Multidimensional, multiphysics simulations of core-collapse supernovae

O E B Messer\(^1\), S W Bruenn\(^2\), J M Blondin\(^3\), W R Hix\(^4\)
and A Mezzacappa\(^4\)

\(^1\) National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6008, USA
\(^2\) Department of Physics, Florida Atlantic University, Boca Raton, FL 33431-0991, USA
\(^3\) Department of Physics, North Carolina State University, Raleigh, NC 27695-8202, USA
\(^4\) Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6354, USA

Abstract. CHIMERA is a multi-dimensional radiation hydrodynamics code designed to study core-collapse supernovae. The code is made up of three essentially independent parts: a hydrodynamics module, a nuclear burning module, and a neutrino transport solver combined within an operator-split approach. We review the code’s architecture and some recently improved implementations used in the code. We also briefly discuss preliminary results obtained with the code in three spatial dimensions.

1. Introduction

The center of a massive star (a star more than 8 or so times the mass of our own Sun) as it nears its demise is composed of iron, nickel, and similar elements. Above this iron core lie concentric layers of successively lighter elements, recapitulating the sequence of nuclear burning that occurred in the star during its lifetime. Unlike prior burning stages, where the ash of one stage became the fuel for its successor, no additional nuclear energy can be released by further fusion in the iron core. No longer can nuclear energy production stave off the inexorable force of gravity. When the iron core grows too massive to be supported against its own self-gravity, the core collapses. This collapse continues until the core reaches densities similar to those of the nucleons in a nucleus, whereupon the hard core of the nuclear interaction renders the core incompressible, halting the collapse. Collision of the supersonically falling overlying layers with this stiffened core produces the bounce shock, which drives these layers outward. However, this bounce shock is sapped of energy by the escape of neutrinos and nuclear dissociation and stalls before it can drive off the envelope of the star; see, for example, [1]. How the shock is revived and proceeds to completely disrupt the star is the central question of supernova theory. A closer examination of some of the known physical processes in the event does provide a short list of probable actors.

After core bounce, \( \sim 10^{53} \) erg of energy in the form of neutrinos and antineutrinos of all three types, or flavors, (electron, muon, and tau) is released from the newly formed proto-neutron star (PNS) at the center of the explosion. The supernova explosion energy is \( \sim 10^{51} \) erg. Past simulations [2; 3] demonstrate that energy in the form of neutrinos emerging from the PNS can be deposited behind the shock and may revive it. This neutrino reheating is central to modern core-collapse supernova models. However, while a prodigious amount of neutrino
energy emerges from the PNS, the neutrinos are weakly coupled to the material directly below the shock, and, in fact, the neutrino heating is very sensitive to the distribution of neutrinos in energy and direction of propagation [4; 5; 6; 7; 8; 9]. Therefore, this ultimately requires neutrino transport algorithms that resolve both the neutrino spectra and the shape of the radiation field at any spatial point in order to compute accurately the neutrino distributions in this region. This renders the core collapse supernova problem a truly multidimensional (space plus neutrino angles and energy), petascale (petaflops, petabytes) problem.

This neutrino heating may also be aided by fluid instabilities (e.g., convection) in the PNS [10; 11; 12; 13; 14], which may boost the luminosity of this central neutrino bulb. Also, convection directly beneath the shock fundamentally alters the nature of neutrino shock reheating [15; 16; 5; 17; 14; 18] relative to the spherically symmetric case, allowing simultaneous downflows that fuel the neutrino luminosities and upflows that bring energy to the shock. A newly discovered instability of the shock wave itself, the Stationary Accretion Shock Instability (SASI), will likely dramatically alter the shock and explosion dynamics [19; 20; 21; 22]. The centrifugal effects of stellar core rotation [17; 14], and other of its effects, will also change supernova dynamics qualitatively and quantitatively, and stellar core magnetic fields, increased perhaps dramatically by compression during collapse, convection (e.g., via a dynamo), and rotation (through wrapping and shear; in the latter case the magnetorotational instability may occur and, if so, would dominate the field evolution), may also play a significant role in driving, and perhaps collimating, core-collapse supernova explosions [23; 24]. The nuclear abundances should be evolved in regions where nuclear statistical equilibrium (NSE) cannot be maintained. This process will enable the potentially observable products of nucleosynthesis to be followed and, most important for the mechanism, the energy released by nuclear burning to be fed back into the computation of the explosion dynamics.

