New Approaches for Modeling Type Ia Supernovae

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Abstract. Type Ia supernovae (SNe Ia) are the largest thermonuclear explosions in the Universe. Their light output can be seen across great distances and has led to the discovery that the expansion rate of the Universe is accelerating. Despite the significance of SNe Ia, there are still a large number of uncertainties in current theoretical models. Computational modeling offers the promise to help answer the outstanding questions. However, even with today’s supercomputers, such calculations are extremely challenging because of the wide range of length and time scales. In this paper, we discuss several new algorithms for simulations of SNe Ia and demonstrate some of their successes.

1. Introduction

The standard theoretical picture of a Type Ia supernova is the thermonuclear explosion of a carbon/oxygen white dwarf that accretes material from a companion star (see [1] for a good review). As the mass of the white dwarf approaches the Chandrasekhar limit—the maximum mass that can be supported by electron degeneracy pressure—the temperature and density reach the point where carbon fusion can take place. When the energy release due to the burning exceeds the local cooling rate (due to expansion and neutrino loss), ignition occurs. The burning front propagates outward from the center of the star as a thermonuclear flame, wrinkling via the Rayleigh-Taylor instability and interactions with turbulence. As it continues to burn through the star, the flame accelerates to a large fraction of the sound speed (and possibly transitions into a detonation), producing large amounts of nickel. The energy release is sufficient to unbind the star.

Large-scale computing has already led to advances in the theoretical understanding of Type Ia supernovae (SNe Ia); however, much more is still unknown. An accurate model of SNe Ia needs to capture physical processes from the scale of the carbon flame, $O(10^{-5} \text{ cm}) - O(10 \text{ cm})$, to the scale of the star, $O(10^8 \text{ cm})$. The temporal scales are equally impressive, from the century of convection leading up to the ignition of the flame to the seconds-long explosion. This is truly a multiscale problem, and even at the dawn of petascale computing, a fully resolved simulation of all these processes is beyond the available resources.

Simulations of SNe Ia can be broken down roughly into two types—large eddy simulations operating on the scale of the star (see [2, 3, 4, 5]), and small-scale simulations that resolve the
thermonuclear flame width and model a small, $< O(100 \text{ cm})$, region of the star (see [6, 7, 8, 9]). These two types of simulations are complementary in constructing a full picture of the explosion.

The large-scale simulations follow the evolution of the full star down to typical resolutions of 1 km. On scales smaller than this, they rely on subgrid models to describe the physics of the flame propagation. The majority of research groups performing full star explosion simulations use the fully compressible piecewise parabolic method [10] for the hydrodynamics. Additionally, they require a way to represent and advance the flame front—typically either thickened flames (see, e.g., [11]) or level-sets [12]. These simulations have successfully showed that a thermonuclear carbon deflagration can release enough energy to unbind the star. However, these pure deflagration models tend to produce weak explosions and leave behind too much unburned carbon. A transition to detonation at the late stages of the explosion has been proposed [13, 14], and may produce more energetic explosions [3]. Detonations are not without their problems, however [15]. In particular, it is unknown if a detonation can develop at all in these environments. This is one of the major outstanding problems in the modeling of SNe Ia.

Another major uncertainty concerns the initial conditions for the explosion. The spatial distribution of the hot spots that seed the flame can have an enormous impact on whether the explosion is successful [16, 4, 5]. In practice, large-scale calculations begin by randomly initializing one or more hot spots on the grid and propagating the flame outward from there. In reality, the white dwarf is convecting from the century or more of smoldering burning that precedes the ignition [17], and burning fronts can ignite over a finite time interval. With few exceptions [18], the large scale calculations ignore the pre-existing convective velocity field. Long-time three-dimensional simulations of the convective period are required to generate more realistic initial conditions for the ignition and resultant explosion.

Simulations on the scale of the flame can be used to formulate and calibrate the subgrid models employed by the full-star calculations. As the flame propagates outward from the center of the star, it encounters lower density fuel and the laminar flame speed decreases and the flame becomes thicker. For most of its life, the flame is in the flamelet regime—characterized by a sharp interface between the fuel and the ash. At densities less than $3 \times 10^7 \text{ g cm}^{-3}$, the flame becomes broad enough that turbulent eddies on this scale can disrupt the structure of the flame directly, without burning away. At this point, a mixed region of fuel and ash develops, and the flame is said to be burning in the distributed burning regime. Small-scale simulations of the distributed burning regime can help answer the question of whether a transition to detonation is possible late in the evolution of the explosion.

In this paper, we discuss new algorithms that allow for efficient simulation of both the small scales and the full star. Our approach exploits the fact that the pre-explosion evolution and flame propagation are subsonic; only in the very late stages of the explosion does the Mach number approach unity. Filtering sound waves allows for much longer time evolution than fully compressible codes and forms the basis for a new generation of SNe Ia evolution codes.

