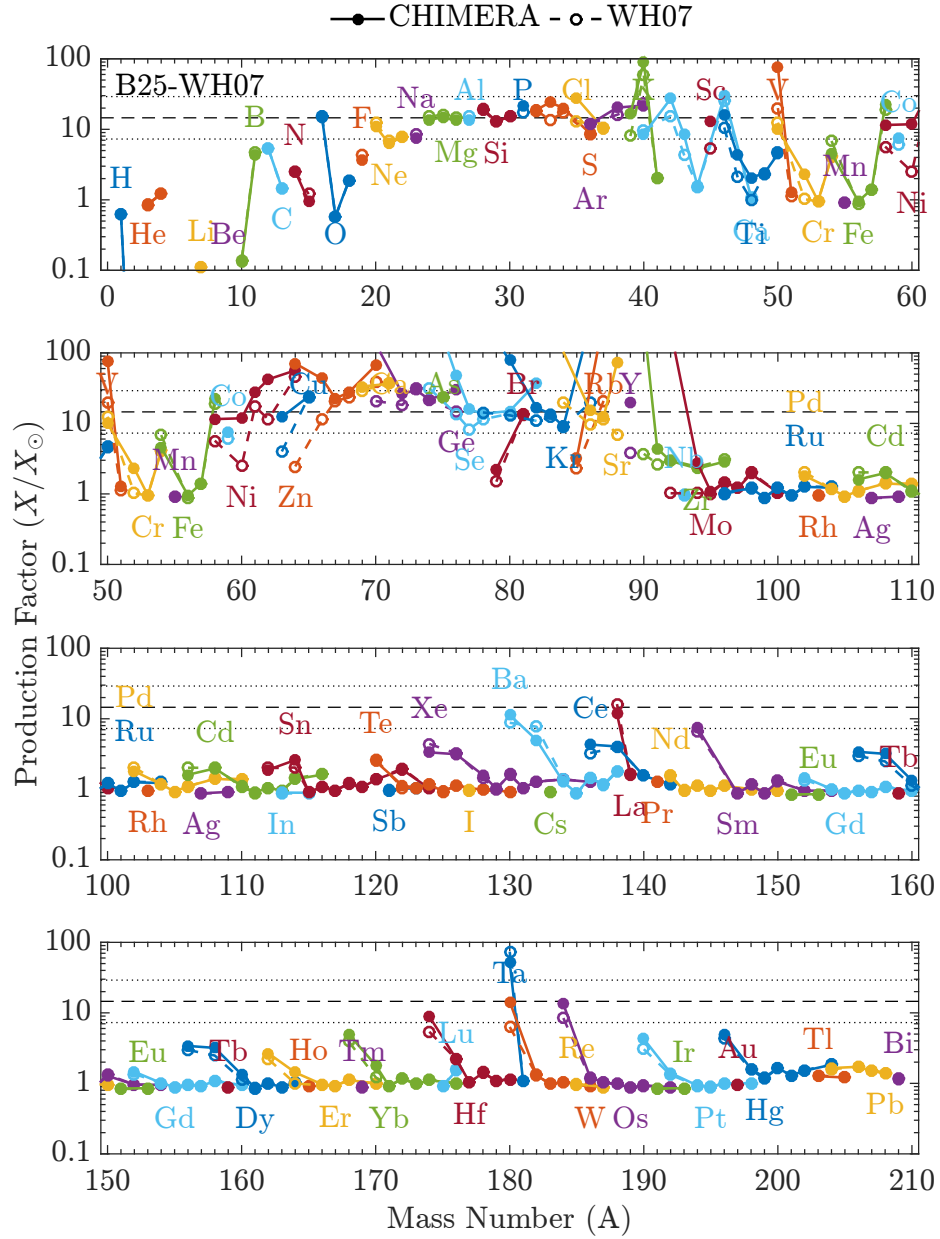


Figure 4.16 Final nucleosynthesis production factors (abundances relative to solar abundances) as a function of mass number at 1 yr after bounce for B25-WH07 (solid lines) and the parameterized 1D explosion model (dashed lines; Woosley and Heger, 2007). Isotopes of a given element are all the same color and connected by lines. Normalization bands (dotted lines) are provided using a factor of two difference in the production factor of ^{16}O .

$^{36,38}\text{Ar}$, ^{42}Ca , and ^{46}Ti , all of which are products of explosive oxygen-burning. B20-WH07 is very similar to B15-WH07 in this regard, albeit the effects are less drastic, possibly the result of a weaker, less asymmetric explosion. The largest differences in B25-WH07 are seen in ^{35}Cl , ^{39}K , ^{42}Ca , and ^{50}V , pointing to both explosive oxygen- and neon-burning as the responsible processes.

4.2.1 Neutron-rich, α -poor ejecta

A particularly fascinating feature of the nucleosynthesis in B12-WH07 relative to that in the WH07 model is the production of the neutron-rich isotopes ^{48}Ca , ^{50}Ti , ^{54}Cr , ^{58}Fe , ^{64}Ni , ^{70}Zn , ^{76}Ge , and ^{82}Se . Given the small amounts of neutron-rich ejecta, which are poorly sampled by the tracer particles (see Figure 3.42), nucleosynthesis uncertainties for these species stemming from tracer particle spatial resolution are likely significant. However, the process that leads to the overproduction of these isotopes in B12-WH07 is, nonetheless, intriguing. Any production of these isotopes could potentially address a long-standing mystery. The astrophysical sites responsible for the observed solar abundances of these isotopes has remained elusive despite more than three decades of investigation (see, e.g., [Hartmann et al., 1985](#); [Meyer et al., 1996](#), and references therein, for more details on the historical background). As a doubly magic stable nuclei ($A = 48, Z = 20$), ^{48}Ca is pivotal to this discussion due to its role as a *quasi-statistical equilibrium* (QSE) “post” for nuclei with $Z > 15$ ([Meyer et al., 1996](#)), wherein the abundances of isotopes in this “group” can be tied directly to the abundance of ^{48}Ca via local equilibrium (see, e.g., [Bodansky et al., 1968](#); [Woosley et al., 1973](#); [Hix and Thielemann, 1996](#), and references therein, for more details on QSE). [Meyer et al. \(1996\)](#) argue that production of ^{48}Ca in CCSNe is directly correlated with the photon-to-nucleon ratio, $\phi \equiv 0.34T_9^3/\rho_5$, in the neutrino-driven ejecta, where T_9 is the temperature in units of 10^9 GK and ρ_5 is the density in units of 10^5 g cm $^{-3}$. The authors conclude by placing the restriction of $\phi \lesssim 1$ for appreciable amounts of ^{48}Ca to be created and subsequently exclude CCSNe as a

production site due to high entropies ($\phi > 1$) in the innermost, neutrino-driven ejecta. [Wanajo et al. \(2013a\)](#) propose that ECSNe are, at least in part, responsible for ^{48}Ca production in ejecta with physical conditions in the transition region between α -poor QSE at low entropies ($\phi \lesssim 1$) and the more common α -rich freeze-out ($\phi \gtrsim 1$). Rare ($\approx 2\%$) varieties of Type Ia supernovae characterized by carbon deflagration at very high densities ($\rho \gtrsim 5 \times 10^9 \text{ g cm}^{-3}$) are thought to be the only other astrophysical site with the conditions necessary to produce ^{48}Ca and the other low-mass neutron-rich isotopes of Ti, Cr, and Fe ([Meyer et al., 1996](#); [Woosley, 1997](#); [Woosley et al., 2002](#)). However, the nucleosynthesis results in B12-WH07 suggest that a small fraction of very neutron-rich matter ($Y_{\text{e,NSE}} \approx 0.42$), or moderately neutron-rich ($Y_{\text{e,NSE}} \approx 0.45$) in the case of ^{54}Cr , in some low-mass Fe-core CCSNe may encounter such conditions in the early ejecta. While no tracer particles in B15-WH07, B20-WH07, or B25-WH07 sample these conditions, there is evidence for such n-rich matter in these models as well.

Close inspection reveals that ^{48}Ca production in B12-WH07 is isolated to three tracer particles with $P^{48\text{Ca}} > 1$: B12-WH07-P1247, B12-WH07-P1485, and B12-WH07-P1616. The thermodynamic histories (T , ρ , Y_{e} , and ϕ_{ν}) of these tracer particles are shown in Figure 4.17. Unlike B12-WH07-P1247 and B12-WH07-P1485, which exhibit the low-entropy, neutron-rich conditions necessary to preserve appreciable amounts of ^{48}Ca produced in NSE, B12-WH07-P1616 is initially characterized by high-entropies typically encountered in α -rich freeze-out and is proton-rich, far from the low Y_{e} necessary to make ^{48}Ca in NSE. At later times, B12-WH07-P1616 decreases in Y_{e} and, in so doing, produces modest amounts of ^{48}Ca . Fortunately, as shown in Figure 4.18, the contributions from this particle are small and the bulk of the ^{48}Ca is produced in the other two particles in a manner consistent with expectations. B12-WH07-P1485 represents the largest contribution to ^{48}Ca , the production of which occurs in NSE with $Y_{\text{e,NSE}} \approx 0.4$, but survives QSE due to a lack of α -particles which would otherwise destroy ^{48}Ca in the process of creating heavier nuclei via reactions like $^{48}\text{Ca}(\alpha, n)^{51}\text{Ti}$. Later in its thermodynamic trajectory, B12-WH07-P1485 slowly

trends upward in Y_e and, in so doing, produces appreciable ^{54}Cr as well. In the case of B12-WH07-P1247, $Y_{e,\text{NSE}} \approx 0.44$ favors the production of ^{54}Cr over ^{48}Ca , but, nonetheless, the low-entropy environment preserves significant amounts of ^{48}Ca throughout its evolution.

This new result merits further studies before any definitive conclusions can be made. The restriction to axisymmetry and limited tracer particle resolution in the B-Series models, as well as other approximations made in CHIMERA (e.g. GR, MGFLD, grid resolution), could be important in determining the quantity of matter that experiences the conditions necessary for such nucleosynthetic processes, particularly in the innermost ejecta. Still, these findings suggest that the community should not yet exclude CCSNe as a possible astrophysical site for the production of these neutron-rich isotopes.

In B12-WH07, increased production of ^{70}Zn , ^{76}Ge , and ^{82}Se relative to what is seen in the WH07 is attributed to a neutron-rich, α -poor QSE. Many of the other isotopes in this mass range are products of a weak s -process (e.g. ^{70}Ge , ^{75}As , $^{79,81}\text{Br}$, $^{80,82}\text{Kr}$, and $^{86,87}\text{Sr}$) and are first produced in the stages of hydrostatic oxygen and carbon shell-burning. In some cases, however, these s -process nuclei are completely destroyed by the passing shock before being recreated (e.g., [Tur et al., 2009](#)), making their production quite sensitive to the conditions in the expanding hot bubble as matter freezes out from QSE.

