Verification and validation of current models of thermonuclear-powered supernovae using large-scale simulations


1CELS Directorate, Argonne National Laboratory
2HEP Division, Argonne National Laboratory
3ALCF, Argonne National Laboratory
4DOE NNSA/ASC Alliance Astrophysical Center for Thermonuclear Flashes, Department of Astronomy & Astrophysics, University of Chicago
5Department of Physics, University of Massachusetts, Dartmouth
6MCS Division, Argonne National Laboratory
7Department of Physics and Astronomy, University of Alabama

Abstract. We report initial results of a verification study to determine the fundamental properties of buoyancy-driven turbulent nuclear combustion and a comprehensive, systematic program to validate current models of Type Ia supernovae.

1. Introduction
Observations using Type Ia (thermonuclear-powered) supernovae (SNe Ia) led to the discovery of dark energy and provide one of the most promising methods for determining its properties. Most scientists believe that using these explosions to accomplish the latter will require a much better understanding of them. Two major challenges face numerical astrophysicists in the Type Ia supernova (SN Ia) field: (1) several key physical processes in these explosions are not fully understood, including buoyancy-driven turbulent nuclear combustion; and (2) very few simulations of the current models of SNe Ia have been done, making it difficult to determine which of these models is favored by observations, and even more, what values of the many parameters specifying these models are consistent with observations. We report the results of extensive large-scale, 3D verification simulations of buoyancy-driven turbulent nuclear combustion for planar flames in a channel, flame bubbles in an open domain, and flame bubbles in a white dwarf star. We have also begun a comprehensive, systematic validation of current models of SNe Ia, using through large-scale, whole-star 3D hydrodynamic simulations of these explosions using FLASH [2] and radiation transfer calculations using Sedona [5] to compare the light curves and spectra predicted by these models with high-quality data obtained by the SDSS-II Supernova Survey team and its collaborators [6]. We describe the initial results of these efforts below.
2. Buoyancy-Driven Turbulent Nuclear Combustion

We are attempting to provide definitive answers to three questions regarding buoyancy-driven turbulent nuclear combustion:

- Is it possible to describe the burning rate of a turbulent flame by a single characteristic turbulent timescale? If so, what scale dominates the flow?
- Under what conditions does a flame transition from the flamelet regime to the distributed burning regime?
- How does buoyancy-driven turbulent nuclear combustion in a stratified medium differ from turbulent nuclear combustion in a homogeneous isotropic turbulent background?

To answer these questions, we have conducted large-scale 3D simulations of (i) planar flames in a rectilinear computational domain in which \( g \) and \( \rho \) are constant; (ii) flame bubbles in an open domain, which we simulate using a rectilinear computational domain having large lateral dimensions, in which \( g \) is constant and \( \rho \) is decreasing; and (iii) flame bubbles in a white dwarf star, in which \( g \) is increasing and \( \rho \) is decreasing. Figure 1 shows a simulation of the first physical situation; Figures 2 and 3 show simulations of the latter two physical situations. We have made the following discoveries about buoyancy-driven turbulent nuclear burning:

- The rate of nuclear burning appears to be governed by the length scale corresponding to the flame polishing length \( \lambda_c \) [7] (see Figure 4).
- “Self regulation” is a physical process in which changes in the area of the flame exactly compensate for changes in the laminar flame speed, causing the nuclear burning rate to be independent of the laminar flame speed. Our simulations suggest self regulation is the result of the fundamental properties of buoyancy-driven turbulent nuclear combustion, and so occurs not only for planar flames in closed computational domains—where it has been observed previously—but also for flame bubbles in open domains, which is directly relevant to the burning that occurs during the deflagration stage of SNe Ia.

Figure 1. Frames showing two different ways of visualizing the physical properties of a simulation of buoyancy-driven turbulent reactive flow at a moment in time for a flame speed \( s = 30 \text{ km s}^{-1} \). Left frame: volume rendering of the flame surface; right frame: volume rendering of the velocity field generated by the flame [10].
Figure 2. Resolution study of simulations of a flame bubble in an open domain (mocked up by a rectilinear domain having large lateral dimensions) in which $g$ is constant and $\rho$ is decreasing.

Figure 3. Resolution study of simulations of a flame bubble in a white dwarf star in which $g$ is increasing and $\rho$ is decreasing.

Figure 4. Flame area as a function of time for different spatial resolutions for flame bubble simulations in an open domain (mocked up by a rectilinear domain having large lateral dimensions) with constant acceleration of gravity $g$ and decreasing density $\rho$. The results demonstrate convergence with resolution for spatial resolutions of 8 km or better; i.e., simulations that resolve the flame polishing length $\lambda_c$. 
• The condition $K_a = 1$, where $K_a$ is the so-called Karlovitz number, has been used in the SN Ia field as the criterion for when a flame transitions from the flamelet regime to the distributed burning regime (see, e.g., [1]). Our simulations show the flame remains in the flamelet regime even for $K_a \gg 1$. This is important because transition to the distributed burning regime is a pre-requisite for initiation of a detonation in the deflagration-to-detonation model.

3. Validation of Current Type Ia Supernovae Models

We have extended our large-scale, whole-star 3D hydrodynamic simulations of SN Ia models using FLASH [2] from the GCD models [9,4,3,8] (see Figure 5) to the pure deflagration and deflagration-to-detonation models. Taking the data from these simulations as input for radiation transfer calculations using Sedona [5], we find the following:

• The light curves predicted by the GCD model can be fit reasonably well by the MLCS2k2 and SALT2 data-driven models the supernova community uses to fit to the light curves of individual SNe Ia [6], showing that the predicted light curves are similar to those observed.

• Preliminary results based on 2D simulations show the light curves predicted by the GCD model are consistent with the Phillips relation between peak B-band magnitude and stretch and the inference from observations that most observed SNe Ia produce 0.5-1 solar masses of nickel (see Figure 6).

• Viewing asymmetric supernovae from different directions may contribute significantly to the anomalous scatter in the calibration of SNe Ia as “standard candles” (see Figure 6).

Figure 5. Images showing extremely hot matter (ash or unburned fuel) and the surface of the star at different times for an 8-km resolution simulation of the GCD model starting from initial conditions in which an 16-km radius hot bubble is offset 80 km from the center of the star. Times are (a) 0.5 s, soon after the bubble becomes Rayleigh-Taylor unstable and develops into a mushroom shape, (b) 1.0 s, as the bubble breaks through the surface of the star, and (c) 2.03 s, when the hot ash has flowed over the surface of the star and has begun to collide, and (d) 2.23 s, as the detonation wave sweeps through the star [9,4,3,8].
Figure 6. Left panel: Points corresponding to 30 different viewing angles predicted by simulations of the GCD model of SNe Ia for three different initial conditions that produce 0.71, 0.91, and 1.26 solar masses of nickel, superimposed on a scatter plot of a simulated SDSS-II sample of SNe Ia in the (stretch, B-band peak magnitude)-plane, where stretch is a measure of the rate an SN Ia fades and B-band peak magnitude is a measure of the peak luminosity of a SN Ia. Right panel: Same, except in the (color, B-band peak magnitude)-plane. These preliminary results, which are based on 2D simulations, show the light curves predicted by the GCD model are consistent with the Phillips relation between peak B-band magnitude and stretch and the inference from observations that most observed SNe Ia produce 0.5–1 solar masses of nickel.

References