Advancements in modeling self-consistent core collapse supernovae with CHIMERA

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Abstract.
We discuss advancements in modeling core-collapse supernovae with our code CHIMERA. We describe the status and details of our tracer particle method and its uses for post-processing nucleosynthesis and as a tool for broad core-collapse supernova (CCSN) model analyses. We also introduce our progress towards expanding a nuclear reaction network beyond the alpha-network for the purpose of accurate in-situ nucleosynthesis, not only for core-collapse supernovae (CCSNe) in general, but for a special sub-class of supernovae called electron capture supernovae (ECSNe), which stem from progenitors stars between 8 and 10 $M_\odot$. By using an advanced nuclear reaction network, our 2D and 3D code will allow for unparalleled studies of CCSNe and ECSNe ejecta.

1. Introduction
The final stage of stellar evolution for stars between roughly 8 and 25 solar masses ($M_\odot$) marks a singularly unique class of phenomena in the observable universe. Within this mass range, a core-collapse supernova (CCSN) occurs when a star’s degenerate core is unable to support itself against gravitational collapse. Once the core reaches super-nuclear densities, the collapse halts and a rebound shock forms, which eventually stalls as its energy is sapped via neutrino losses and nuclear dissociation. Self-consistent computer simulations attempt to describe how neutrino energy deposition, aided by the convection of neutrino-heated material between the stalled shock and gain radius, eventually re-energizes the stalled shock towards explosive energies. This process accelerates as instabilities increase the size of the heating region until enough matter is energized to turn the collapse around and become gravitationally unbound — thus creating a supernova. Without question, we know CCSNe are complex multi-dimensional events; and years of theoretical and computational development have shown that the codes we develop to model them must follow suit.

The ORNL/UTK group, in strong collaboration with Florida Atlantic University and NC State University, have built a tightly coupled radiation hydrodynamic code called CHIMERA. The code’s primary modules are designed to evolve the stellar gas hydrodynamics (VH1), compute the “ray-by-ray-plus” neutrino transport (MGFLD-TRANS), and solve the...
thermonuclear kinetics (XNet) [1]. These three heads are augmented by a sophisticated equation of state for nuclear matter (e.g. Lattimer & Swesty [2]) and a self-gravity solver capable of an approximation to general-relativistic gravity. A more general description of CHIMERA and general features of our recent two-dimensional simulations have been reported in Messer et al. (2007) [3] and Bruenn et al. (2010) [4].

This report features our use of tracer particle to expand the CHIMERA models and highlights two CHIMERA advancements not addressed in Bruenn et al. (2010). These advancements are (1) the development of a larger nuclear reaction network beyond the popular 14-species alpha-chain within CHIMERA, which allows for (2) the recent progress toward modeling electron capture supernovae (ECSNe) of $8 - 10 M_\odot$ progenitors with ONeMg cores. ECSNe are unique in that they require more detailed burning treatments to address their initial composition of oxygen, neon, and magnesium, which differ from larger iron core progenitors. We want to model ECSNe because theoretical and observational studies are still subject to many uncertainties [5, 6, 7, 8].

Regardless of the initial mass, the prime motivation for modeling realistic CCSNe abundances is to reconstruct observables for the purpose of understanding the origin of the elements. This means we cannot simply "follow" chemical abundances throughout the evolution, but we must properly treat the feedback of thermodynamic energy generation upon the overlying hydrodynamic model. Since this energy generation can have a local effect upon the hydrodynamics, potentially affecting whether individual mass elements are ejected, it should be directly included among the physical processes associated with the explosion mechanism [9, 10].

2. The Tracer Particle Method (TPM)

CHIMERA’s Eulerian grid makes it difficult to obtain the necessary data to calculate realistic ejecta abundances via post-processing, as what is needed are time histories of thermodynamic conditions for mass elements. A Lagrangian grid would provide us with this useful information, but these schemes quickly become tangled in the multi-dimensional hydrodynamic flows inherent in any realistic supernova calculation. As a solution to this problem, we have recovered a Lagrangian perspective by implementing massless tracer particles to keep track of thermodynamic histories which we use for post-processing nucleosynthesis using thousands of nuclear species [11]. We are currently running state-of-the-art 2D models with CHIMERA towards explosions and we will have a plethora of tracer particle data to analyze. Although the tracer particles were primarily developed to perform post-processing nucleosynthesis calculations, we have also found use for them as a tool to search for possible code problems manifested in physical quantities during code development.