2. Small-scale flame modeling

2.1. Low Mach number approach

The laminar flame speed of a thermonuclear carbon flame is very subsonic, with Mach numbers less than $10^{-2}$. Efficient simulation of turbulent flames on small scales requires a code well-suited to low Mach number flows. The algorithm described below was developed originally for low-speed terrestrial combustion, which shares the common feature that the flame speed and fluid speed are both much less than the speed of sound. On small scales, the background stratification of the star is negligible, and the pressure in the domain can be assumed constant. By expanding the state variables in powers of Mach number, $M$, the pressure can be decomposed into a dynamic component, $\pi$, and thermodynamic component, $p_0$, the ratio of which is $O(M^2)$. In the low Mach number model we replace the total pressure, $p$, by $p_0$ everywhere except in the
momen\textsuperscript{t}um equation; this substitution decouples pressure and density variations and has the
effect of removing sound waves from the system. The thermodynamic constraint that $p = p_0$
can be recast, by differentiating the equation of state along particle paths, as a constraint on
the velocity field:
\[
\nabla \cdot \vec{U} = S
\]
In this equation, the source term, $S$, represents the compressibility effects due to thermonuclear
energy release and thermal diffusion.

We solve the low Mach number system using a second-order accurate approximate projection
method originally developed for solving the incompressible Navier-Stokes equations [19],
extended to low Mach number combustion [20], and explained in detail for SNe Ia in [21].
Since sound waves are filtered from the system, the timestep is limited only by the bulk velocity,
not the soundspeed. For low Mach number flows, this means that a factor of $\sim \frac{1}{M}$ fewer
timesteps are needed relative to fully compressible formulations.

The low Mach number formulation is solved in an adaptive mesh refinement framework in
order to focus the spatial resolution on the regions of the flow that are of particular interest,
such as a flame front. The gains in efficiency due to the combination of the low Mach number
formulation and adaptive mesh refinement have opened up a previously inaccessibly suite of
small-scale SNe Ia flame problems. Shown in Figure 1, for example, is a portion of a calculation
of a Rayleigh-Taylor unstable flame. The boxes represent the different levels of the adaptive
grid hierarchy. Simulations like this [8, 9] have captured the transition to distributed burning
in detail and have shown that the turbulence obeys isotropic Kolmogorov scaling.

2.2. The transition to distributed burning
More recent simulations include those that focus on the transition to distributed burning through
a parameter study of turbulent flame sheets. Figure 2 shows the response of a flame to inflowing
turbulence fuel at two different densities. In both cases, the domain width is 50 flame thicknesses
in the lateral directions. The structure of the flame is resolved with 5 zones in its thermal
thickness ($l_f = \Delta T/\max(\nabla T)$). A turbulent velocity field is generated in an incompressible
code and inflowed into the domain. The turbulent inflow properties correspond to a Kolmogrov
cascade from an integral scale of $10^6$ cm with a corresponding velocity of $10^7$ cm s$^{-1}$—these numbers are chosen to match the expected turbulent intensity in SNe Ia [13]. Active control is used to vary the inflow velocity to ensure that the flame remains statistically stationary in the domain as it accelerates.

By varying the density of the flame we can sample different regimes of combustion, from the flamelet to distributed burning. At the higher density ($3 \times 10^7$ g cm$^{-3}$), with these turbulence parameters, the flame is right at the point to transition to the distributed regime. The flame surface appears relatively smooth, with some large-scale wrinkling. The flame can simply burn through the smaller-scale turbulent eddies. At the lower density ($1.5 \times 10^7$ g cm$^{-3}$), the flame is wrinkled on a much larger range of scales. The goal with this study is to create a model for how large the mixed region of fuel and ash can grow, and from that, determine whether it is possible for a transition to detonation. These are the first ever three-dimensional simulations of distributed burning in SNe Ia.

3. Full-star low Mach number algorithms
Addressing the ignition of Type Ia supernovae requires a hydrodynamics algorithm that can follow the $M \sim 0.01$ convection for many turnover times on the scale of the full star. Previous work by research groups studying convection in SNe Ia includes a two-dimensional implicit approach [22] and use of the anelastic approximation in three-dimensions [23]. By contrast, we extend the low Mach number model described above for small-scale flows to include compressibility effects due to the stratification of the star. The ultimate goal is the development of a new simulation code, MAESTRO, that is able to carry the evolution from the convective
phase, through ignition, into the explosion phase.