4.2.2 Light element primary process

In each of the B-Series models, we also see a consistent increase in the production of several p-nuclei (e.g. ^{88}Sr , ^{90}Zr , ^{92}Mo , ...) which had been consistently under-produced by the WH07 models. The origin of these isotopes is often tied to the *lighter element primary process* (LEPP), the nature of which has yet to be determined ([Pruet et al., 2006](#)). There are several proposed scenarios for the LEPP—e.g., a weak s -process in low-metallicity, fast-rotating, massive stars ([Pignatari et al., 2008](#)), the

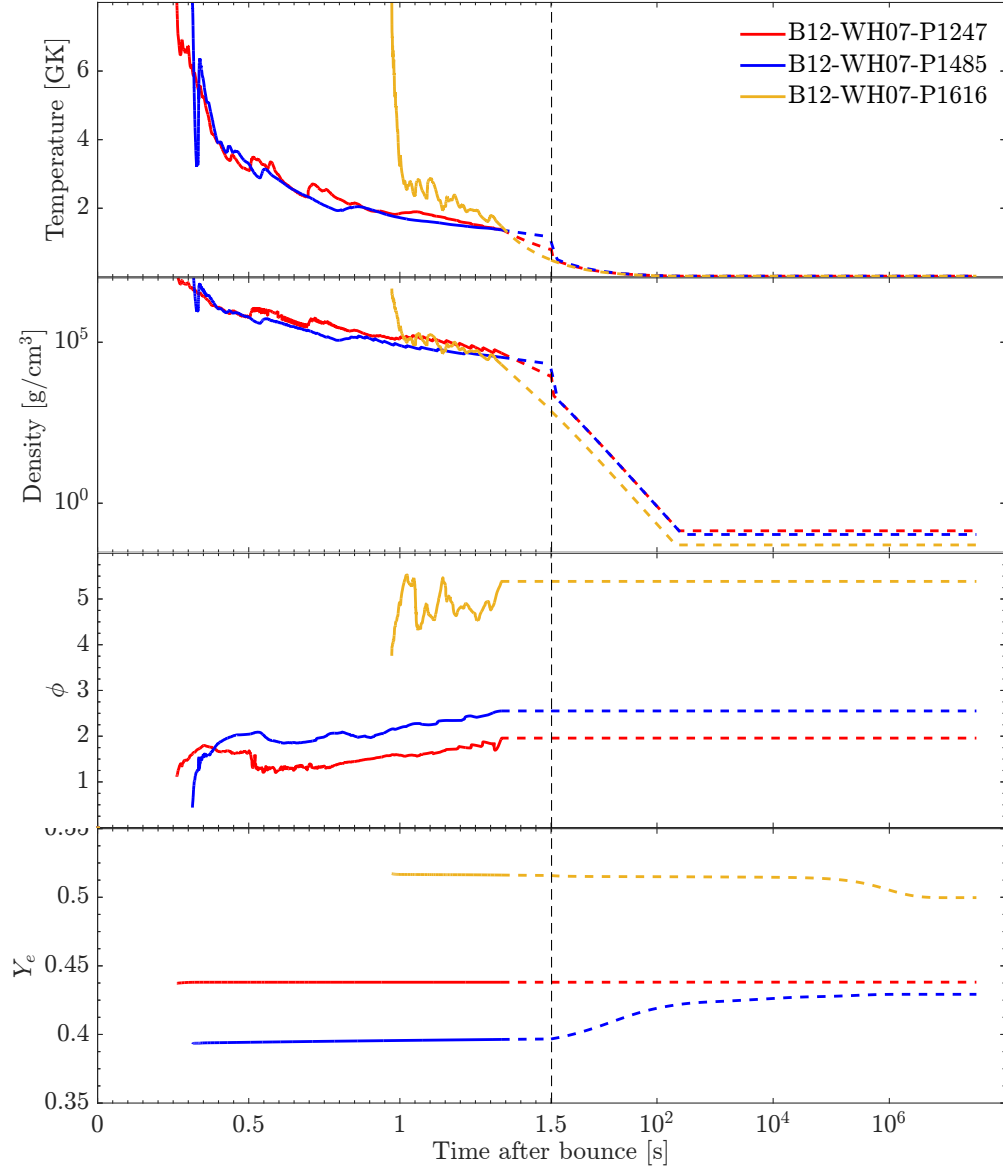


Figure 4.17 In order of top to bottom: temperature, density, photon-to-nucleon ratio, and electron fraction histories beginning at the transition out of NSE at $T = 8$ GK for the tracer particles contributing to ^{48}Ca production above solar values in B12-WH07. The dashed, colored lines signify the switch to a parameterized thermodynamic profile. The dashed, black line marks the switch to a logarithmic scale for the time axis.

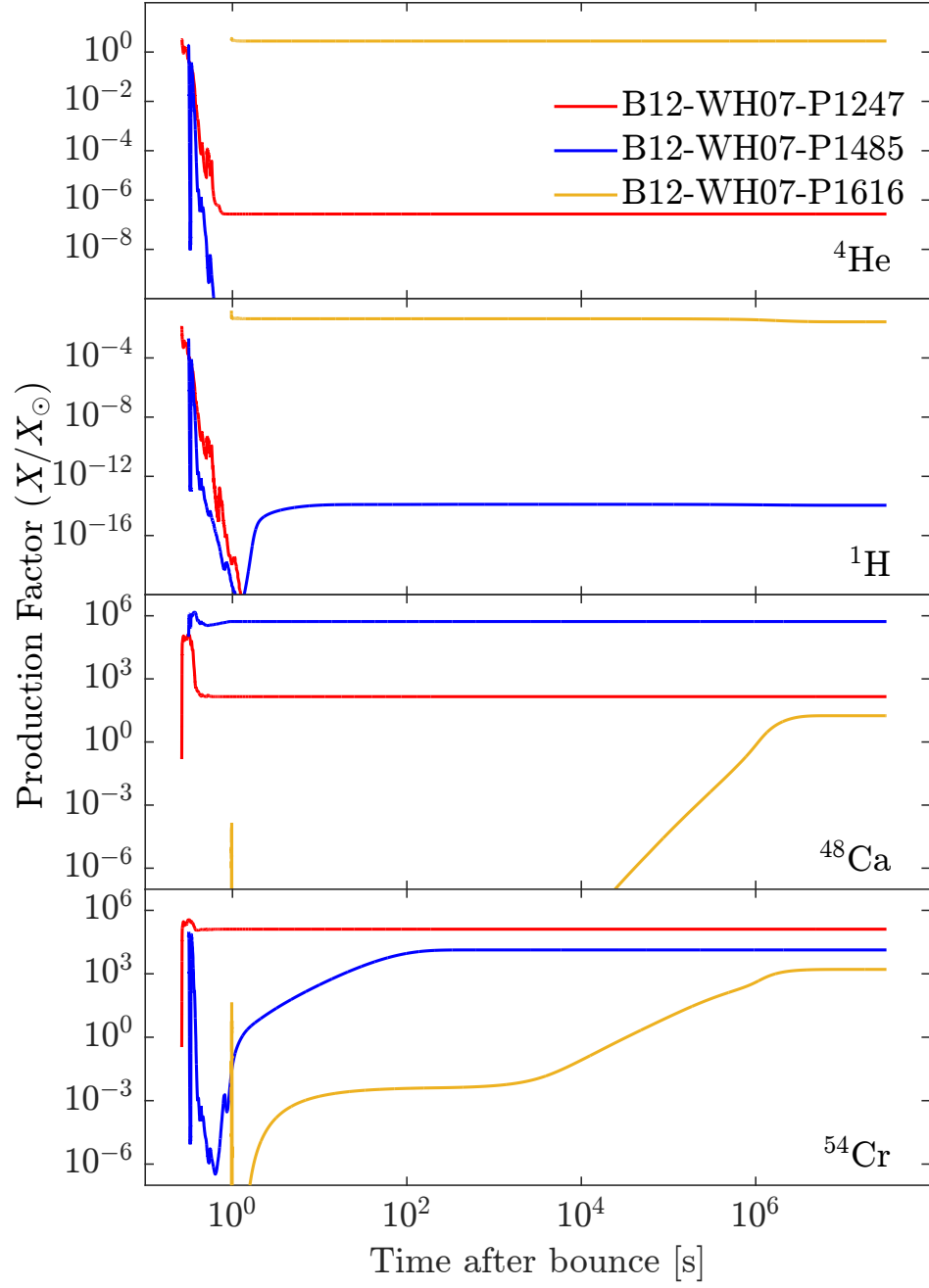


Figure 4.18 In order of top to bottom: production factors for ${}^4\text{He}$, ${}^1\text{H}$, ${}^{48}\text{Ca}$, and ${}^{54}\text{Cr}$ beginning at the transition out of NSE at $T = 8$ GK for the tracer particles contributing to ${}^{48}\text{Ca}$ production above solar values in B12-WH07.

νp -process in proton-rich neutrino-driven winds of CCSNe (Fröhlich et al., 2006a), incomplete α -rich freeze-out in high-entropy winds (HEW) from the newly-formed proto-NS (Woosley et al., 1994; Farouqi et al., 2009). In the absence of a fully developed neutrino-driven wind, the HEW scenario seems most similar to what is observed in the B-Series models, though these models do not reach entropies as large as those typically associated with the HEW. As illustrated in Figure 4.19, the production of ^{92}Mo in the B-Series models occurs in moderately neutron-rich ejecta ($0.45 \lesssim Y_{\text{e,NSE}} \lesssim 0.48$) and is confined to a narrow entropy range, the limits of which vary between models. Unlike the products of the very neutron-rich, α -poor freeze-out discussed earlier (e.g. ^{48}Ca), the process responsible for ^{92}Mo production occurs in many tracer particles.

In Figure 4.20 and Figure 4.21, we track the production of ^{92}Mo (dashed, orange line) and other related isotopes throughout freeze-out for the two particles in B12-WH07 with the largest contributions to the ejected ^{92}Mo mass (B12-WH07-P1293 and B12-WH07-P1531). As ^{92}Mo and other p-nuclei, like ^{64}Zn (solid, cyan line), ^{80}Kr (solid, pink line), ^{88}Sr (dashed, black line), and ^{90}Zr (dashed, red line), are created, products of neutron-rich NSE (e.g. ^{54}Cr ; solid, green line) are destroyed in the QSE phase due to the availability of α -particles. Once the α -reactions cease, the production shifts solely to isotopes like ^{64}Zn , ^{80}Kr , ^{90}Zr , and ^{92}Mo as species similar to ^{75}As , ^{74}Ge , ^{84}Kr , and ^{88}Sr are squeezed out by the changing QSE landscape.

4.2.3 γ -process

Through a combination of (γ, n) , (γ, p) , and/or (γ, α) photo-disintegrations, lingering s -process nuclei from hydrostatic and explosive oxygen- and neon-burning can serve as seeds for many of the p -process nuclei. This γ -process (Arnould, 1976; Woosley and Howard, 1978; Rayet et al., 1990, 1995; Rauscher et al., 2002) accounts for many of the neutron-deficient isotopes for $A > 90$ (namely $^{112,114}\text{Sn}$, $^{124,126}\text{Xe}$, $^{130,132}\text{Ba}$, $^{136,138}\text{Ce}$, ^{138}La , ^{144}Sm , ^{168}Yb , ^{174}Hf , ^{180}Ta , ^{180}W , ^{184}Os , and ^{196}Hg), the production of

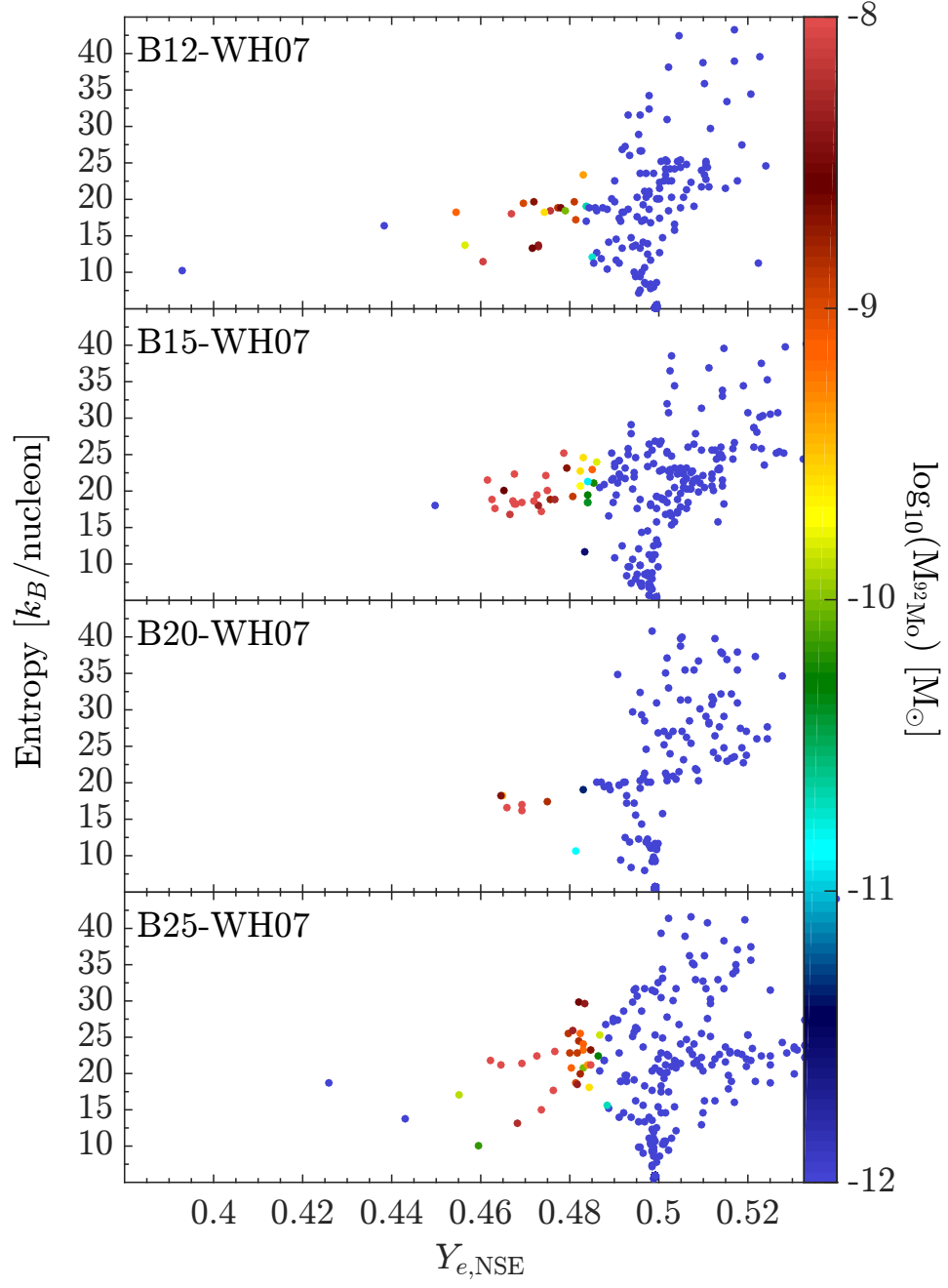


Figure 4.19 Tracer particles in $\mathbb{P}_+(t_f)$ for each B-Series simulation and positioned according to Y_e and entropy at the transition to nuclear burning from NSE and colored by ^{92}Mo mass at 1 yr after bounce.