“Ray-by-ray” simulations [25; 26; 14; 18] capture much of the transport realism in multidimensional models, neglecting only contributions from lateral neutrino transport, which will likely be important only below the neutrinospheres in the proto-neutron star where the neutrinos and matter are strongly coupled and the flow may be highly nonspherical. The ray-by-ray approximation allows a substantial amount of physical fidelity in simulations that remain tractable on petascale platforms. The addition of a prescription for nuclear burning to a multidimensional ray-by-ray radiation hydrodynamics scheme allows much of the known physics in the problem to be competently addressed.

All of these facts make realistic modeling of the core-collapse supernova mechanism a computational challenge that is nearly unrivaled. Indeed, though the seminal paper of [27] was among the very first examples of computational astrophysics (if not, arguably, computational science in general), the explosion mechanism remains unsure even today, more than 40 years later. The explosion mechanism is apparently inherently multidimensional, with all the attendant difficulties of multidimensional modeling. Furthermore, the mechanism itself must be regarded as energetically marginal. The observed explosion energy of ≈1 B (1 bethe [B] = 10^51 ergs) is only 1 percent of the internal energy residing in the immediate post-collapse core, and the near negative of this in the form of gravitational binding energy. Thus, simulations must be energy conserving to high accuracy if we are to take their outcomes seriously. Ultimately ≈300 B in energy is released by the core in neutrinos of all flavors, and their interaction with the stellar core and mantle will either power the explosion itself or play a major role in the explosion dynamics. An inaccurate treatment of neutrino transport can qualitatively change the results of a simulation. Neutrinos interact with matter in a variety of energy-dependent ways, and it is generally accepted that this demands that both the neutrino transport and the interactions receive a full spectral implementation, rather than having the neutrino spectrum prescribed. The angular distribution of the neutrinos is also important to compute accurately. In particular, it affects the neutrino heating, and the latter is primarily determined in a region where the angular
distribution can neither be assumed to be isotropic nor radially free streaming. The nuclear abundances should be evolved in regions where NSE cannot be maintained. This will enable the potentially observable products of nucleosynthesis to be followed and, most importantly for the mechanism, the energy released by nuclear burning to be fed back into the computation of the explosion dynamics. Moreover, general relativistic effects must be incorporated as they influence the size of the neutrino heated region, the rate of matter advection through this region, and the neutrino luminosities and RMS energies [28], and can therefore profoundly affect the dynamics. Computational work over the past 40 years has generally consisted of several generations of simulations, each generation containing more physical fidelity than the last, where, as computational power has increased, the treatment of one or more of these myriad physical inputs has been refined. Modern petascale platforms will, for the first time, allow the inclusion of all currently known important physics in supernova simulations. This will mark a watershed moment in supernova simulation, ushering in a new era of predictive capability.

2. Code architecture

Our code, CHIMERA, incorporates most of the aforementioned criteria for realistic core-collapse modeling. At the same time it is efficient enough to evolve progenitors from the onset of collapse to roughly 1-second postbounce, given present state-of-the-art computational resources, such as the Cray XT4. It conserves total energy (gravitational, internal, kinetic, and neutrino) to well within 0.5 B.

CHIMERA can well be described as a “chimera” of three separate, rather mature codes. The codes are tightly coupled in a single executable through a set of interface routines that provide each of the code components access to global variables for use (cf. the FLASH code [29], where each code module “checks out” copies of global variables from a central database structure, uses or evolves them, and then “checks them back in.”) The primary code modules are designed to evolve the stellar gas hydrodynamics (VH1), the “ray-by-ray-plus” neutrino transport (MGFLD-TRANS), and the thermonuclear kinetics (XNET). These three “heads” are augmented by a sophisticated equation of state for nuclear matter (e.g., LS-EOS [30]) and a self-gravity solver capable of an approximation to general-relativistic gravity. The hydrodynamics is directionally split, and the ray-by-ray transport and the thermonuclear kinetics solve occur after the radial sweep occurs, when all the necessary data for those modules is local to a processor (see Figure 1). The individual modules are algorithmically coupled in an operator split approach. This approach is well motivated, as the characteristic time scales for each module are widely disparate. Specifically, during the radial sweep of the hydrodynamics, the neutrino transport and the thermonuclear burning are computed along each radial ray, using only data that is local to that ray and, therefore, local to the current process.