2.1. Tracer Data

The tracer particles record thermodynamic, hydrodynamic, gravitational energy, nuclear binding energy, and neutrino energy deposition rates and flux quantities for the parcels of matter which they represent throughout the evolution of the supernova. To gain a representative picture of our simulations, we initially distribute tracer particles uniformly within the inner core layers from iron to oxygen (in our iron core models). Depending on the size of the progenitor and the dimensionality of the simulation, we distribute between several thousand tracer particles in 2D and hundreds of thousands in 3D. As an example, a run containing $\sim 8,000$ tracer particles produces approximately 400 GB of processed data, of which 47 GB will be used for post-processing, while the rest is used for general analysis. Each tracer particle is represented by one file since the tracer’s physical movement causes it to move from processor to processor through CHIMERA’s domain decomposition. This can mean we must handle upwards of 100,000 individual files. For these reasons, we must carefully consider proper data management, efficient processing, and long-term storage.
2.2. The Tracer Particle Reader
To handle the tracer particle data management and processing, we have developed a tracer particle “reader,” (TPR) to (1) read-in the binary tracer files; (2) digest and pre-process the data; (3) perform automated analysis of CHIMERA not necessarily associated with nucleosynthesis; and (4) organize the resultant information into suitable formats for post-processing nucleosynthesis by our general purpose nuclear kinetic solver XNet. The TPR also helps us perform many service tasks such as finding bad tracers (tracers whose data may have become corrupt due to I/O or file system issues), and hunting down tracers of particular interest. Without this effective data management, sorting through 8000 − 100,000 files for the location of, for example, the non-spherical shock and the location of the boundary between NSE & non-NSE matter to determine which particles (an thus what parcel of matter) becomes unbound, would be a daunting task.

There are many ways of utilizing tracer particles as a tool to understand and interpret our models, but we highlight three examples here. Figure 1 shows tracers superimposed over the entropy of the matter in a simulation of a 15 $M_\odot$ star approximately 300 ms after core bounce. The tracers are shown with their color code indicating the amount of neutrino heating or cooling. The pattern of the tracers illustrates how infalling matter is concentrated into the low entropy downflows as it flows towards the proto-neutron star. The neutrino heating occurs predominately in the inner 100 km, but the heated matter, with its entrained tracers, rises to form low density plumes which push the stalled shock outward. Figure 2 shows the location of tracers at $\sim$1000 ms post-bounce for our 25 $M_\odot$ simulation. The color coding of the tracers indicates the layer in the progenitor from which that tracer originated. This illustrates the difficulty in translating the “mass-cut” of spherically symmetric models to multi-dimensions, pointing out that the term is really a misnomer. This figure also indicates the complexity of mixing issues relative to the initial composition distributions. CHIMERA overestimates microscopic mixing due to zone interpolation, while the tracers underestimate fluid mixing because of their Lagrangian nature. Figure 3 provides a different perspective on this issue, which highlights the trajectories of six tracer particles from the same initial radius but different angular latitudes; two of these tracers are captured by the proto-neutron star (PNS) while the other four escape to possibly become ejecta — depicting clearly that one-dimensional models can not capture the complex behavior of the inner most supernova ejecta.

2.3. Alternate Use of Tracers: Gravitational Waves
The TPM method can also be used to explore multi-dimensional effects, in general, that stem from anisotropies, instabilities, and fluid mixing. We have used the unique Lagrangian perspective of the tracer particles to assist in the analysis of gravitational wave (GW) signatures from our non-parameterized, 2D, 12 – 25 $M_\odot$ core-collapse supernovae models [12]. In these models, each particle is assigned a constant mass ($1/4000^{th}$ – $1/8000^{th}$ of the mass of the progenitor in the region of interest where the tracers were deployed), and the GW signal their movement produces is calculated. Comparing the GW signal corresponding to a given group of tracers with the signal produced by the bulk-matter motion (captured on the Eulerian grid) has allowed us to identify what part of the fluid generates a specific GW feature. We have calculated the contribution to the signals produced by both baryonic matter motion and anisotropic neutron emissions up to 530 ms after bounce for all four progenitors. This analysis matches the predictions based on the parameterized models by Murphy et al. [13]. However, given the development of non-parameterized explosions in our models, we were able to compute the waveforms through explosion and to determine more precisely the per-explosion amplitudes and timescales. In doing so, we have decomposed the GW signal and determined which mass motions contribute to the various components of the waveforms. As a result, we have been able to explore the prompt signal, which is generated by two independent phenomena. Prompt
Figure 1. Tracer particles plotted over an entropy colormap. Here, the tracers are colored to represent the superposition of neutrino-heating.