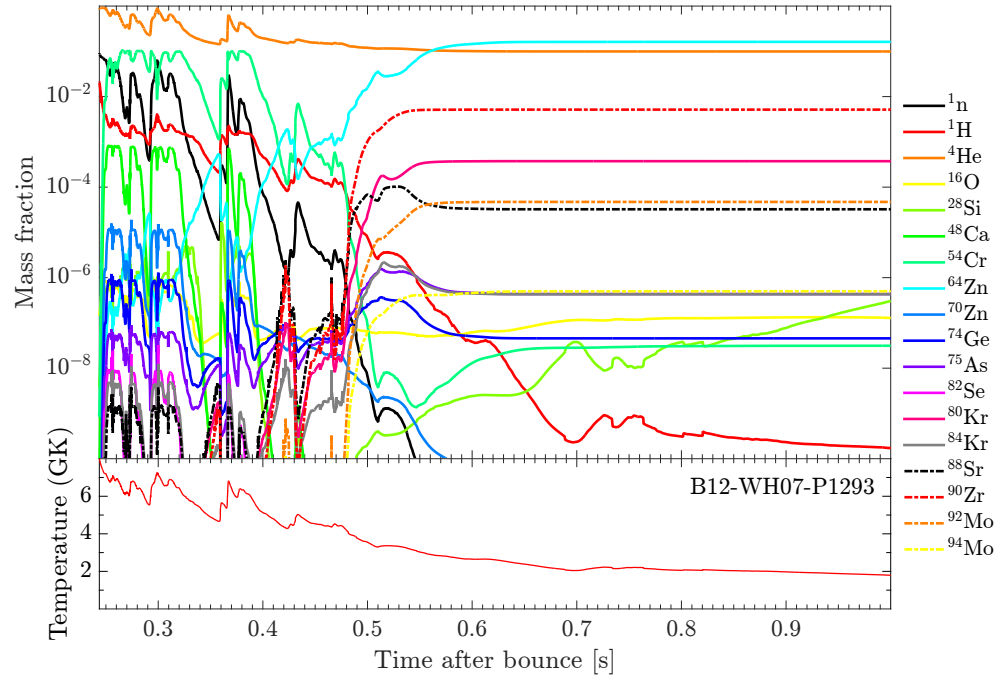


Figure 4.20 Evolution of composition (top) and temperature (bottom) for B12-WH07-P1293, a particle with a large contribution to the ejected ^{92}Mo mass (dashed, orange line).

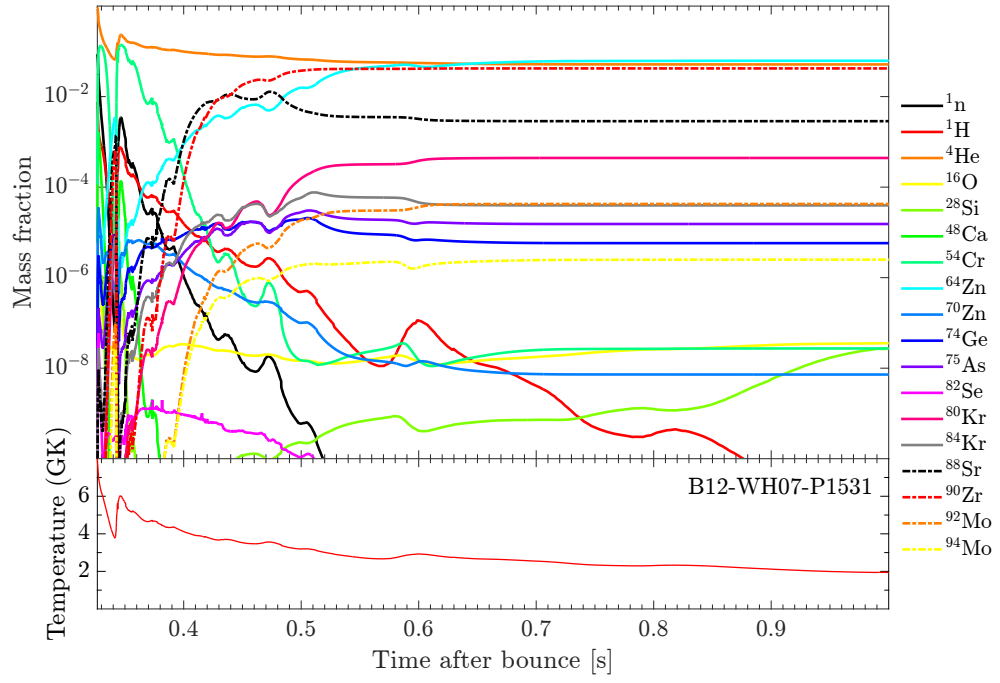


Figure 4.21 Evolution of composition (top) and temperature (bottom) for B12-WH07-P1531, a particle with a large contribution to the ejected ^{92}Mo mass (dashed, orange line).

which is significantly altered in the B-Series models, with the quantitative differences varying between progenitor mass. Alterations to the production of these heavy p -process nuclei suggests that the dynamics of the supernova explosion could account for previously noted deficiencies in 1D models.

4.2.4 r -process

Conspicuously absent in both the B-Series and WH07 models is the r -process; nevertheless, the lack of a true neutrino-driven wind leaves the production of r -process elements in these models an open question.

4.3 Comparisons to observation

Ultimately, self-consistent nucleosynthesis models need to be able to reproduce what is observed in nature. Computationally, this process is referred to as validation. However, the enormous computational challenge of evolving the nucleosynthesis of a massive star throughout the stages of stellar evolution and core-collapse demands that certain physical approximations and parameterizations be made (see Chapter 3 for more details). Observational data must then be used as a tool to constrain and refine the assumptions of the prescribed nucleosynthesis model. Also, reasonable agreement for observable isotopes gives us confidence in the yields of the remaining, unobservable nuclei. In Table 4.1, several isotopic yields from observed SN remnants (SNR) are provided from the literature. In this section, I highlight a few such comparisons and discuss the insight provided therein.

Constraining the zero-age main-sequence mass, M_{ZAMS} , of observed SNe and SN remnants is a process fraught with systematic errors and uncertainties, complicated even further by the poorly understood effects of mass-loss and binarity in stellar evolution. In the interest of providing a simple, yet informative comparison of the B-Series nucleosynthesis results with observations, we assume the progenitor stars of

Table 4.1. Measured yields of CCSNe

Measurement	$M_{\text{ej}}(^{44}\text{Ti})$ [$\times 10^{-4} M_{\odot}$]	$M_{\text{ej}}(^{56}\text{Ni})$ [$\times 10^{-2} M_{\odot}$]	$M_{\text{ej}}(^{57}\text{Ni})$ [$\times 10^{-3} M_{\odot}$]	References
Cas A				
CGRO	$\sim(1.0, 3.0)^{\text{a}}$	...	...	1
COMPTEL	$(1.3 \pm 0.25, 3.3 \pm 0.63)^{\text{b}}$	...	...	2
BeppoSAX	$1.2^{+1.3}_{-0.4}$	...	...	3
XMM-Newton	...	$>5.8^{\text{c}}$	...	4
UVOIR	...	<20	...	5
INTEGRAL	$1.6^{+0.6}_{-0.3}$	...	...	6
NuSTAR	1.25 ± 0.3	...	...	7
INTEGRAL	1.5 ± 0.4	...	...	8
SN 1987A				
UVOIR	$(0.5, 1.0, 2.0)$	6.9 ± 0.3	~ 3.3	9
Chandra	<2.0	...	...	10
HST	1.5 ± 0.5	...	...	11
INTEGRAL	3.1 ± 0.8	...	...	12
UVOIR	0.55 ± 0.17	7.1 ± 0.3	4.1 ± 1.8	13
NuSTAR	1.5 ± 0.3	...	...	14

^a $t_{1/2} = (66.6, 46.4)$ yr

^b[distance, $t_{1/2}$] = [(2.8, 3.4) kpc, (96.1, 78.2)] yr

^cAssuming iron in X-ray emitting plasma of Cas A is from ejecta and primarily composed of ^{56}Fe

References. — (1) [The et al. \(1996\)](#); (2) [Iyudin et al. \(1997\)](#); (3) [Vink et al. \(2001\)](#); (4) [Willingale et al. \(2003\)](#); (5) [Young et al. \(2006\)](#); (6) [Renaud et al. \(2006\)](#); (7) [Grefenstette et al. \(2014\)](#); (8) [Siegert et al. \(2015\)](#); (9) [Fransson and Kozma \(2002\)](#); (10) [Leising \(2006\)](#); (11) [Jerkstrand et al. \(2011\)](#); (12) [Grebenev et al. \(2012\)](#); (13) [Seitenzahl et al. \(2014\)](#); (14) [Boggs et al. \(2015\)](#);

both [Woosley and Heger \(2007\)](#) and the models used to calculate M_{ZAMS} of observed SN remnants to exhibit similar explosive nucleosynthesis signatures.

Calculations for the initial mass of SN 1987A typically involve varying merger scenarios ([Podsiadlowski, 1992](#); [Podsiadlowski et al., 1993](#)), but all produce helium core masses consistent with that of a single star model with $15^{+4}_{-1} M_{\odot}$ ([Smartt et al., 2009](#)), which we employ hereafter. Efforts to determine the initial mass for the progenitor of Cassiopeia A are similarly challenging. Now known to be a Type IIb SNe ([Krause et al., 2008](#)), constraints based on the total mass of the supernova ejecta ([Hwang and Laming, 2012](#)) and matter recently ejected by the progenitor star into the circumstellar medium ([Hwang and Laming, 2009](#); [Patnaude and Fesen, 2009](#)) agree with other Type IIb SNe of initial mass in the range $(15 \pm 3) M_{\odot}$ ([Smartt, 2015](#)). However, contrary to other Type IIb SNe for which a companion star has been observed (e.g. SN 1993J), the lack of evidence for a companion star begs the question of how the star lost its hydrogen envelope. In the absence of further evidence, we take the progenitor of Cassiopeia A to be that of a $15\text{--}25 M_{\odot}$ star that loses its envelope via binary interaction ([Young et al., 2006](#)).

4.3.1 ^{56}Ni

Through the decay-chain of $^{56}\text{Ni} \rightarrow ^{56}\text{Co} \rightarrow ^{56}\text{Fe}$ with half-lives of 6.1 days and 77.3 days, respectively, ^{56}Ni is largely responsible for the observed light-curves of CCSNe and is strongly correlated with the explosion energy ([Hamuy, 2003](#)), making it a key, first-order target for both nucleosynthesis and explosion models. Indeed, ^{56}Ni observations of SN 1987A have long been used to tune 1D explosion models (e.g., [Woosley et al., 2002](#); [Woosley and Heger, 2007](#); [Perego et al., 2015](#)).

Bolometric light-curve analysis from SN 1987A UVOIR observations at 1,854 days reveal an ejected ^{56}Ni mass of $(6.9 \pm 0.3) \times 10^{-2} M_{\odot}$ ([Fransson and Kozma, 2002](#)).

By scaling time-extended B-, V-, and R-band data and performing a non-linear, non-weighted least-squares fit to the composite light-curve, [Seitenzahl et al. \(2014\)](#) obtain a similar value of $(7.1 \pm 0.3) \times 10^{-2} M_{\odot}$.