The hydrodynamics module in CHIMERA is a modified version of the PPM code VH-1, which has been widely used in astrophysical fluid dynamics simulations and as an important benchmark code for a variety of platforms. VH-1 is a Lagrangian remap implementation of the Piecewise Parabolic Method (PPM) [31]. Being third order in space (for equal zoning) and second order in time, the code is well suited for resolving shocks, composition discontinuities, etc. with modest grid requirements. To avoid the odd-even decoupling and carbuncle phenomenon for shocks aligned parallel to a coordinate axis, we have employed the local oscillation filter method of Sutherland et al. (2003) which subjects only a minimal amount of the computational domain to additional diffusion. We have also found it necessary to incorporate the geometry corrections of [32] in the hydrodynamics module to avoid spurious oscillations along the coordinate axes. Redshift and time dilation corrections are included in both the hydrodynamics and neutrino transport (to be described later). A moving radial grid option, where the radial grid follows the average radial motion of the fluid, makes it possible for the core infall phase to be followed with good resolution. The hydrodynamics equations to be solved can be replaced by the
magnetohydrodynamics equations, enabling the inclusion of stellar magnetic fields in CHIMERA simulations. This change would enable inclusion of all known important physical processes in CHIMERA supernova simulations.

The equation of state (EOS) of [30] is currently employed for matter at high densities. The EOS provides a relationship between the matter density and pressure, closing the system of radiation hydrodynamics equations. At densities below about $1.7 \times 10^8$ g cm$^{-3}$ the state of the matter is described by mixture of 4 nuclei (neutrons, protons, helium, and a representative heavy nucleus) in a highly modified version of the EOS described by [33]. For regions not in NSE (at even lower densities), an EOS with a nuclear component consisting of 14 alpha particle nuclei ($^4$He to $^{60}$Zn), protons, neutrons, and an ironlike nucleus is used. An electron-positron EOS with arbitrary degeneracy and degree of relativity spans the entire density-temperature regime of interest. The nuclear composition in the non-NSE regions is evolved by the thermomuclear reaction network of [34]. The thermomolecular network is a set of coupled ODEs describing the various nuclear processes that serve to define the isotopic composition of the matter. This is a fully implicit, general-purpose reaction network. Currently, however, we have implemented only a so-called $\alpha$-network; that is, only reactions linking the 14 alpha nuclei from $^4$He to $^{60}$Zn are used. Data for these reactions is drawn from the REACLIB compilations [35], the world standard for reaction data in simulations of this type. Because the 14 element $\alpha$ reaction network neglects reaction flows involving neutron-rich nuclei, it provides only estimates of the energy generation rates for nuclear burning stages encountered in the supernova $\pm 50\%$ for oxygen burning and $\pm 10\times$ for silicon burning; [36]. Detailed nucleosynthesis requires evolving 150 or more nuclear isotopes throughout the matter that is ultimately ejected. Simple replacement of the 14-element network with 150 isotopes in the fully implicit Backward Euler integration scheme represents a several hundredfold increase in the computational cost. Given

![Schematic CHIMERA flowchart.](image)
the current ≈5% of execution time required by the alpha network in the current simulations, this cost is prohibitive if implemented naively. New thermonuclear kinetic methods can achieve factors of 6–12 decrease in the computational cost of the thermonuclear network during the most computationally expensive supernova burning phases by employing local partial equilibria (termed quasi-equilibrium or QSE) to reduce size of the system of equations which must be integrated [37]. With modest further refinement, these QSE-reduced networks will enable self-consistent nucleosynthesis within the radiation-transport problem at a cost only a few times the current simulations. We have also finished the initial development of a tracer particle tracking module in CHIMERA to allow more detailed postprocessing nucleosynthesis calculations to be performed [38].