Figure 2. Tracer particles from a 25 $M_\odot$ model at $\sim 1000$ ms post-bounce have diverged from initial spherical symmetry illustrating that the definition of a “mass-cut” is not well defined in multi-dimensions. This figure also indicates the complexity of mixing issues relative to the initial composition distributions.

Convection inside the PNS generates a high-frequency signal that is superimposed on a lower frequency component. There is a hint of this in the inset of Figure 4, where the signal for our 15 $M_\odot$ run has been split into the contributions from two different regions, but it is in the tracer analysis of Figure 5 (right) where this becomes most evident. The matter-generated GW (solid red) is closely tracked by the GW generated by the infalling tracer particles deflected by the shock (dashed blue), some of which are shown in the left panel. Although the hydrodynamic resolution (256 radial and 256 angular zones) for this suite of runs was significantly finer than the
Figure 3. The time history of 6 example tracers from an initial spherically symmetric distribution within a 15 $M_\odot$ star. Two tracers are captured onto the PNS while the other four are possibly ejected through convection.

tracer-matter resolution (50 x 100 tracers), we identified a low-frequency signal from 20 to 60 ms after bounce originating at the shock radius, which is at $\sim 100$ km at this time and well outside the PNS. The results presented here are preliminary: a new set of 2D simulations performed with an enhanced version of our CHIMERA code is currently ongoing [4], and will explore the use of tracer particles to investigate the GW signal at lower frequencies with post-bounce dynamics.

3. Nuclear Networks

As detailed in Timmes et al. (2000) [18], since the implicit solution of a nuclear reaction network is, at its heart, the solution of a matrix equation, the computational cost grows non-linearly with the number of nuclei included in the calculation. For this reason, an alpha-network, or even a simpler “flashing” scheme, is typically used to evolve the composition where conditions are not in nuclear statistical equilibrium (NSE). Because the alpha-network neglects reaction flows involving neutron-rich (or proton-rich) nuclei, it cannot fully represent accurate compositions, and it provides incomplete estimates of the energy generation from nuclear burning encountered in CCSNe. Detailed nucleosynthesis calculations can be performed by post-processing methods, but only if the temporal evolution of matter is present (see section 2). To avoid the need for post-processing, accurate nucleosynthesis in-situ can be obtained by evolving 150, or more, nuclear isotopes throughout the matter that is ultimately ejected. A large network would also explore the importance of composition mixing, and facilitate the testing of post-processed results.

As additional motivation for improving the nuclear kinetics within CHIMERA, Pruet et al. [19, 20] and Fröhlich et al. [17, 21] have studied the inner ejecta layers showing that neutrino-powered explosions (using spectral neutrino transport) result in decreased neutronization, and that the electron fraction ($Y_e$) has a dominate effect on nucleosynthesis. This finding is at odds with the prediction of previous models, all of which neglect this important piece of physics. The decreased neutronization removes the overproduction of neutron-rich iron and nickel isotopes commonly seen in parameterized bomb and piston models [22, 23]. The simulations of Pruet et al. and Fröhlich et al. also show enhanced production of Sc, Cu, and Zn, elements which observations of metal-poor stars (see, [24, 25]) suggest are 3 – 10 times more abundant than previous models predicted. Finally, a significant neutrino driven flow to proton-rich nuclei above $A > 64$ is seen,
suggesting that the innermost ejecta of core-collapse supernovae may be the production site of the light p-process nuclei [17]. This agreement with galactic and solar $\nu p$-process abundances at later times generates a small abundance of neutrons, which helps explain things like strontium in otherwise metal-poor stars [17].

Within our ongoing runs, the equation of state (EOS) of Lattimer and Swesty [2] is employed in CHIMERA for matter at high densities. For smaller densities, an electron-positron EOS, with arbitrary degeneracy and degree of relativity, spans the entire density-temperature regime of interest. For regions not in nuclear statistical equilibrium (NSE), we use an EOS with a nuclear component consisting of a 14-species alpha-network ($^4$He to $^{60}$Zn) which carries the protons, neutrons, and an iron-like nucleus. Here, the composition is evolved by XNet, the

**Figure 4.** Contributions to the matter-generated GW signal from two different regions for the 15 $M_\odot$ model: the PNS ($r < 30$ km) and the region above the PNS ($r > 30$ km). The latter includes the region of neutrino-driven convection, the SASI, and the shock. [12]

**Figure 5.** Left: trajectories of the tracer particles. The clear deflection of infalling particles through the shock that collectively produce a low-frequency high-amplitude component of the GW signal shown on the right panel. Right: comparison between the matter signal (solid red) and signal calculated using the tracers (dashed blue). Both panels correspond to our 15 $M_\odot$ simulations. [12]
Figure 6. Another way of looking at the alpha-network’s inability to represent abundance values at a constant temperature and density profile. As indicated, the thick dashed line representing the 150-isotope network chosen to accommodate neutron-rich nuclei of significant abundances.

thermonuclear reaction network [14]. Data for these reactions is drawn from the REACLIB compilations [15].