Constraining the ejected ^{56}Ni mass of Cassiopeia A is somewhat more challenging and relies on constructing limits from indirect evidence. Following the work of [Young et al. \(2006\)](#), the comparisons which follow assume a lower limit to the ^{56}Ni mass of $5.8 \times 10^{-2} M_{\odot}$, obtained by assuming that the iron in observations of the X-ray emitting plasma of Cassiopeia A originated from the supernova ejecta and is primarily composed of ^{56}Fe ([Willingale et al., 2003](#)). An upper limit of $0.2 M_{\odot}$ can be constructed from light-curve models by constraining the total ejecta mass and using a parameterization which errs on the side of larger ^{56}Ni mass ([Young et al., 2006](#)).

Much work has been done in modeling the late-time velocity and spatial distributions of ^{56}Ni as ejecta propagates through the stellar envelope towards homologous expansion and is subjected to hydrodynamical instabilities and the reverse shock (e.g., [Hammer et al., 2010](#); [Wongwathanarat et al., 2015b](#), and references therein). The distribution of ^{56}Ni in the B-Series models is contingent on further hydrodynamic evolution; thus, it is left as the subject of future study. For now, only the total ^{56}Ni yield of the ejecta is considered.

The synthesis of ^{56}Ni via complete silicon-burning, resulting in NSE, is the dominant nuclear process in the early stages of the explosion development ($t_{\text{pb}} \lesssim 500$ ms). Its production can continue into later epochs via incomplete explosive silicon-burning for $T \gtrsim 4$ GK in the passing shock and hot bubble but is essentially complete by t_{f} in each of the B-Series models. In earlier work, $M_{\text{C}}^{56\text{Ni}}$, the mass of ^{56}Ni synthesized via the *in situ* α -network in zones for which $\varepsilon_{\text{tot}} > 0$, is compared with well-observed supernova remnants for each model (see Figure 27 in [Bruenn et al., 2014](#)). As previously illustrated in Figure 3.43, ^{56}Ni production is reasonably well-represented by the α -network, but the *in situ* nucleosynthesis can mis-estimate the total ^{56}Ni mass due to an unphysical assumption of NSE in CHIMERA. The amount of ejected ^{56}Ni reported by [Bruenn et al. \(2014\)](#) is consistently and moderately

under-produced relative to observations, albeit within observational uncertainties. In Figure 4.22, ^{56}Ni masses from the 1D WH07 models (red squares) and B-Series *in situ* calculations (blue diamonds) are compared against post-processing calculations performed with the full reaction network (Section 2.2.5) and initiated from an NSE transition temperature $T_{\text{NSE}} = 8$ GK (black circles). The error bars on the *in situ* results are merely a representation of uncertainty stemming from identifying the ejecta (Section 3.1.1), with the lower limit the result of applying the additional constraint $v_r > 0$ in calculating the ejected ^{56}Ni mass. For the post-processed results, a correction factor from spatial resolution considerations, $f_{\Delta\mathbf{r}}^{56\text{Ni}} = 10^{\delta_{\Delta\mathbf{r}}^{56\text{Ni}}}$, is also applied, where it is assumed that changes in network size will have negligible impact on the values of $\delta_{\Delta\mathbf{r}}^i$ (see Section 3.1.4 for details on the estimation of $\delta_{\Delta\mathbf{r}}^i$ and Table 3.1 for values). However, the post-processed results suggest that the previously inferred ^{56}Ni masses in Bruenn et al. (2014) may be underestimated by as much as $\approx 20\%$, bringing them in better agreement with observations. With the possible exception of B15-WH07, there is a tendency for the B-Series models to under-produce ^{56}Ni relative to the parameterized explosion models of Woosley and Heger (2007), a feature that is consistent with explosion energies in the B-Series models below those of the WH07 models, which are fixed at 1.2 B and possibly overdriven.

4.3.2 ^{44}Ti

Recent high-energy X-ray and γ -ray observations of the radioactive decay-chain $^{44}\text{Ti} \rightarrow ^{44}\text{Sc} \rightarrow ^{44}\text{Ca}$ provide an unparalleled glimpse into the otherwise hidden central engine of CCSNe (see, e.g., Grefenstette et al., 2014; Boggs et al., 2015). Much like ^{56}Ni , ^{44}Ti measurements provide powerful constraints on CCSN models. To date, there have only been two measurements of ^{44}Ti in definitive core-collapse remnants (SN 1987A and Cassiopeia A).

The most recent spectroscopic observations of SN 1987A by the Nuclear Spectroscopic Telescope Array (NuSTAR; Boggs et al., 2015) place the ^{44}Ti yield

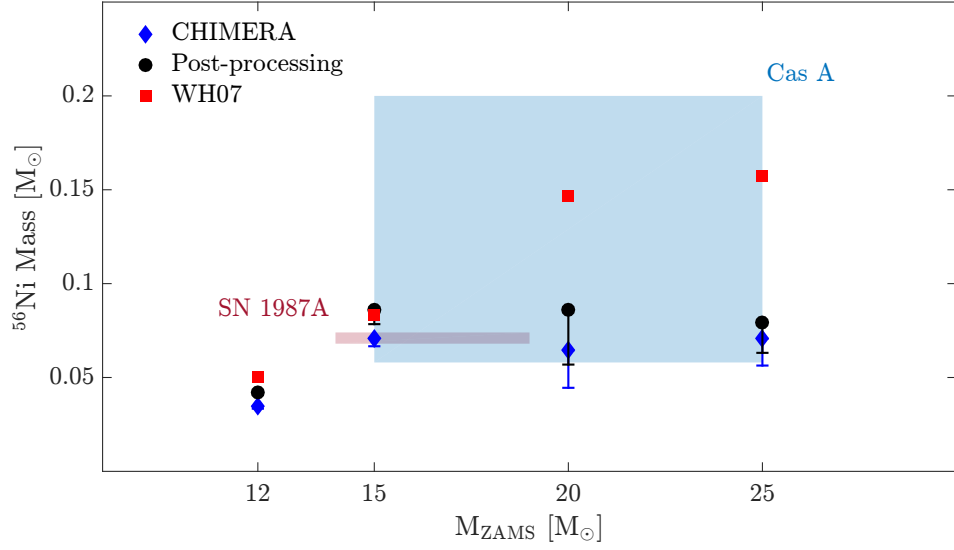


Figure 4.22 Total unbound ^{56}Ni mass at t_f for the B-Series simulations as a function of zero-age main-sequence mass (M_{ZAMS}) as calculated from the *in situ* α -network in CHIMERA (blue diamonds), post-processing with 7,852 species reaction network transitioned out of NSE at 8 GK (black circles), and original 1D WH07 explosion models (red squares). The large colored rectangles correspond to observational constraints for SN 1987A (red) and Cassiopeia A (blue). Error bars represent uncertainty pertaining to identification of the ejected matter.

at $(1.5 \pm 0.3) \times 10^{-4} M_{\odot}$, which is inconsistent with previous measurements by INTEGRAL of $(3.1 \pm 0.8) \times 10^{-4} M_{\odot}$ (Grebenev et al., 2012), but consistent with an upper limit of $2 \times 10^{-4} M_{\odot}$ inferred from earlier measurements by the Chandra X-ray Observatory Advanced CCD Imaging Spectrometer (ACIS; Leising, 2006).

NuSTAR observations of Cassiopeia A (Grefenstette et al., 2014) imply a ^{44}Ti yield of $(1.25 \pm 0.3) \times 10^{-4} M_{\odot}$, consistent with prior observations by CGRO ($\sim 1.0 \times 10^{-4} M_{\odot}$; The et al., 1996), INTEGRAL ($1.6^{+0.6}_{-0.3} \times 10^{-4} M_{\odot}$; Renaud et al., 2006), COMPTEL ($(1.3 \pm 0.25) \times 10^{-4} M_{\odot}$; Iyudin et al., 1997), and BeppoSAX ($1.2^{+1.3}_{-0.4} \times 10^{-4} M_{\odot}$; Vink et al., 2001). Siegert et al. (2015) combined these results, reporting a ^{44}Ti mass of $(1.37 \pm 0.19) \times 10^{-4} M_{\odot}$ for Cassiopeia A.

Unlike ^{56}Ni , ^{44}Ti , the production of which predominately occurs in regions of α -rich freeze-out originating in the deepest layers of the ejecta, is quite sensitive to the hydrodynamic conditions of the expanding, convective hot bubble between the proto-NS and the shock. Therefore, it is not surprising that attempts to reproduce observed ^{44}Ti yields with spherically symmetric models have been largely unsuccessful (see, e.g., Perego et al., 2015, and references therein for historical discussion). In Figure 4.23, we compare ejected ^{44}Ti masses from each of the B-Series and WH07 models at 1 yr after bounce (black circles and red squares, respectively) with existing ^{44}Ti yield measurements from SN 1987A and Cassiopeia A. The error bars on the B-Series results are merely a representation of uncertainty stemming from identifying the ejecta (Section 3.1.1), with the lower limit the result of applying the additional constraint $v_r > 0$. A correction factor from tracer particle spatial resolution considerations, $f_{\Delta\mathbf{r}}^{44\text{Ti}} = 10^{\delta_{\Delta\mathbf{r}}^{44\text{Ti}}}$, is also applied, where it is assumed that changes in network size beyond the α -network species will have negligible impact on the values of $\delta_{\Delta\mathbf{r}}^i$ (see Section 3.1.4 for details on the estimation of $\delta_{\Delta\mathbf{r}}^i$ and Table 3.1 for values).

From these estimates, the B-Series models exhibit a slight overproduction of ^{44}Ti relative to observations. It is also likely susceptible to a certain amount of fallback from the reverse shock, which has not been accounted for in these models. Despite this overproduction, these axisymmetric, self-consistent ^{44}Ti mass calculations are

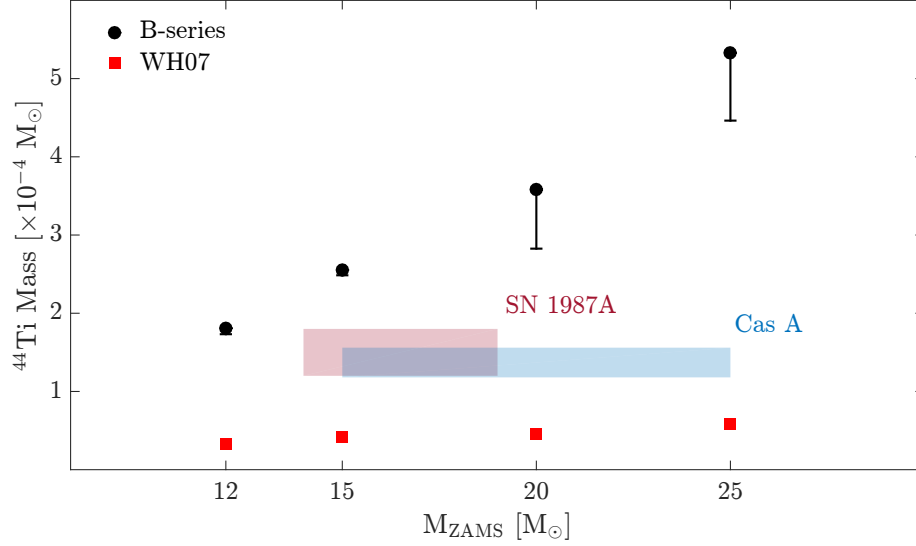


Figure 4.23 Total unbound mass of ^{44}Ti at 1 yr after bounce for the B-Series simulations (black circles) and 1D WH07 explosion models (red squares) as a function of zero-age main-sequence mass (M_{ZAMS}). Error bars represent uncertainty pertaining to identification of the ejected matter. Observational measurements of ^{44}Ti mass in Cassiopeia A (blue rectangle) and SN 1987A (red rectangle) are provided for reference.

much more optimistic than those from their spherically symmetric counterparts. It remains to be seen whether extending these models to 3D or evolving them until the explosion morphology is fully determined brings the predictions of CCSN explosion simulations into better agreement with nucleosynthesis observations.