Ideally, neutrino transport would be implemented with full multidimensional Boltzmann transport. This important development, however, lies beyond the petascale and will require at least exascale computing to fully realize. We compromise by implementing a “ray-by-ray-plus” approximation (see [14]) for neutrino transport, whereby the lateral effects of neutrinos such as lateral pressure gradients (in optically thick conditions), neutrino advection, and velocity corrections are taken into account, but transport is performed only in the radial direction. Transport is computed by means of multigroup flux-limited diffusion with a flux limiter that has been tuned to reproduce Boltzmann transport results to within a few percent [39]. All $O(v/c)$ observer corrections have been included. The transport solver is fully implicit and solves for four neutrino flavors (types) simultaneously (i.e., $\nu_e$’s, $\bar{\nu}_e$’s, $\nu_\mu$’s and $\nu_\tau$’s (collectively $\nu_x$’s), and $\bar{\nu}_\mu$’s and $\bar{\nu}_\tau$’s (collectively $\bar{\nu}_x$’s)), allowing for neutrino neutrino scattering and pair-exchange, and different neutrino and antineutrino opacities. The PPM technology has been directly applied to both the spatial and energy advection of neutrinos in both the radial and lateral directions. The neutrino opacities employed for the simulations are the standard ones described in [40], with the isoenergetic scattering of nucleons replaced by the more exact formalism of [41], which includes nucleon blocking, recoil, and relativistic effects, and with the addition of nucleon–nucleon bremsstrahlung [42] with the kernel reduced by a factor of five in accordance with the results of [43].

3. Current code development
We have recently implemented a new spatial domain decomposition for the hydrodynamics module used in CHIMERA to enable three-dimensional simulations to be performed. The new spatial domain decomposition divides the computational domain into a series of “pencils” along each coordinate direction. This is in contrast to the original VH-1 “slab” decomposition, where a 2D slice through the computational domain was transposed after each directional sweep. Importantly, the pencil decomposition makes use of a series of data transposes (specifically, using MPI_Alltoall) that are performed over row and column subcommunicators. Therefore, although all processes participate in communication roughly simultaneously, producing contention, the actual data movement is significantly less than would be seen an global collective.

Though the preponderance of the work involved in each timestep is performed by the thermonuclear burning and neutrino transport modules, the performance of the hydrodynamics module must also be improved to ensure scalability to tens of thousands of processes, at least. Our choices of ray-by-ray transport and dimensionally split hydrodynamics simplify this task to a large extent but also constrain the methods we use to achieve good scalability. The data transposes between dimensional sweeps and the possibility of overlapping communication and computation in these transposes mark the primary areas of possible improvement.

As these improvements and extensions are added to CHIMERA, the computational infrastructure around the hardware platform will also continue to grow. This growth is inevitable, as the data volumes generated on petascale platforms will dwarf even the most ambitious simulation environments of today. We anticipate each CHIMERA simulation will
produce more than 10–100 TB of data per run, the exact number depending strongly on the size of the thermonuclear network used for the nuclear burning and the phase space resolution (20 or more energy groups) of the neutrino transport employed. Robust and straightforward I/O and data workflow tools will be essential to obtain scientific insight from these petascale simulations.

4. Two-dimensional simulations
The current version of CHIMERA has been used to model core-collapse supernovae in two spatial dimensions (for a recent example, see figure 2) [18]. The outcomes in these simulations are promising and have forged a deeper and, in certain important respects, new understanding of the supernova mechanism. We find, as others do, that the shock wave initially stalls and becomes a quasi-stationary accretion shock after propagating out to less than 200 kilometers (the iron core is about 1000 kilometers in size). 200–500 milliseconds then elapse (depending largely on the progenitor), during which time large-scale convective motions develop in the neutrino heated region below the shock, as expected. Distinct, rising high-entropy (hotter) plumes grow and become separated by narrower, low-entropy (cooler) downflows. The rising high-entropy plumes begin to push the shock outward, causing local dome-like distortions. As the evolution continues, these plumes merge and grow, distorting the shock even more. By 140 milliseconds for an 11 solar mass progenitor, or 200 milliseconds for a more massive progenitor, two or three plumes dominate the flow. Significantly, at this time the shock begins to exhibit global distortions of a quasi-oscillatory time-dependent character, which we attribute to the \( l = 1 \) SASI mode. The shock continues to undulate in a global low-order mode until the oxygen layer, which has been infalling with the matter outside the shock, begins to impinge on one of the extended lobes of the shock. This happens by 180 milliseconds after bounce for an 11 solar mass progenitor, and by 300–500 milliseconds for more massive progenitors. When it does, the energy generated by the oxygen burning of the shock-heated material causes the shock undulations to rapidly grow and a highly asymmetric explosion to occur in the 11 Solar mass case. Simulations beginning with 15 and 20 Solar mass progenitors are ongoing, and the final outcomes are not yet determined but are, nonetheless, promising.