To improve the nucleosynthesis results while reducing the energy-generation uncertainty, we have improved CHIMERA’s nuclear network by allowing for the substitution of the alpha-network with a larger, 150-isotope network. Figure 6 shows the alpha-network’s inability to represent abundance values for the given temperature and density profile. It is important to note that the three most abundant species — protons, \(^{54}\)Fe, and \(^{58}\)Ni — are not members of an alpha-network. It is also clear that the alpha-network does not span the entire regime of interest whereas a 150-isotope network is much more inclusive. The downside is that a simple replacement of the 14-species alpha-network with 150-isotopes in the fully-implicit backward-Euler integration scheme represents a several hundred-fold increase in the computational cost. Given the current ~ 5% of execution time required by the alpha network in the current simulations, this cost is prohibitive if implemented naively. Figure 7 illustrates two 15 \(M_\odot\) radial composition profiles of the significant nuclear species using an alpha-network (solid lines) and a large-network (dashed lines) within CHIMERA. While the alpha-network reproduces the general abundance patterns, there are many examples where it simply does not represent the composition.

To increase the physical fidelity, yet have calculations that complete in a reasonable time, we have improved the speed of these calculations by using the shared-memory parallel-programming API OpenMP. We plan to further decrease our computational time by adaptively managing the nucleosynthesis by taking advantage of quasi-statistical equilibrium (QSE), a precursor to NSE, to reduce the size of the system of equations where conditions apply. This adaptive QSE-network has been developed in-house and is expected to be become a CHIMERA module within the coming year [9]. With our improvements to CHIMERA’s nuclear kinetic module, we hope to expand upon the recent work on by Pruet et al. (2005, 2006) [19, 20] and Fröhlich et al. (2006a,
2006b) [17, 21]

Figure 7. An example of a radial composition profile of significant nuclear species highlighting the difference between an alpha (solid) and 150-isotopes (dashed) network early during the collapse our $15 \, M_\odot$ model.

4. ECSN and ONeMg Progenitors

With our self-consistent, multi-dimensional, tracer-laden code, and a network extended beyond 14-species (to 150 species enabling us to follow the neutronization) we can expand the scope of our studies with progenitors of various masses and compositions. One such investigation is exploring the lower mass range ($\sim 8 - 10 \, M_\odot$) of CCSN progenitors whose cores are composed of oxygen, neon, and magnesium. These supernova are called electron capture supernovae (ECSNe) since they can undergo collapse via extreme deleptonization within the degenerate core, where stellar oxygen burning is not favored. There is a large interest in resolving the specific explosion mechanism of ECSNe as they have been suggested as the source of the r-process [26], though more recent models suggest only a light r-process as the origin of elements heavier than Zn, potentially up to Cd [8].

The large network will play a unique role in these models because the core is not in NSE and are composed of oxygen, neon, sodium, and magnesium, as previously stated. Lacking significant mass for gravitational contraction, the core cannot progress beyond the production of magnesium and it becomes physically inert. The H- and He-burning shells continue to deposit mass until the core reaches the Chandrasekhar mass ($M_{CH} \sim 1.37 \, M_\odot$) [7]. Here, extreme deleptonization begins through sequential electron captures on $^{24}\text{Mg}$, $^{23}\text{Na}$, $^{20}\text{Ne}$, and the core begins to collapse [27]. The coincident oxygen deflagration is unable to stop the collapse and the core reaches nuclear densities. The subsequent explosion mechanism is moderately under debate, though most recent studies point towards a requirement for neutrino energy deposition
behind a stalled shock [6, 8]. Observationally, the explosion associated with these less massive stars is relatively weak (\(\sim 10^{50}\) ergs), they have a larger Ni/Fe ratio (\(\sim 1 - 2\)) than their iron core counterparts, and they eject a much smaller amount of \(^{56}\)Ni [7, 27].