4.3.3 Ratio of ^{44}Ti to ^{56}Ni

Given that the B-Series models may still be susceptible to a certain amount of fallback, either prompt or resulting from the reverse shock, a particularly useful quantity to compare against observations is the ratio of ^{44}Ti to ^{56}Ni in the ejecta. As shown in Figure 4.24, the radial velocity distributions of ^{44}Ti (green) and ^{56}Ni (red) in the unbound ejecta are strongly correlated. This suggests that while fallback may be a concern for properly calculating the ejected ^{44}Ti mass, for example, the $^{44}\text{Ti}/^{56}\text{Ni}$ ratio should remain relatively unaffected. These velocity distributions are noticeably

different than that of ^{28}Si (blue), which tails off at higher velocities, likely indicating an increased susceptibility for ^{28}Si to late-time fallback.

In Figure 4.25, we compare the normalized ^{44}Ti to ^{56}Ni ratio, $[\text{}^{44}\text{Ti}/\text{}^{56}\text{Ni}] \equiv [X_{\text{unb}}(^{44}\text{Ti})/X_{\text{unb}}(^{56}\text{Ni})]/[X_{\odot}(^{44}\text{Ca})/X_{\odot}(^{56}\text{Fe})]$, calculated from the B-Series (black circles) and WH07 (red squares) models, to measured values in Cassiopeia A (blue rectangle) and SN 1987A (red rectangle). The large area of the Cas A measurement is a consequence of the wide range of values permitted within the ^{56}Ni upper and lower limits. The error bars on the B-Series results are merely a representation of uncertainty stemming from identifying the ejecta. All four of the B-Series models have a much larger $[\text{}^{44}\text{Ti}/\text{}^{56}\text{Ni}]$ ratio than the WH07 explosion models, a consequence of both less ^{56}Ni (see Figure 4.22) and more ^{44}Ti (see Figure 4.23) in the ejecta. The calculated $[\text{}^{44}\text{Ti}/\text{}^{56}\text{Ni}]$ ratio in our models could be a slight overestimate, yet both B15-WH07 and B20-WH07 agree with measured values within uncertainties in the models stemming from accurately determining the multi-dimensional mass-cut. This is a promising result, especially given the very different explosion morphologies of B15-WH07 and B20-WH07 (Bruenn et al., 2014) and suggests that $[\text{}^{44}\text{Ti}/\text{}^{56}\text{Ni}]$ may not be as sensitive to the details of the explosion development as, for example, ^{44}Ti .

One of the major results from recent NuSTAR observations of Cassiopeia A is the discovery of significant amounts of ^{44}Ti interior to the reverse shock, the spatial distribution of which is not correlated with either the reverse shock-heated Fe K-shell emission or cool, dense iron visible in the optical/infrared spectral bands (Isensee et al., 2010). This suggests that any remaining iron in the ejecta exists in low-density ^{56}Ni bubbles interior to the reverse shock, an implication consistent with the inferred bubble-like interior from near-infrared observations of [S III] emission (Milisavljevic and Fesen, 2015). In Figures 4.26–4.29, the positions of tracer particles shocked by the primary shock are shown at t_f for each B-Series model. The sizes of the particles are scaled according to the mass density of ^{44}Ti and colored by the mass fraction ratio of ^{44}Ti to ^{56}Ni , which is responsible for the bulk of the iron production via decay to ^{56}Fe . While these models are much too early in the development of the explosion to make

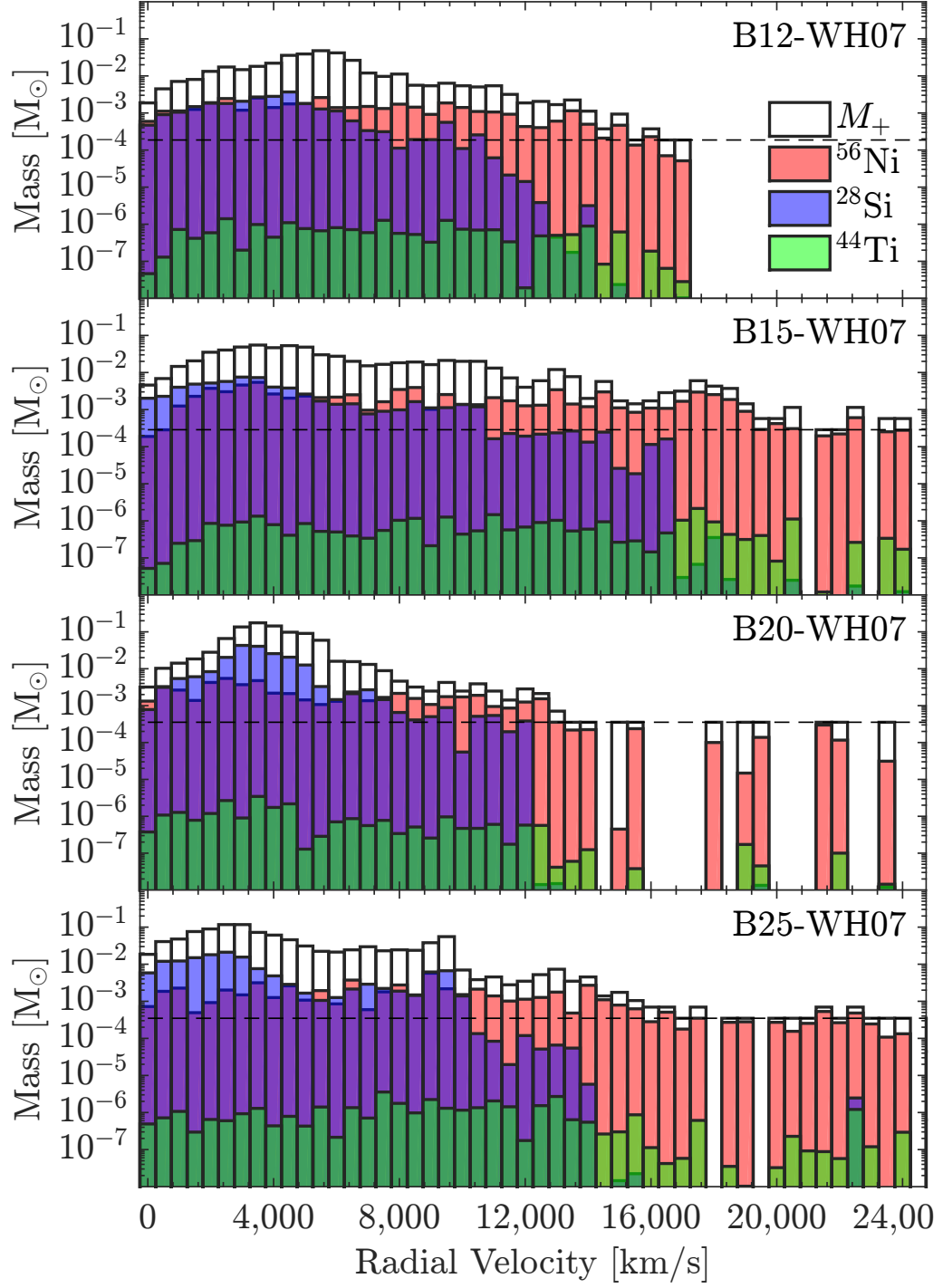


Figure 4.24 B-Series radial velocity distributions of ²⁸Si (blue), ⁴⁴Ti (green), and ⁵⁶Ni (red) in the unbound ejecta mass M_+ (white) at 100 s after bounce. The mass represented by one Lagrangian tracer particle is given by the dashed line.

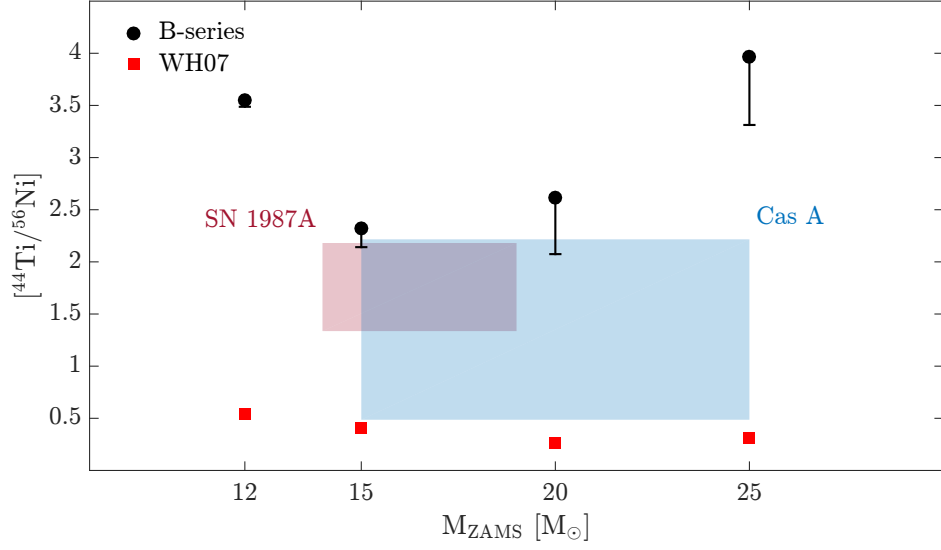


Figure 4.25 $^{44}\text{Ti}/^{56}\text{Ni}$ ratio in ejected matter and normalized to the solar abundance ratio of the decay products $^{44}\text{Ca}/^{56}\text{Fe}$ at 1 yr after bounce for the B-Series simulations (black circles) and 1D WH07 explosion models (red squares) as a function of zero-age main-sequence mass (M_{ZAMS}). Error bars represent uncertainty pertaining to identification of the ejected matter. Observational measurements of the $[^{44}\text{Ti}/^{56}\text{Ni}]$ ratio in Cassiopeia A (blue rectangle) and SN 1987A (red rectangle) are provided for reference.

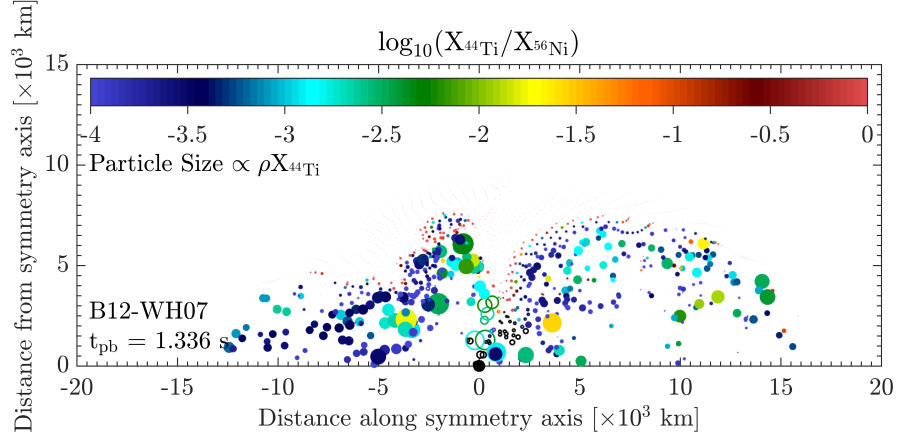


Figure 4.26 B12-WH07 shocked tracer particles in $\mathbb{P}_+(t_f)$ (solid, colored circles), $\mathbb{P}_-(t_f)$ (open, colored circles), $\mathbb{P}_{\text{bound}}(t_f)$ (open, black circles), and those located in the proto-NS (solid, black circles) at t_f , placed at their locations at t_f and sized in proportion to the mass density of ^{44}Ti at $t_{\text{pb}} = 1$ yr. Particles in $\mathbb{P}_{\text{umb}}$ are colored by the mass fraction ratio of ^{44}Ti to ^{56}Ni at $t_{\text{pb}} = 1$ yr on a log-scale.

definitive statements about the spatial distribution of ^{44}Ti , there are variations in the ratio $^{44}\text{Ti}/^{56}\text{Ni}$ as large as 2–3 orders of magnitude at different regions in the star. This ratio will remain roughly unchanged as the model continues to evolve, since the production of both of these isotopes has ceased. Particles with large ^{44}Ti abundances tend to be located in the expanding hot bubble behind the shock. Regions with the largest ^{44}Ti -to- ^{56}Ni ratio are confined to cut-off downflow boundaries and episodic high-entropy winds coming off of the proto-NS. In all of the models, the ^{44}Ti -to- ^{56}Ni ratio is $\lesssim 0.1$ for any tracer particle with significant ^{44}Ti mass, suggesting that the observed lack of correlation in the spatial distributions is a consequence of “hidden” iron, which will become visible as it is heated by the reverse shock. The development of nickel bullets and/or “bubbles” (Li et al., 1993) remains an open question for these models, and will need to be addressed in future multi-dimensional hydrodynamics simulations which extend the evolution through the stellar envelope.