A critical time scale between the stall of the shock and its subsequent rejuvenation is needed in order to explain observed supernova element synthesis, large-scale asymmetry, and remnant neutron star masses. For example, models that explode too quickly [5; 44; 45; 46; 17; 47] do not develop low-mode distortions, which lead to large-scale asymmetries. In our proposed scenario, as briefly described above, this critical time scale is naturally provided by the time required for the oxygen layer to reach the shock. Until that time has elapsed, neutrino energy deposition, aided by convection, supports the shock at a mean radius of several hundred kilometers, but is not able to revive it. The oxygen burning, which commences when the oxygen layer is advected through the shock, provides an additional source of energy. This is sufficient to initiate a shock revival. Moreover, the time to reach the oxygen layer is greatly reduced by the SASI.

5. Three-dimensional simulations
The current state of supernova modeling must move to 3D. Virtually all 2D models exhibit large, low-order deviations from spherical symmetry, which appear as sloshing modes (\( l=1 \)) along the symmetry axis [18]. The work reported in [49] has shown that this mode may not persist in three dimensions, and surprising results can appear in 3D [50]. In 3D simulations, the standing accretion shock instability (SASI) leads to the growth and development of a “spiral mode” with an attendant redistribution of angular momentum below the shock. This spiraling flow beneath the supernova shock is capable of depositing significant angular momentum onto the PNS, causing it to spin up. The predicted spin periods are \( \sim 50 \) ms, in the range of the observed spin periods of young pulsars [51; 49; 50]. Moreover, such spins can be generated
beginning with nonrotating progenitors, complicating the link between progenitor characteristics and final neutron star properties. These simulations provide specific evidence that core-collapse supernova models must be performed in three dimensions.

No three-dimensional models to date have included all of the following: (1) multifrequency neutrino transport, (2) convection and other fluid instabilities, (3) rotation, (4) nuclear burning, and (5) magnetic fields. In particular, no three-dimensional core-collapse supernova models exist that include at least multifrequency neutrino transport, regardless of other physics included—that is, that satisfy the criterion for realism discussed earlier in this section. (2) and (3) have been included in models without neutrino transport or with gray (frequency-integrated) neutrino transport [17; 51; 49; 52].

We have recently undertaken three-dimensional simulations using CHIMERA. These simulations are evolved through core bounce in one spatial dimension. The profound spherical symmetry seen during core collapse and the absence of symmetry breaking processes like neutrino-driven and PNS convection and the SASI during the infall epoch make this strategy perfectly reasonable. Figure 3 is a snapshot of matter entropy and electron fraction for one of these simulations shortly after the evolution has moved from 1D to 3D (at roughly 19 ms post core bounce). As the evolution proceeds, convection and the SASI will break the apparent spherical symmetry in the matter configuration. These simulations will mark the world’s first fully three-dimensional supernova simulations incorporating spectral neutrino transport and detailed nuclear burning capable of modeling realistic nuclear energy release. Though stellar rotation and magnetic fields must be added to future simulations to account for the full panoply of known physics in the problem, these initial simulations mark an important milestone in supernova modeling.
Figure 3. Rendering of the matter entropy (orange colormap) and the electron fraction (blue colormap) in a three-dimensional supernova simulation using CHIMERA. The snapshot is taken roughly 5 ms from the relaxation of spherical symmetry (see text). The spatial resolution of the simulation is 304 radial zones, 76 azimuthal zones, and 152 longitudinal zones; 20 energy groups were used to resolve the neutrino spectra.

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