Kitaura et al. (2008) [6] have performed spherically symmetric ECSN models up to one second after bounce finding a delayed neutrino-driven explosion instead of the prompt-shock mechanism as described by Hillebrandt et al. (1984) [28]. Although Kitaura et al. carefully considered a description of weak interaction, they were still limited by a seven species alpha-chain network. As with all alpha-networks, important abundances that may be present in the core, such as \(^{23}\)Na [29], are simply omitted. This of course ignores important reaction channels for nucleosynthesis. Kitaura et al. project ECSNe to produce neutron-rich eject with \(Y_e\) as low as \(\sim 0.2\) and entropies down to \(\sim 10k_B\) [6].

The 2D model of Janka et al. (2007) [5] was somewhat more energetic due to convective overturn in the gain layer while using the same network of Kitaura et al. [6]. Although they determine that neutrino energy deposition within the gain region is the primary source for reviving a temporarily stalled shock, their model fails to create conditions to support the r-process scenario by having too modest entropies and/or not sufficient temperatures. Janka et al. [5] point out that their thermonuclear energy production is approximate and a full reaction network is desired in order to take electron capture rates into consideration.

Also in contrast to Kitaura et al. [6], Wanajo et al. (2010) [8] found that a multi-dimensional model produces neutron-rich ejecta due to convective overturn that could otherwise not be seen in 1D cases. They performed the first nucleosynthesis study on the basis of self-consistent 2D models (while using tracer particles for post-processing), and have found neutron-rich lumps with electron fractions down to 0.40, which can lead to nuclei up to \(A \sim 80\). Ultimately, they hypothesize that a 3D model may eject a tiny amount of matter with a \(Y_e\) as low as \(0.35 - 0.30\) leading to the creation of Cd. Wanajo et al. were also unfortunately limited by resolution and dimensionality constraints, as well as the small network, and could not exclude weak r-process elements beyond \(N = 50\) up to Pd, Ag, and Cd [8].

We are presently modeling the collapse and explosion of the ONeMg core of Nomoto et al. (1987) [27] — the same pre-collapse core used in the Prometheus-Vertex models of Hillebrandt et al. [28], Kitaura et al. [6], Janka et al. [5], and Wanajo et al. [8]. Previous 2D, \(12 - 25\) \(M_\odot\) models in CHIMERA have resolved up to \(512 \times 256\) zones and we can extend this resolution to ECSNe. We are working on the evolution of a 1D model out to \(\sim 1000\) ms post-bounce to ensure CHIMERA's compatibility with a progenitor it was not explicitly designed to evolve. This study will use an alpha-network as a baseline for comparison to the 150-isotope network. The alpha-network model alone will produce physically meaningful results, but the 150-isotope network will go far beyond any previous study.

As previously stated, a large network in 2D is too taxing given the current scheme in CHIMERA, so our in-situ alpha-network will rely on the post-processing of tracers to model the nucleosynthesis. After the adaptive QSE-network is installed we can perform a nucleosynthesis study between an alpha-network and a large-network in the context of a multi-dimensional simulation. In parallel to these two network runs, we would like to perform a detailed study on how the thermonuclear energy from burning and nucleon recombination feeds back into the hydrodynamics. This will help us understand the effect thermonuclear energy release has on the outward propagating shock and supernova dynamics.

Ultimately, we would like to run ECSNe with an adaptive QSE-network and a yin-yang grid — a pole-free 3D grid unlike the typical spherical-polar grid. As with any realistic hydrodynamic model, a self-consistent 3D model would provide a verification of 2D results. But most importantly, as stated by Wanajo et al. [8] and Pumo et al. [7], a 3D run is required to not only study the creation of nuclei within ECSN, but to understand the composition of the ejecta due to a more realistic determination of convective processes afforded by the move to 3D.
5. Conclusion
We seek to extend existing core-collapse supernova (CCSN) models to examine nucleosynthesis in a self-consistent fashion. Self-consistency requires, among other things, a code that evolves explosions without parameterized methods to obtain delayed neutrino heated shock revival and late time ejecta that match CCSNe morphologies and galactic-abundance contributions from CCSNe. The tracer particles have been (and continue to be) a vital tool in our efforts to improve the physical fidelity of our models. Since observations can only be confronted by computational investigations, over the next few of years, the CHIMERA team has an ambitious agenda of running many 2D and 3D models to examine the effects of progenitor mass, rotation rate, and micro-physics input on CCSN evolution and the explosion mechanism. It must be stressed that these analyses will be incomplete without the improvements and efforts highlighted in this paper to our nucleosynthesis studies.

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