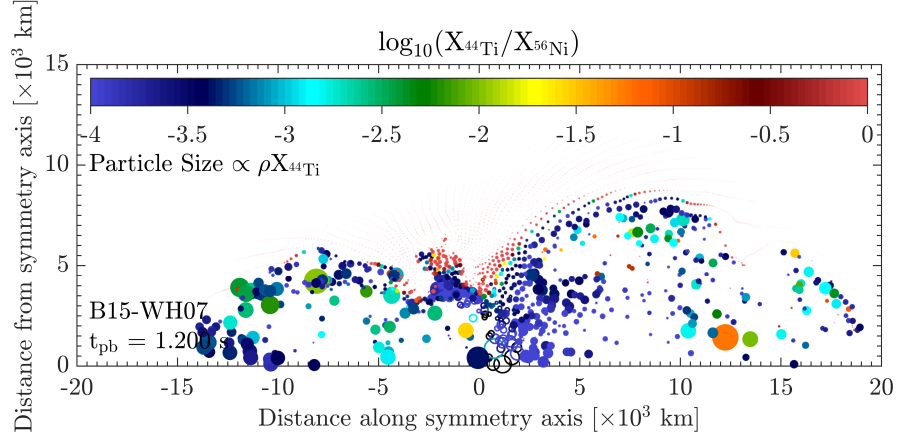


Figure 4.27 B15-WH07 shocked tracer particles in $\mathbb{P}_+(t_f)$ (solid, colored circles), $\mathbb{P}_-(t_f)$ (open, colored circles), $\mathbb{P}_{\text{bound}}(t_f)$ (open, black circles), and those located in the proto-NS (solid, black circles) at t_f , placed at their locations at t_f and sized in proportion to the mass density of ^{44}Ti at $t_{\text{pb}} = 1$ yr. Particles in $\mathbb{P}_{\text{unb}}$ are colored by the mass fraction ratio of ^{44}Ti to ^{56}Ni at $t_{\text{pb}} = 1$ yr on a log-scale.

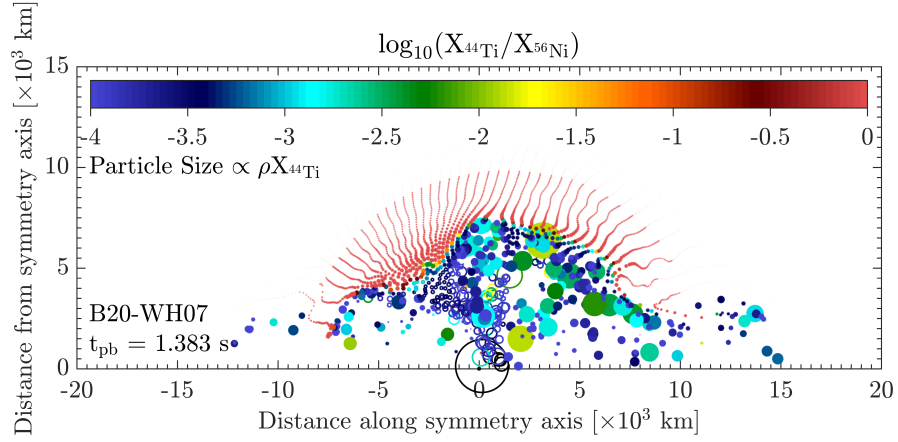


Figure 4.28 B20-WH07 shocked tracer particles in $\mathbb{P}_+(t_f)$ (solid, colored circles), $\mathbb{P}_-(t_f)$ (open, colored circles), $\mathbb{P}_{\text{bound}}(t_f)$ (open, black circles), and those located in the proto-NS (solid, black circles) at t_f , placed at their locations at t_f and sized in proportion to the mass density of ^{44}Ti at $t_{\text{pb}} = 1$ yr. Particles in $\mathbb{P}_{\text{unb}}$ are colored by the mass fraction ratio of ^{44}Ti to ^{56}Ni at $t_{\text{pb}} = 1$ yr on a log-scale.

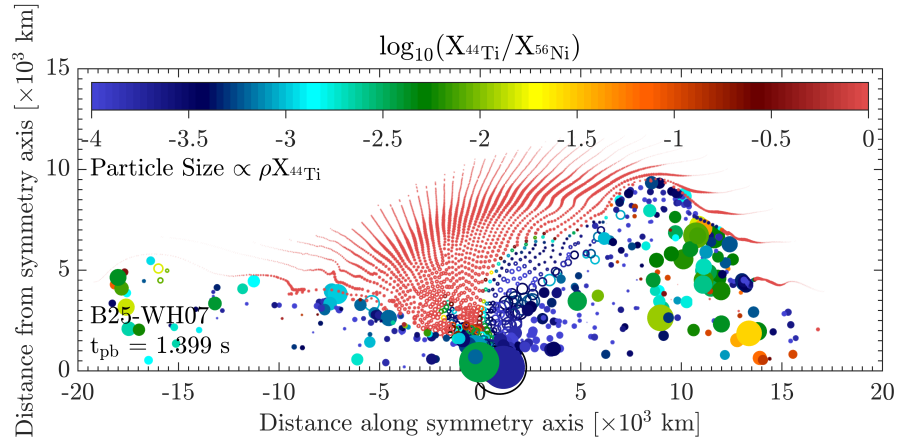


Figure 4.29 B25-WH07 shocked tracer particles in $\mathbb{P}_+(t_f)$ (solid, colored circles), $\mathbb{P}_-(t_f)$ (open, colored circles), $\mathbb{P}_{\text{bound}}(t_f)$ (open, black circles), and those located in the proto-NS (solid, black circles) at t_f , placed at their locations at t_f and sized in proportion to the mass density of ^{44}Ti at $t_{\text{pb}} = 1$ yr. Particles in $\mathbb{P}_{\text{unb}}$ are colored by the mass fraction ratio of ^{44}Ti to ^{56}Ni at $t_{\text{pb}} = 1$ yr on a log-scale.

Chapter 5

Improvements to Chimera

5.1 Nuclear kinetics

The fully implicit nature of XNet, our nucleosynthesis code, necessitates the choice of a suitable integration scheme. Previous work (Thielemann, 1993) has shown the simple first-order backward Euler method to be very efficient in advancing nuclear abundances within the constraints of the CCSN problem. With this scheme, nuclear abundances, $\vec{Y}$, are evolved by some change, $\Delta\vec{Y}$, of the system over a timestep, $\Delta t = t^{(n+1)} - t^{(n)}$, according to

$$\vec{Y}^{(n+1)} = \vec{Y}^{(n)} + \Delta\vec{Y}. \quad (5.1)$$

This is done using the Newton-Raphson method, based on the Taylor series expansion of $\vec{Y}^{(n+1)} = \vec{Y}^{(n)} + f(\vec{Y}^{(n+1)})\Delta t$, where

$$\begin{aligned}
f(Y_i^{(n+1)}) &\equiv \frac{\partial Y_i^{(n+1)}}{\partial t} \\
&= \sum_j \mathcal{N}_j^i \lambda_j Y_j^{(n+1)} \\
&\quad + \sum_{j,k} \mathcal{N}_{j,k}^i \rho N_A \langle j, k \rangle Y_j^{(n+1)} Y_k^{(n+1)} \\
&\quad + \sum_{j,k,l} \mathcal{N}_{j,k,l}^i \rho^2 N_A^2 \langle j, k, l \rangle Y_j^{(n+1)} Y_k^{(n+1)} Y_l^{(n+1)}.
\end{aligned} \tag{5.2}$$

N_A is Avogadro's number, λ_j is the decay-rate, and $\langle j, k \rangle$ and $\langle j, k, l \rangle$ are cross-sections for two- and three-body reactions, respectively. $\mathcal{N}_j^i = N_i$, $\mathcal{N}_{j,k}^i = N_i / \prod_{m=1}^{n_{j,k}} |N_m|$, and $\mathcal{N}_{j,k,l}^i = N_i / \prod_{m=1}^{n_{j,k,l}} |N_m|$ provide for proper accounting of numbers of nuclei, where N_i specify how many particles of species i are created or destroyed in a reaction, and $n_{j,k}$ and $n_{j,k,l}$ denote the number of different species destroyed in the reactions. This reduces to iteratively solving a linear system ($\mathbf{A}\vec{x} = \vec{b}$) in the form

$$\left(\frac{\mathbf{I}}{\Delta t} - \mathbf{J} \right) \Delta \vec{Y}^{[m]} = - \frac{(\vec{Y}^{(n+1),[m]} - \vec{Y}^{(n+1),[0]})}{\Delta t} \tag{5.3}$$

$$\begin{aligned}
&\quad + f(\vec{Y}^{(n+1),[m]}); \\
\vec{Y}^{(n+1),[m+1]} &= \vec{Y}^{(n+1),[m]} + \Delta \vec{Y}^{[m]},
\end{aligned} \tag{5.4}$$

for $m = 0, 1, \dots$, with a suitable initial guess $\vec{Y}^{(n+1),[0]}$, where $\mathbf{J} = \partial f(\vec{Y}^{(n+1),[m]}) / \partial \vec{Y}^{(n+1),[m]}$ is the Jacobian of $f(\vec{Y}^{(n+1),[m]})$ and $\mathbf{I}$ is the identity matrix. Iteration continues until the solution converges according to nucleon number conservation or a predefined convergence criteria, $\|\vec{E}\|_1 < \varepsilon$, is satisfied. In all calculations presented herein, we

use a tolerance $\varepsilon = 1 \times 10^{-4}$ and define

$$E_i \equiv \begin{cases} 0 & \text{if } Y_i^{[m]} < Y_{\min}; \\ |\Delta Y_i^{[m]}|/Y_i^{[m]} & \text{otherwise,} \end{cases} \quad (5.5)$$

where $Y_{\min} = 1 \times 10^{-25}$.

Each Newton-Raphson iteration requires computing the full set of abundance derivatives, calculating all reaction rates, evaluating the Jacobian, evaluating the right-hand side, and then performing one LU decomposition ($\sim \frac{2}{3}N^3$ floating-point operations) and one backsubstitution ($\sim N^2$ floating-point operations). Extremely large variations in timescales between strong, electromagnetic, and weak reactions make nuclear reaction networks extraordinarily stiff (Hix and Meyer, 2006). The extreme degree of stiffness in astrophysical nuclear reaction networks has thus far limited the use of more sophisticated methods developed for solving stiff equations in chemical kinetics. Complicating the computation itself is indirect memory addressing and loop carried dependencies associated with building the Jacobian. Double-precision floating-point arithmetic is required for the calculation, as the approach to equilibrium at various stages of the burning can lead to the near-cancellation of large reaction fluxes.

5.1.1 Improving post-processing nucleosynthesis

A major limitation of post-processing nucleosynthesis is inherent in the accuracy of the rate of nuclear energy released by the smaller *in situ* reaction network. Since the nucleosynthesis depends on the thermodynamic conditions and, consequently, nuclear energy generation, a feedback exists that cannot be captured with post-processing, significantly affecting, for example, the abundances of species such as ^{44}Ti , ^{57}Fe , ^{58}Ni , and ^{60}Zn produced in the α -rich freeze-out (Woosley and Weaver, 1995). As a result of this feedback, Magkotsios et al. (2010) find strong differences in the α -richness

between supernova models, fundamentally altering the conditions of α -rich freeze-out which are also subject to neutronization in the bath of neutrinos near the core. Calculations which cannot track neutronization in the composition (e.g. α -network) are intrinsically limited in their ability to calculate realistic nucleosynthesis. This deficiency cannot be completely redressed via post-processing with larger networks. Furthermore, post-processing is not capable of capturing the observed mixing of the chemical elements due to the lack of coupling of abundances to the hydrodynamics. Thanks to prior work (Chertkow, 2012), CHIMERA can utilize an arbitrarily chosen nuclear reaction network. The SN150-network described in Section 2.2.5 is the next logical step for *in situ* nucleosynthesis calculations.

With the computational cost of evolving the network using a dense matrix solution being $\mathcal{O}(N^3)$, the advancement from an α -network to the more realistic SN150-network makes the nucleosynthesis computation more expensive than the neutrino transport that heretofore dominated the numerical cost. Initial analysis reveals that increasing the number of species from 14 to 150 more than doubles the cost of a CHIMERA simulation. To prevent the computational cost from limiting the scope of our studies, we have incorporated recent advancements in programming interfaces and computational architectures—specifically, shared-memory parallelism (OpenMP) and general purpose graphical processing units (GPGPUs) (e.g. CUDA, OpenACC, ...).

