Type Ia supernovae: advances in large scale simulation

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Abstract. Using the newly developed petascale codes, MAESTRO and CASTRO, the Computational Astrophysics Consortium is simulating the explosion of white dwarf stars as Type Ia supernovae. Since the outcome is sensitive to where the nuclear runaway ignites, three sorts of calculations are being carried out. In the first, the presupernova convection of rotating and non-rotating white dwarfs is followed for several hours (star time), using MAESTRO, in order to determine just where the first sparks ignite. The turbulent nuclear combustion of the explosion is then followed using the compressible hydro code CASTRO in two other studies that assume either central or off-center ignition. Current calculations are running on 4000 – 12000 CPU, but larger studies, on a greater number of CPU, will be required to increase the Reynolds number of the ignition study and the fidelity of the turbulence in the explosion studies.

1. Introduction

Type Ia supernovae (SN Ia) happen when a white dwarf in a binary star system accretes a critical mass and explodes [3]. These are among the brightest explosions in the universe and, because they always starts with the same critical mass, roughly the Chandrasekhar mass, 1.38 solar masses, SN Ia light curves are usually very similar to one another. This makes them excellent "standard candles" for cosmology. There is some diversity however, because not the same fraction of every star burns, and, within that fraction, the composition may vary. Particularly important is the production of radioactive ^{56}Ni, whose decay (6.1 d halflife) to ^{56}Co and ^{56}Co to ^{56}Fe (77.1 d halflife) powers the emissions of the supernova. Indeed, the observed diversity of SN Ia luminosities chiefly reflects their variable ^{56}Ni production. About three-fourths of the iron in nature has been made as ^{56}Ni in these sorts of explosions.

The fraction of the white dwarf that burns depends upon where it is ignited and how fast it burns. If it ignites in the center, then burning proceeds in a large solid angle and the star will become unbound, even without a subsequent detonation. If it ignites off-center, then a buoyant burning bubble of hot ashes floats off to one side, and only a small fraction of the star is consumed before the burning reaches the surface and is quenched. Such a supernova would either not blow up at all or explode very weakly unless there was a lot of burning after this initial breakout. This fast late time burning must occur as a detonation wave, and the two-stage explosion where this happens is sometimes referred to as a "delayed detonation supernova." A displacement of ignition of only 10–20 km from the center of a star with an initial radius of 1700 km suffices to separate the two classes of models [11]. The actual physics of the detonation transition itself is still uncertain and is debated [6,4,9,2].

2. Ignition

The convective phase of the SN Ia problem is characterized by highly subsonic flow. With a fully compressible hydrodynamics algorithm, the time step would be dictated by the propagation of sound waves, and evolving the system would require a large number of steps and lose accuracy. By filtering out the sound waves while still retaining the compressibility effects important to the flow, the time step is based instead on the fluid velocity itself, giving an enormous efficiency boost. This was the motivation for the development of the low Mach number hydrodynamics code, MAESTRO [5]. With MAESTRO, we performed the first full-star, three-dimensional simulation of the final hours of convection leading up to the ignition of the first flame [10]. Subsequent calculations including rotation (Figure 1) have demonstrated a sensitivity to stellar parameters that may translate into variations in the supernova properties (see also [8]).
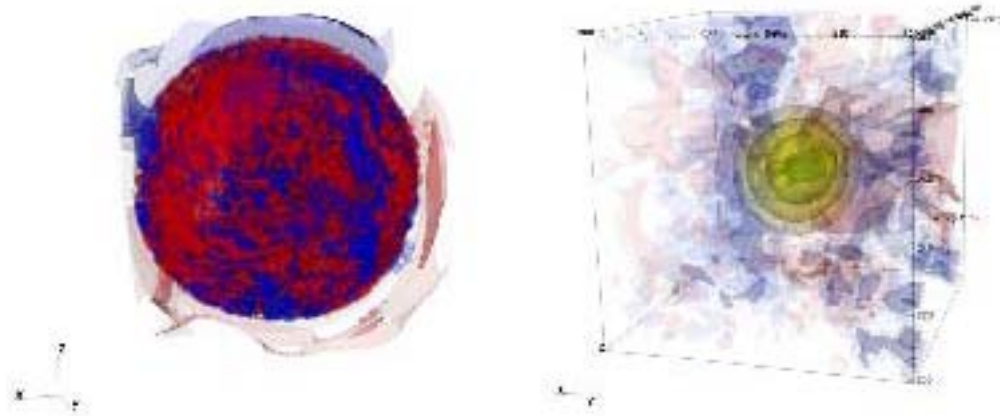