Following the same procedure as on the small scale, but now allowing the thermodynamic pressure to vary with time and in the radial direction, i.e., \( p_0 = p_0(r, t) \), where \( r \) is the radial direction and \( t \) is time, we obtain a constraint on the velocity field of the form [24, 25]:

\[
\nabla \cdot \vec{U} + \frac{1}{\Gamma_1 p_0} \vec{U} \cdot \nabla p_0 = S - \frac{1}{\Gamma_1 p_0} \frac{\partial p_0}{\partial t}.
\]

(2)

Here, \( \Gamma_1 = d(\log p)/d(\log \rho) \) with \( s \) the entropy of the fluid, and \( S \) is as in (1). The \( \vec{U} \cdot \nabla p_0 \) term represents the compressibility due to the stratification. Defining

\[
\beta_0(r, t) = \beta(0, t) \exp \left( \int_0^r \frac{1}{(\Gamma_1 p_0)} \frac{\partial p_0}{\partial r} dr' \right),
\]

(3)

(see [24]) we can rewrite the constraint as

\[
\nabla \cdot (\beta_0 \vec{U}) = \beta_0(S - \frac{1}{\Gamma_1 p_0} \frac{\partial p_0}{\partial t}).
\]

(4)

The time evolution of \( p_0 \) is calculated as a hydrostatic adjustment driven by the average heating in each radial layer; the details are given in [25].

In the absence of any heating, the background stratification remains fixed, and the constraint becomes:

\[
\nabla \cdot (\beta_0 \vec{U}) = 0.
\]

(5)

If we consider an ideal gas, then \( \Gamma_1 = \gamma \) (the ratio of specific heats), and if we take the background to be isentropically stratified, then this constraint can be written as

\[
\nabla \cdot (p_0^{1/\gamma} \vec{U}) = \nabla \cdot (\rho_0 \vec{U}) = 0,
\]

(6)

which is the constraint used in the anelastic approximation. Comparisons between the low Mach number approach and the anelastic approximation [24] show excellent agreement in the regime where the anelastic approximation is valid.

We note that although the low Mach number formulation reduces to the anelastic equation set in the case of small-scale heating where the variations in temperature and density are small, the low Mach number formulation has much more general applicability. The anelastic approximation assumes a fixed background state and small variations in temperature and density from that background state. The stratified low Mach number formulation allows the background state to vary in time in response to large-scale heating [26, 25], and allows large variations in temperature and density from the background values.

The low Mach number equation set is solved with a second-order accurate, approximate projection method as in the case of the small-scale low Mach number approach. Figure 3 shows results of a comparison between a fully compressible code and the stratified low Mach number algorithm for a test case that included both large-scale and localized heat sources. Detailed comparisons between results using the low Mach number approach and those using fully compressible solvers, both with and without external heat sources, show excellent agreement between methods. As expected, the compressible solver takes many more timesteps than the low Mach number method for flows such as this that start from a quiescent state. The low Mach number approach has been demonstrated to be both accurate and efficient for long-time evolution of astrophysical phenomena [24, 25].

Future development of MAESTRO will focus on formulating the algorithm to handle non-grid aligned gravity (i.e. spherical stars), and improving the robustness of the algorithm at the edge of the star where the density drops off suddenly in the radial direction. In addition to the target problem of ignition in SNe Ia, this algorithm can be applied to classical novae and Type I X-ray burst simulations (see also [27]).
Figure 3. Comparison of a fully compressible algorithm (black contours) and the stratified low Mach number algorithm (green contours) [25]. Here we focus on a single two-dimensional plume driven by a localized heating source at $(1.2 \times 10^8, 8.5 \times 10^8)$ cm. We see good agreement for the height and width of the rising plume between the two algorithms.

4. Summary

The multiscale nature of Type Ia supernovae makes them challenging to simulate numerically. As for many multiscale problems, advances in our understanding of the physical phenomena require not just advances in computer hardware, but new algorithms that respect the physical and mathematical nature of the phenomena. This paper outlines several new algorithms for studying SNe Ia based on the low Mach number approach, and several of the successful computations which have resulted. Future work includes applying these algorithms in the hope of answering questions about the nature of ignition in SNe Ia and whether transition to detonation is possible.

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References

[1] Wolfgang Hillebrandt and Jens C. Niemeyer. Type Ia supernova explosion models. *Annu. Rev. Astron. Astrophys.*, 38:191–230, 2000.

[2] F. K. Röpke and W. Hillebrandt. The distributed burning regime in Type Ia supernova models. *Astronomy and Astrophysics*, 429:L29–L32, January 2005.

[3] V. N. Gamezo, A. M. Khokhlov, and E. S. Oran. Three-dimensional Delayed-Detonation Model of Type Ia Supernovae. *Astrophysical Journal*, 623:337–346, April 2005.

[4] T. Plewa, A. C. Calder, and D. Q. Lamb. Type Ia supernova explosion: Gravitationally confined detonation. *Astrophysical Journal*, 612:L37–L40, September 2004.