5.1.2 Reaction kinetics on the GPU in Chimera

The evolution of the nuclear kinetics for one global timestep on a single radial ray in CHIMERA can be modeled as such:

1. Choose a zone in the radial ray over which to subcycle, if necessary.
2. Calculate the reaction rates from the REACLIB database.
3. Determine the necessary network timestep.

4. Build the left- and right-hand sides of Equation 5.3.
5. Perform a single LU decomposition (DGETRF) and triangular back-substitution (DGETRS).
6. Update the nuclear abundances with the solution vector, $\Delta\vec{Y}$, representing the trial change in abundances for one network timestep.
7. Continue subcyclng of nuclear burning until reaching the global timestep.

There is a great deal of task-level parallelism to be exploited in this problem. Relatively small problem sizes limit the degree of data-level parallelism for which GPGPUs are excellent at handling. GPU optimized libraries such as MAGMA, CULA, and Cray’s LibSci accelerated BLAS and LAPACK routines provide a general framework for us to utilize the GPU effectively. However, these libraries are limited in their ability to effectively task a single GPU from multiple processes and/or threads due to the lack of use of CUDA streams in all of the aforementioned packages.

Modern NVIDIA GPUs employ a technology dubbed “Hyper-Q”, which provides up to 32 independent work queues between the CPU and GPU. Another crucial technology only now available is CUDA “Dynamic Parallelism”, which allows kernels executing on the GPU to launch other kernels. None of the library packages mentioned above utilize this capability in the DGETRF or DGETRS routines. In order for CHIMERA to effectively task the GPU, each thread must be able to launch independent kernels on the GPU. As part of this effort, I have modified the necessary routines in MAGMA to utilize streams. Consequently, each thread is now able to evolve the nuclear network independently from other threads on the same processor. This represents a significant improvement over prior attempts at tasking the GPU from multiple threads, wherein the calculation was serialized. The performance results from this improvement are shown in Figures 5.1–5.3.

The ability for each thread to be able to task the GPU independent from other threads represents a significant step forward in our effort to use a realistic network

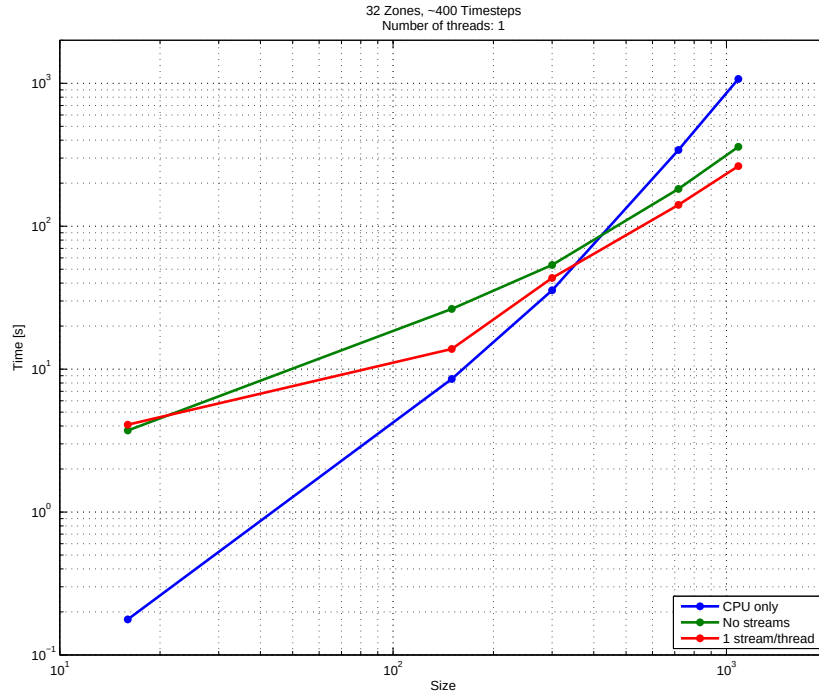


Figure 5.1 XNet timing results using a single OpenMP thread for a sample thermodynamic profile emulating the nuclear network’s computational behavior encountered in a typical CHIMERA simulation. Improvements to the MAGMA DGETRF and DGETRF routines have significantly helped make the cost for a realistic network manageable by using the GPU.

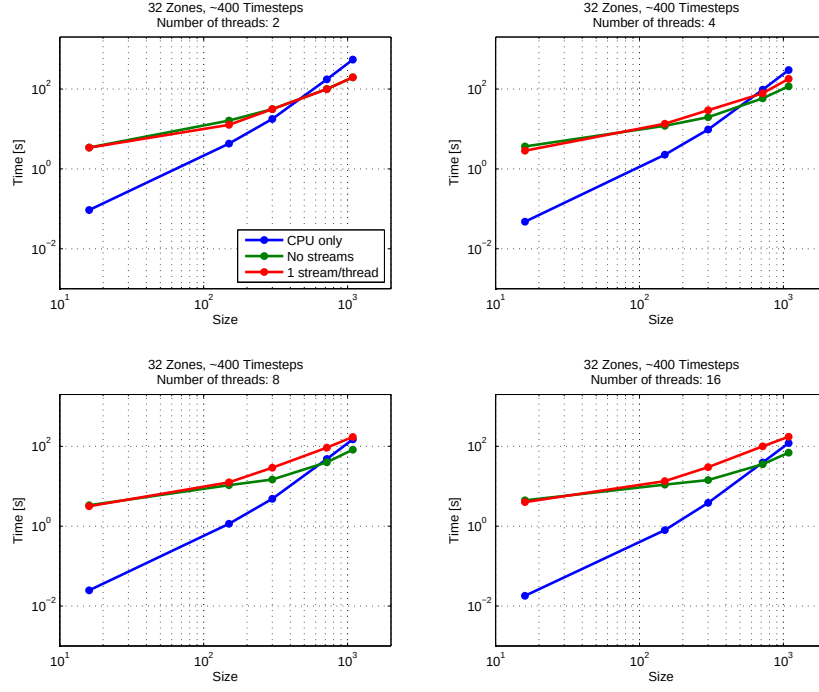


Figure 5.2 XNet timing results for the same thermodynamic profile used in Figure 5.1. As we increase the number of threads communicating with the GPU and, consequently, CUDA streams, we see the performance begin to degrade due to inefficient task scheduling on the GPU. We should be able to eliminate this effect by batching zones together to be solved on the GPU.

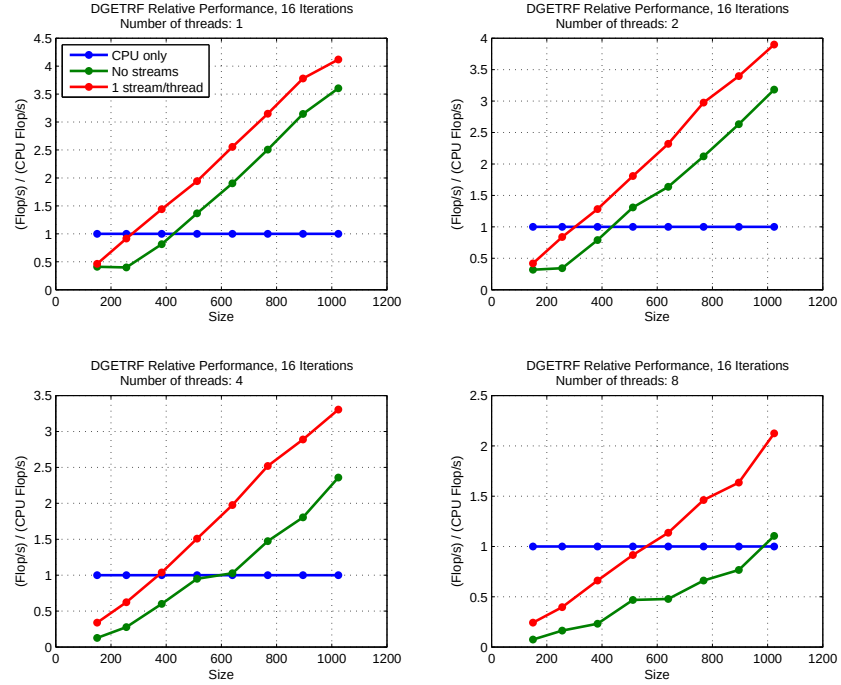


Figure 5.3 Performance results for the modified MAGMA DGETRF routine (LU decomposition), which represents the bulk of the computational cost of a nuclear timestep. Incorporating streams into this routine allows for asynchronous execution between multiple CPU threads. As a direct result, we are able to more efficiently task the GPU.

in CHIMERA. Even with this improvement, we must do more to efficiently utilize the GPU for the SN150-network. This *occupancy problem* is at the crux of optimizing the nucleosynthesis solution and is a reflection on the imbalance between task-level and data-level parallelism, which can be somewhat ameliorated with *batching*. By grouping the independent systems of Equation 5.3 into batches of sufficient size, we can shift this imbalance so that we exploit the relevant computational tool. The problem of optimization can then be framed as an attempt to balance task-level parallelism on the CPU with threads (OpenMP) and data-level parallelism on the GPU (CUDA). Batching the zones in the radial zone-loop directly address the issue of occupancy by only launching a kernel when there is sufficient computation for the GPU to perform.

5.1.3 Benchmarking test

XNet is now capable of evolving a 150-species, *in situ* nuclear network with GPUs in CHIMERA at a comparable or slightly decreased cost to that of sparse solvers (Dong et al., 2014). In Figure 5.4, I show timing results from tests of zone-batching in XNet conducted using 419 zones representing conditions along a radial ray in CHIMERA. The test problem was carried out on a single node of Titan, a Cray XK7 hybrid (CPU/GPU) system. Further examination is required for multiple node performance. Each compute node consists of a single AMD Opteron 6274 “Interlagos” processor and a single CUDA-enabled NVIDIA Tesla K20X GPU accelerator module comprised of a single Kepler GK110 GPU. Details of these architectures are listed in Table 5.1. The GPU and CPU are connected by a PCI Express Gen 2.0 bus with a maximum bandwidth of 8.0 GB/s.

An individual Interlagos processor is comprised two NUMA (non-uniform memory access) memory domains, each with four “Bulldozer modules” comprised of two integer cores with independent L1D cache, shared L2 cache, and a single float-point scheduler with access to a shared 256-bit FMAC. Each integer core can use the entire

Table 5.1. Architectural details for Titan (Cray XK7)

Hardware specifications		
AMD Opteron 6274 “Interlagos”		
	Single-stream	Dual-stream
Cores	16	8
Frequency	2,200 MHz	
FP ops/cycle	4	8
Data Width	64 bit	
L1 Cache per core	16 KB	
L2 Cache per core	1,024 KB	2,048 KB
L3 Cache	16,384 KB	
L1 Cache Latency	4 cycles	
L2 Cache Latency	18–20 cycles	
L3 Cache Latency	55–60 cycles	
Memory	32 GB	
(per core)	2 GB	4 GB
Theoretical Peak	140.8 Gflop/s	
(per core)	8.8 Gflop/s	17.6 Gflop/s
NVIDIA Tesla K20X Kepler GK110		
Streaming multiprocessors (SMX)	14	
CUDA Cores per SMX	192	
Frequency	732 MHz	
Threads per Warp	32	
Max Warps / SMX	64	
Max Threads / SMX	2,048	
32-bit Registers / SMX	65,536	
Max Registers / Thread	255	
Max Threads / Thread Block	1,024	
Shared Memory / L1 Cache configurations	16 KB/48 KB	
	32 KB/32 KB	
	48 KB/16 KB	
Theoretical Peak (Double precision)	1.31 Tflop/s	
Memory Bandwidth	250 GB/s	
Memory size	6 GB	

FMAC with AVX instructions. We can specify whether to use one or both of the integer cores for each Bulldozer module (single-/dual-stream). Each NUMA domain has an independent 8 MB L3 data cache and two DDR3 synchronous DRAM channels.

The GPU is composed of 15 streaming multi-processor units (SMX) and six 64-bit memory controllers. Each SMX features 192 single-precision CUDA cores. The SMX schedules threads in groups of 32 parallel threads called warps. Double-precision is improved from previous generations of Tesla GPUs by allowing other instructions to be paired with floating-point instructions. Most notable for the purposes of our problem is the ability to launch concurrent kernels via CUDA streams, MPI processes, or multiple threads within a process. The latter two abilities are only available on NVIDIA GPUs with a compute capability of at least 3.5. The GPU employs a technology NVIDIA has dubbed "Hyper-Q", which provides up to 32 independent work queues between the CPU and GPU. Another crucial technology only now available is CUDA "Dynamic Parallelism", which allows kernels executing on the GPU to launch other kernels. Each of the Kepler SMXs has one 64 KB cache which can be configured in one of three shared memory/L1 cache configurations. The GK110 also has 1536 KB of dedicated L2 cache memory.

