Petascale Supernova Simulation with CHIMERA

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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 describe some major algorithmic facets of the code and briefly discuss some recent results. The multi-physics nature of the problem, and the specific implementation of that physics in CHIMERA, provide a rather straightforward path to effective use of multi-core platforms in the near future.

1. Introduction
Twenty years ago, the nearest supernova since the invention of the telescope was observed in the Large Magellanic Cloud. This supernova, SN 1987a, provided a raft of important observables that have served to shape the computational modeling of core-collapse supernovae in the intervening years. The historic detection of roughly two dozen neutrino events from the explosion served to confirm the fundamental paradigm of stellar core collapse and the attendant weak interaction physics that accompany the formation of a neutron star \([1]\). The lightcurve and spectra of the explosion \([1]\) and the morphology and evolution of the SN 1987a remnant \([2]\) have been cited as strong evidence that the explosion mechanism itself is asymmetrical, inducing strong mixing in the inner precincts of the star and producing global deformations. Over the same twenty years, the considerable growth in computing power has begun to shape our understanding of the explosion mechanism, both in helping us meet the observational constraints provided by SN 1987a and other supernovae and by providing new, wholly computational discoveries (e.g. see \([3]\)). We can count ourselves fortunate to be standing on the edge of the petascale computing era, as modern understanding of core-collapse supernovae has made it all too clear that the explosion mechanism is a fundamentally multi-dimensional, multi-scale, and multi-physics phenomenon \([4; 5; 6]\), with a complexity found in few other physical problems. We are developing a code, CHIMERA, to attack this problem on current and near-future platforms, incorporating as much physical fidelity as possible given the resources available and the need to explore the parameter space of possible physical and astrophysical inputs.
Figure 1. Schematic of CHIMERA’s assumed geometry. The hydrodynamics is evolved in the three-dimensional space defined by \( r, \theta, \phi \). At each point along each \( r \), a neutrino phase space is evolved as well, spanned by 2 neutrino propagation angles, \( \Theta \) and \( \Phi \), and a neutrino energy, \( \epsilon \). The heart of the “ray-by-ray-plus” approximation lies in the assumption that each ray, \( r \), can, for the most part, be decoupled from neighboring rays during the transport step, requiring only integral corrections (e.g. lateral pressure gradients). We assume the imposed boundary conditions on each radial transport solution mimic the effects of neighboring rays. The additional degrees of freedom provided by the nuclear network are not shown. (Diagram from H.-T. Janka)

2. Code Architecture

CHIMERA solves the equations of radiation hydrodynamics using a “ray-by-ray-plus” approximation for the neutrino transport coupled to directionally split hydrodynamics. Ideally, neutrino transport should be implemented with full multi-D Boltzmann transport. However, this ideal will be computationally expensive indeed, if not prohibitive, even on petascale platforms for highly-resolved simulations. We compromise by implementing a ray-by-ray-plus approximation (cf. [9]) 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 (see Figure 1). 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 [10].

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 [7], 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/MVH3), the “ray-by-ray-plus” neutrino transport (MGFLD-TRANS), and the nuclear kinetics (XNET). These three “heads” are augmented by a sophisticated equation of state for nuclear matter (e.g. LS-EOS [8]) and a self-gravity solver capable of an approximation to general-relativistic gravity. Here, we describe two development efforts currently underway in CHIMERA: our implementation of the method of Müller & Steinmetz [11] for determining the gravitational field in our three-dimensional simulations and our improvements to the nuclear kinetics solver in the code.
3. Poisson Solver

The use of a spherical grid to facilitate the neutrino transport calculations leads us naturally to the algorithm of Müller & Steinmetz [11] for solving Poisson’s equation in spherical coordinates. Their approach begins with the integral form of Poisson’s equation,

\[
\Phi(\mathbf{x}) = -G \int \frac{\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} d^3\mathbf{x}',
\]

and expands the integrand in terms of spherical harmonics, \(Y_{lm}(\theta, \phi)\). This approach has the distinct advantage of requiring only a single global sum across processors. Furthermore, the computational work per zone scales only as \(N_r(L+1)^2\), where \(N_r\) is the number of zones in the radial direction and \(L\) is the order of the highest spherical harmonics used in the expansion of the above integral. As a result, this algorithm is both efficient and highly scalable.