Figure 1. Calculation using MAESTRO of ignition in a rotating Chandrasekhar mass white dwarf shown just seconds before the first flame ignites. In this model, the ratio of centrifugal force to gravity is 1.5% at the equator. The left frame shows radial velocity iso-surfaces. Red indicates outward speeds of 12 (faint red) or 20 km s^{-1} (dark red); blue indicates inward speeds in the same range. The right frame also shows radial velocities with red again indicating motion outwards and blue, inwards. It additionally shows surfaces of constant nuclear energy generation rate (0.32, 1, 3.2, 10, and 32×10^{13} erg g^{-1} s^{-1}) at a time close to the point of run away. Only the inner 1000 km are shown. This calculation required 0.6 M CPU hr on Jaguar at ORNL. Zoning was 3843 which is good for the resources available, but not enough to give a turbulent numerical Reynolds number or to well resolve the ignition radius.

As in past studies, we find that the convective flow demonstrates spontaneous symmetry breaking. An axis for the flow is arbitrarily established that is maintained for a few convective periods, then a rapid migration occurs to another angle. Small amounts of rotation break this pattern. We performed a number of simulations varying the resolution and rotation rate and found ignition radii ranging from essentially central ignition to 85 km off center. This suggests that explosion calculations need to consider both central and strongly off-center ignition.

These calculations are computationally demanding. The calculations using a 384^3 grid required about 0.6 million CPU-hours on 1728 processors to evolve the system for a few hours, and at this resolution, we were still not adequately resolving the turbulence that dominates the convective flow. Our estimates suggest that a resolution of at least 1536^3 will be required both to resolve the inertial range of turbulence and to give an accurate measure (more than a few zones) of the ignition displacement. If uniformly gridded, achieving this higher resolution would increase the necessary computational resources by 4^4 to about 150 M CPU-hours. Keeping work-per-processor constant, such a calculation would run on ~110k processors—MAESTRO is capable of scaling to this regime [1].

Recently however [5], adaptive mesh refinement (AMR) has been added to MAESTRO, resulting in an anticipated savings of about a factor of 6 for this problem and putting the needed resources at 25 M CPU-hours. Even with this savings though, this is a petascale problem.

To date, our calculations end at the ignition of the first flame. However, the ignition process itself may continue, with ignition occurring at multiple points separated closely in time. At the point of the first ignition, the energy release is large enough that the low Mach number approximation breaks down. Over the next year, we will explore ways around this, including modifying the behavior of the reaction network at the point of ignition, adding a simple flame model, and exploring the addition of long-wavelength acoustic information. We have also begun the work necessary to transfer a model [1] from MAESTRO to our compressible hydrodynamics code CASTRO. This can provide another mechanism to explore the potential for subsequent ignition events as well as allow for an exploration of the explosion dynamics with realistic ignition conditions.

3. Explosion

Once born, nuclear burning produces bubbles and sheets of hot ash embedded in cooler, denser fuel. The ash floats, producing Rayleigh-Taylor and Kelvin-Helmholtz instabilities and, ultimately, turbulence. These instabilities, which feed back on the flame sheet, folding and distorting it, govern the rate at which the burning progresses, and, ultimately, the power and brightness of the supernova.