The performance test was conducted using four different libraries for the linear algebra component of XNet: standard machine-optimized LAPACK (MKL; blue), batched LU decomposition on the GPU (cublasDgetrfBatched; green), direct sparse solver (MA48; red), and an open-source implementation of a hybrid CPU/GPU linear algebra library (MAGMA 1.5.0; red). MA48 was found to outperform other direct sparse solvers that are publicly available (e.g. PARDISO), but this result is restricted to the relatively small matrix sizes in our simulations. For larger nuclear networks used in post-processing calculations, PARDISO was much faster, but these types of calculations are not the motivation for this study. For the batched LU decomposition on the GPU, the left- and right-hand sides of Equation 5.3 were computed on the CPU before being transferred asynchronously to the GPU. After the batched LU

decomposition, the resulting solution vector was sent back to the CPU for the back-substitution. MAGMA did not have batched routines available when these tests were performed but has since added this capability in MAGMA 1.6.0. Some of the preliminary results for batching with MAGMA are discussed in [Dong et al. \(2014\)](#) and reveal significant speedup relative to the cuBLAS batched routines on a single CPU process. However, as previously discussed, MAGMA has a fundamental flaw for our application due to its lack of support for concurrent execution among several CPU processes sharing a single GPU. The batched cuBLAS LU decomposition outperforms MKL for batch sizes ≥ 8 , and approaches MA48 for batch sizes ≥ 32 . While not representative of the level of improvement in performance necessary to categorically replace the α -network with a larger, more realistic reaction network, this improved efficiency is sufficient to warrant a small set of axisymmetric models with realistic nucleosynthesis calculations.

5.2 D-series models

In addition to larger-network models, the next series of CHIMERA simulations, hereafter referred to as the D-Series set of models, also incorporate improvements to the NSE and nuclear burning infrastructures, which now identify grid cells approaching equilibrium on an individual basis and properly evolve the composition as zones transition out of NSE. We were previously limited in the B-Series simulations to a single interface between the NSE region and the non-NSE region in which the nuclear burning is active and, consequently, may have been misrepresenting the nucleosynthesis in certain conditions (e.g. α -rich freeze-out). The D-Series simulations also incorporate general performance improvements not related to GPUs, including improved utilization of OpenMP to parallelize local computations performed on each MPI task (e.g. neutrino transport and nucleosynthesis) and reductions in the overall memory-footprint. The overall effect of this is that CHIMERA is now able to

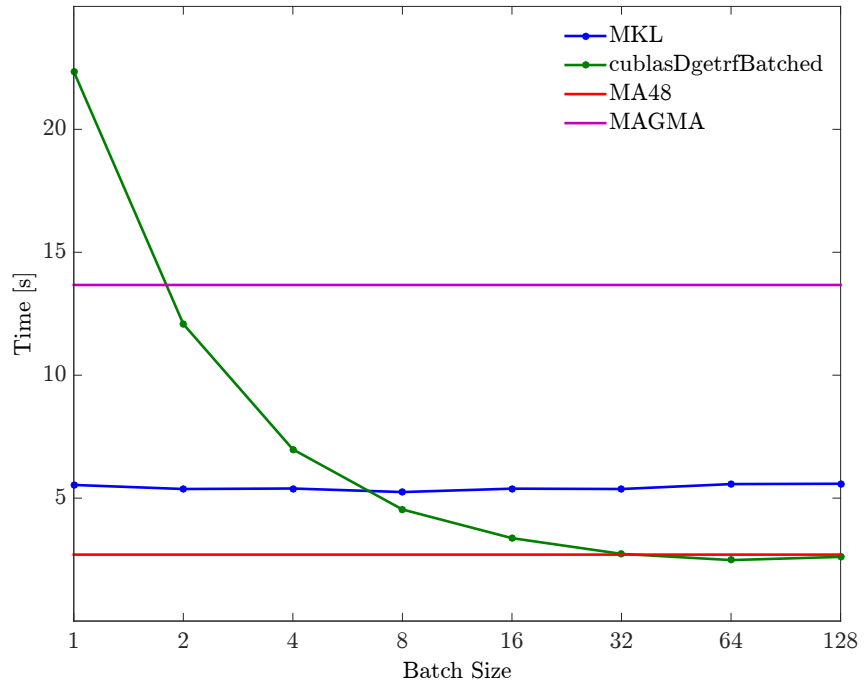


Figure 5.4 XNet wall-clock times for different batch sizes using various linear algebra libraries to evolve 419 zones with initial conditions defined by a single radial ray in CHIMERA through a typical global timestep (5.0×10^{-6} s).

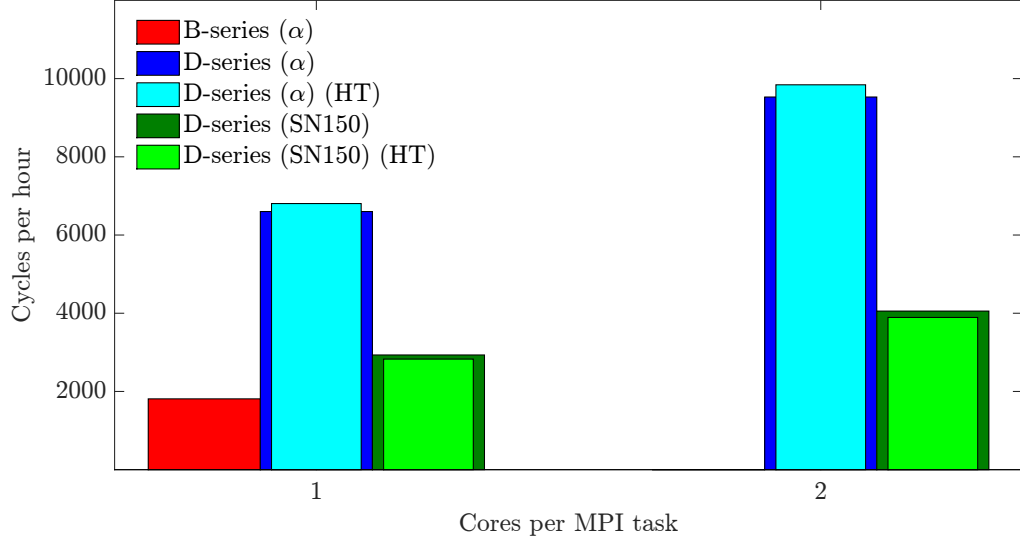


Figure 5.5 CHIMERA D-Series performance improvements compared to equivalent B-Series simulations as measured on Darter, a Cray XC30 with two Intel 8-core Xeon E5-2600 (Sandy Bridge) Series processors per compute node (see [NICS, 2015](#), for details about this architecture).

perform a simulation $\approx 3\text{--}4$ times faster than an equivalent B-Series simulation (see [Figure 5.5](#))

As I alluded to in [Section 3.1.4](#), we need an *in situ* large network simulation in order to truly understand the α -network's limitations. At less than twice the cost of a B-Series simulation, even before considering sparse linear solvers or recent GPU advances in the nuclear burning, it behooves us to incorporate a realistic nuclear reaction network in at least some of our models.

Chapter 6

Conclusions

The key to understanding the role of CCSNe in galactic chemical evolution lies in self-consistent, multi-dimensional radiation-hydrodynamics simulations which incorporate realistic nucleosynthesis calculations and follow the *full* development of the neutrino-driven explosion and consequent morphology. CHIMERA represents a significant milestone to this end.

With 1.2–1.4 s of post-bounce evolution, the B-Series models have been evolved much further than other efforts of similar numerical sophistication and physical fidelity but must still rely on some extrapolation via parameterized thermodynamic trajectories to allow nucleosynthesis calculations of all elemental contributions to the ISM. These calculations are subject to various uncertainties which were discussed in detail in Chapter 3. Namely, the early termination complicates the identification of ejecta via the determination of the multi-dimensional mass-cut. Also, despite temperatures generally below the threshold for explosive burning ($T_f \lesssim 2$ GK), deviations from isentropic expansion in the parameterization of the thermodynamic trajectories can incur non-trivial uncertainties for products of secondary nuclear processes and neutrino-induced nucleosynthesis. Furthermore, the effectiveness of Lagrangian tracer particles in reproducing the *in situ* nuclear burning conditions of

the original B-Series simulations is significantly reduced in regions of α -rich freeze-out, which are characterized by high-entropy (i.e. low-density) outflows in the rapidly expanding ejecta. Future investigations made possible by the lessons learned in this work will address all of these concerns by extending the simulations to the freeze-out conditions of nuclear burning with notable increases in the number of tracer particles and utilizing a larger *in situ* nuclear network.

As discussed in detail in Chapter 4, the B-Series models provide an unprecedented insight to the nuclear processes characterizing CCSN nucleosynthesis. By lifting the restriction of spherical symmetry and including realistic neutrino fluxes, CHIMERA simulations obviate the need to invoke a contrived energy source to launch an explosion and produce qualitatively different nucleosynthesis results, addressing some long-standing questions in the community. In particular, the production of the most neutron-rich stable isotopes between $A = 48$ and $A = 90$ (i.e. ^{48}Ca , ^{54}Cr , ...) via a neutron-rich, α -poor freeze-out in B12-WH07 renews the viability of Fe-core CCSN, which had otherwise been excluded based on 1D nucleosynthesis simulations, as an astrophysical production site for these isotopes. As seen in B12-WH07 and the other B-Series models, if made in α -rich regions, these nuclei will be destroyed, producing ^{92}Mo and other light p -process nuclei traditionally tied to a light element primary process. The persistent overproduction relative to solar abundances of the most neutron-rich and proton-rich isotopes between $A = 60$ and $A = 90$ raises additional questions but could be explained by a tracer particle distribution which does not sufficiently resolve the ejecta where the production of these isotopes occurs. Comparisons of the B-Series nucleosynthesis results to measured yields, specifically those of ^{44}Ti and ^{56}Ni , from light-curve analyses and supernova remnant spectroscopy demonstrate a level of qualitative agreement well beyond that of prior simulations. Furthermore, the highly asymmetric distribution of ^{44}Ti in the interior regions of the ejecta, though correlated with that of ^{56}Ni , reveals a $^{44}\text{Ti}/^{56}\text{Ni}$ ratio which varies by several orders of magnitude.

These unique results demonstrate the importance of self-consistent, multi-dimensional nucleosynthesis models but, nonetheless, are contingent upon an imposition of axisymmetry and other physical approximations, like the α -network, that must ultimately be lifted by three-dimensional simulations with even better microscopic physics. Improvements to computational prowess, like those discussed in Chapter 5, will eventually make such simulations possible.

The findings presented herein suggest that the predication of the larger astrophysical community's interpretation of CCSN nucleosynthesis on spherically symmetric models is flawed. Modern observations of anisotropies in the explosion mechanism and subsequent nucleosynthesis, coupled with models of increasing physical fidelity, are beginning to aptly transform this understanding but will ultimately require a fundamental shift towards a CCSN nucleosynthesis paradigm grounded in an intrinsic awareness of the multi-dimensionality inherent to CCSNe.

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Vita

James Austin Harris was born in Madisonville, KY on March 4, 1987 to the parents of Doug and Jayne Harris as the youngest of three children, including one brother, Adam, and one sister, Christine. After graduating from Hopkins County Central High School in 2005, Austin attended Murray State University in Murray, KY, where he majored in both Engineering Physics with a Mechanical Engineering concentration and Mathematics and Statistics. In 2009, he graduated *summa cum laude* and received his B.S. degree. During the course of his time at MSU, Austin opted for a shift in career track and decided to pursue a Ph.D. in Physics at The University of Tennessee, Knoxville, TN. In the years that followed, he received his M.S. degree in Physics in 2012 and joined the astrophysics research group, a partnership between UT–Knoxville and Oak Ridge National Laboratory. As part of his research, he utilizes high-performance computing to study the topics of computational and nuclear astrophysics in the context of self-consistent core-collapse supernova (CCSN) simulations. He expects to complete his Ph.D. in Physics in August, 2015, with an Interdisciplinary Graduate Minor in Computational Science. Upon receipt of his degree, Austin will continue pursuing his academic interests in computational and nuclear astrophysics as a post-doctoral scholar at Lawrence Berkeley National Lab in Berkeley, CA, where he will continue to study CCSN nucleosynthesis and extend his research to the topic of nucleosynthesis in neutron star mergers.