The details of this algorithm are carefully described by Müller & Steinmetz [11], so we only briefly describe the method here. We begin by expanding the Poisson integral in spherical harmonics:

\[
\Phi(r, \theta, \phi) = -G \sum_{l=0}^{\infty} \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_{lm}(\theta, \phi) \int_{4\pi} d\Omega' Y_{lm}(\theta', \phi') \left( \int_0^r r' r'^{l+2} \rho(r', \theta', \phi') + r^l \int_r^\infty dr' r'^{l-1} \rho(r', \theta', \phi') \right).
\]

One then need only calculate the local zone integrals

\[
A_{ijk}^{lm} = \int_{\phi_{k-1}}^{\phi_{k-1}} \int_{\theta_{j-1}}^{\theta_{j-1}} \sin \theta d\theta d\phi Y_{lm}^* (\theta, \phi) \int_{r_{i-1}}^{r_i} dr r^{l+2} \rho(r, \theta, \phi),
\]

\[
B_{ijk}^{lm} = \int_{\phi_{k-1}}^{\phi_{k-1}} \int_{\theta_{j-1}}^{\theta_{j-1}} \sin \theta d\theta d\phi Y_{lm}^* (\theta, \phi) \int_{r_{i-1}}^{r_i} dr r^{l-1} \rho(r, \theta, \phi),
\]

and sum them over the 3D spherical grid

\[
C_{n}^{lm} = \sum_{i=1}^{n} \sum_{j=1}^{N_\theta} \sum_{k=1}^{N_\phi} A_{ijk}^{lm},
\]

\[
D_{n}^{lm} = \sum_{i=1}^{n} \sum_{j=1}^{N_\theta} \sum_{k=1}^{N_\phi} B_{ijk}^{lm}.
\]

The potential at any grid point can then be generated by a sum of the spherical harmonics weighted by these coefficients. Note that the only global communication occurs in the summation to produce \(C_{n}^{lm}\) and \(D_{n}^{lm}\).

In practice, one assumes the density is a slowly varying function of \((\theta, \phi)\), such that the angular zone integrals in Eqn. 3 can be pre-computed assuming a constant density within each zone. Beer & Podsiadlowski [12] assume a locally linear density profile in computing the radial integral in Eqn. 3, while Müller & Steinmetz [11] assume a constant density within the zone such that the integral can be solved analytically.

Both authors report maximum errors of order 1% in the computed potential of an oblate spheroid, and find no significant improvement beyond \(l = 14\). This spectral Poisson solver is augmented in CHIMERA with general-relativistic corrections to the spherical component as described in [13].
Figure 2. A portion of the nuclear N-Z plane important for supernova nucleosynthesis. The color map gives the abundance of each species at the indicated density and temperature (roughly $6 \times 10^5$ g/cm$^3$ and 4.7 billion K, respectively). The locations of the current 14 isotope network species are marked with $\alpha$’s. The extents of the 150 isotope network are circumscribed by the dashed line, exhibiting the good, but not complete, coverage for the chosen conditions.

4. Nuclear Reaction Network
The nuclear composition of the stellar matter in CHIMERA is followed using a hierarchy of methods. For regions where Nuclear Statistical Equilibrium (NSE) applies (generally temperatures $> 5.5$ GK), the equation of state (EOS) of Lattimer and Swesty [8] provides the composition for densities $> 1.7 \times 10^8$ g cm$^{-3}$. Below this density, matter in NSE is described similarly by 4 nuclei (neutrons, protons, helium, and a representative heavy nucleus) in a highly modified version of the EOS described by Cooperstein [14]. For regions not in NSE, the nuclear composition is evolved using the thermonuclear reaction network of Hix & Thielemann [15]. In the current models, this fully implicit general purpose reaction network employs only reactions linking the 14 alpha nuclei from $^4$He to $^{60}$Zn (see Figure 2). Data for these reactions is drawn from the REACLIB compilation [16]. An additional iron-like nucleus is included to accommodate a neutron-rich freezeout, which the alpha network is unable to follow, as all included nuclei have equal numbers of neutrons and protons.

While this 14 element reaction network is sufficient to schematically follow the major nuclear burning stages encountered in the supernova event, it is insufficient to study the detailed supernova nucleosynthesis as it is revealed in astronomical observations and terrestrial composition. Neither is the representative nucleus scheme of [8] and [14] sufficient for this purpose, though it is advantageous for providing the bulk EOS properties [17]. Detailed
nucleosynthesis requires evolving 150 or more nuclear isotopes throughout the matter which is ultimately ejected. Simple replacement of the 14 element network with 150 isotopes in the fully implicit Backward Euler integration scheme represents a several hundred-fold increase in the computational cost. Given that \( \approx 5\% \) of the execution time is spent in the alpha network in current simulations, this cost is prohibitive. However, recently developed methods [18] can decrease the computational cost of the network during the most computationally expensive supernova burning phases by factors of 5 or more by employing local partial equilibria (termed quasi-equilibrium or QSE) to reduce size of the system of equations which must be integrated. 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.

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