[5] D. García-Senz and E. Bravo. Type Ia Supernova models arising from different distributions of igniting points. *Astronomy and Astrophysics*, 430:585–602, February 2005.

[6] J. C. Niemeyer and W. Hillebrandt. Microscopic Instabilities of Nuclear Flames in Type Ia Supernovae. *Astrophysical Journal*, 452:779–784, October 1995.

[7] F. K. Röpke, J. C. Niemeyer, and W. Hillebrandt. On the Small-Scale Stability of Thermonuclear Flames in Type Ia Supernovae. *Astrophysical Journal*, 588:952–961, May 2003.

[8] J. B. Bell, M. S. Day, C. A. Rendleman, S. E. Woosley, and M. Zingale. Direct numerical simulations of Type Ia supernovae flames II: The Rayleigh-Taylor instability. *Astrophysical Journal*, 608:883–906, 2004.

[9] M. Zingale, S. E. Woosley, C. A. Rendleman, M. S. Day, and J. B. Bell. Three-dimensional Numerical Simulations of Rayleigh-Taylor Unstable Flames in Type Ia Supernovae. *Astrophysical Journal*, 632:1021–1034, October 2005.

[10] P. Colella and P. R. Woodward. The piecewise parabolic method (ppm) for gas-dynamical simulations. *Journal of Computational Physics*, 54:174–201, 1984.

[11] A. M. Khokhlov. Propagation of turbulent flames in supernovae. *Astrophysical Journal*, 449:695, 1995.

[12] M. Reinecke, W. Hillebrandt, J. C. Niemeyer, R. Klein, and A. Gröbl. A new model for deflagration fronts in reactive fluids. *Astronomy and Astrophysics*, 347:724–733, July 1999.

[13] J. C. Niemeyer and S. E. Woosley. The thermonuclear explosion of chandrasekhar mass white dwarfs. *Astrophysical Journal*, 475:740–753, February 1997.

[14] A. M. Khokhlov, E. S. Oran, and J. C. Wheeler. Deflagration-to-Detonation Transition in Thermonuclear Supernovae. *Astrophysical Journal*, 478:678–688, March 1997.

[15] J. C. Niemeyer. Can deflagration-detonation transitions occur in type Ia supernovae? *523:L57–L60*, September 1999.

[16] J. C. Niemeyer, W. Hillebrandt, and S. E. Woosley. Off-Center Deflagrations in Chandrasekhar Mass Type Ia Supernova Models. *Astrophysical Journal*, 471:903–914, November 1996.

[17] S. E. Woosley, S. Wunsch, and M. Kuhlen. Carbon ignition in Type Ia supernovae: An analytic model. *Astrophysical Journal*, 607:921–930, 2004.

[18] E. Livne, S. M. Asida, and P. Höflich. On the Sensitivity of Deflagrations in a Chandrasekhar Mass White Dwarf to Initial Conditions. *Astrophysical Journal*, 632:443–449, October 2005.

[19] A. S. Almgren, J. B. Bell, P. Colella, L. H. Howell, and M. L. Welcome. A conservative adaptive projection method for the variable density incompressible Navier-Stokes equations. *Journal of Computational Physics*, 142:1–46, May 1998.

[20] M. S. Day and J. B. Bell. Numerical simulation of laminar reacting flows with complex chemistry. *Combust. Theory Modelling*, 4(4):535–556, 2000.

[21] J. B. Bell, M. S. Day, C. A. Rendleman, S. E. Woosley, and M. A. Zingale. Adaptive low Mach number simulations of nuclear flame microphysics. *Journal of Computational Physics*, 195(2):677–694, 2004.

[22] P. Höflich and J. Stein. On the thermonuclear runaway in Type Ia supernovae: How to run away? *Astrophysical Journal*, 568:779–790, April 2002.

[23] M. Kuhlen, S. E. Woosley, and G. A. Glatzmaier. Carbon Ignition in Type Ia Supernovae. II. A Three-dimensional Numerical Model. *Astrophysical Journal*, 640:407–416, March 2006.

[24] A. S. Almgren, J. B. Bell, C. A. Rendleman, and M. Zingale. Low mach number modeling of type Ia supernovae. I. hydrodynamics. *Astrophysical Journal*, 637:922–936, February 2006.

[25] A. S. Almgren, J. B. Bell, C. A. Rendleman, and M. Zingale. Low mach number modeling of type Ia supernovae. II. energy evolution. *Astrophysical Journal*, 2006. in press.
[26] A. Almgren. A new look at the pseudo-incompressible solution to Lamb’s problem of hydrostatic adjustment. *Journal of Atmospheric Sciences*, 57:995–998, April 2000.

[27] D. J. Lin, A. Bayliss, and R. E. Taam. Low Mach number modeling of Type I X-ray burst deflagrations. *ArXiv Astrophysics e-prints, astro-ph/0606207*, 2006.