This turbulent nuclear combustion of the explosion was followed using the compressible hydro code CASTRO. Both central and off-center ignition are considered (Figure 2). The initial computational domain was 8,192 km in each dimension, but this was remapped to a larger domain as star expanded. Initially, the base grids of the calculations were 512^3 with 4 levels of AMR and refinement ratios of 2. As the star expanded, the refinement was allowed to decrease. The burning front was modeled as a thick flame and a carbon fraction between 0.1 and 0.4 indicated the location of the flame surface. This and the density were two criteria for AMR refinement. Active flame surface was always tracked at the finest resolution, less than 1 km at the beginning and 4 km at the end, thus the number of finest grids increases rapidly with flame propagation and stellar expansion. Ten species were carried in the calculations, along with two-stage nuclear burning networks calculated both on the flame surface and in the hot ash.
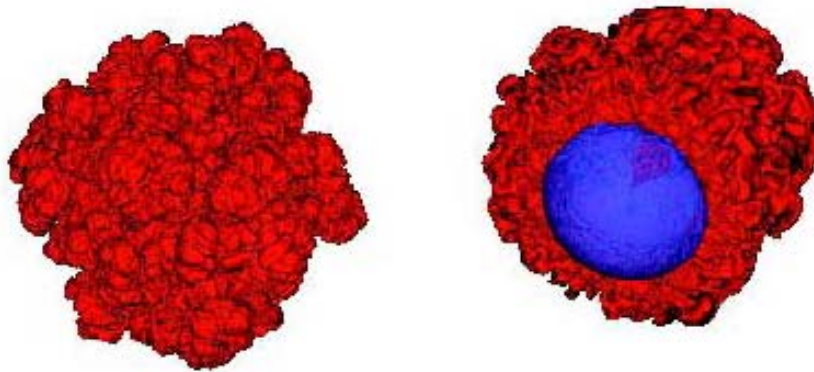

Figure 2. Two 3D simulations of SN Ia explosions using CASTRO. The left figure is of a centrally ignited deflagration with 4 levels of AMR. Red color indicates the flame surface. Initially matter within 100 km was set as hot ash with a perturbed surface. The figure shows the flame surface at a star time of 1 second when the flame has extended to 2500 km away from the center. 0.65 solar masses of iron-group elements have been synthesized. The right frame shows the results of a study of off-center ignition at a time just before the collision of ejecta on the far side, and blue color indicates the star surface. This run has a resolution of 5 km around the flame surface. Only about 0.08 solar masses of iron group elements were produced prior to the collision.

Because of its larger solid angle the central ignition case was more costly. Our first calculation ran on 4096 to 8192 CPU on Franklin and 12288 CPU on Jaguar for about 1.9 MCPU hr. Even though we dropped the finest resolution to 2 km then to 4 km, the total number of cells exceeded 1.5 billion. At a star time near 1.5 second, nuclear burning was essentially over and 0.70 solar masses of iron-group elements and 0.1 solar masses of intermediate elements (Si, S, Ar, Ca) had been produced. The star was exploding with a projected final kinetic energy of 8×10^{50} erg. This energy and iron mass are comparable to what was obtained in a previous study by the Munich group [7], but the synthesis of intermediate mass elements here is much lower. Our calculation needs to be done with greater resolution in order to reduce sensitivity to the flame model, but the Munich result for low density burning may be questionable. A calculation that fully resolved the turbulent integral scale, about 10 km, during the critical late stages of the explosion would require about 40 MCPU hr and run on 125 k CPU.

The off-center case, on the other hand, sends up a burning vortex ring to one side whose ashes erupt and roll around the star. We are looking to see whether a detonation will develop when a collision occurs on the far side of the star, as has been suggested by the Chicago FLASH team. We have studied this problem in 2D and 3D for two different choices of resolution, but are still in an exploratory phase using only moderate resolution. Our 2D results agree with both Chicago and Munich in that only a small amount of white dwarf expansion occurs during the initial rise of the bubble to the surface and spread to the far side. A vigorous collision could ignite a detonation. Our 3D calculations, however show more burning and a result that is very sensitive to just where the ignition occurs. For the small ignition radius implied by the MAESTRO studies just discussed (∼30 km), the collision on the far side of the star may be weaker than Chicago has estimated. Typical burned masses before the collision happens are 0.08 M⊙, not enough to unbind the star, but enough to cause significant expansion. However, we need to do our calculations at higher resolution and study a variety of ignition radii before drawing strong conclusions here. Fortunately, given the computer resources, we can do that. A definitive study that resolved the turbulence during the deflagration stage would take about 20 MCPU hr on 80 k CPU.

Because the flame surface tracked at the finest level occupies only a small fraction of the star, a typical simulation of the pre-detonation phase here spans 1.3 seconds of star time and has used only 0.4 MCPU hr, i.e., five times less than the central ignition study. Multiple time steps and AMR speed up the study a lot. The resolution at the flame early in the study was less than 1 km and was 5 km at late times. We plan to increase the late time resolution by a factor of at least two in the near future and to finely resolve the collision of the ashes on the far side of the white dwarf.

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