Numerical Stability of Detonations in White Dwarf Simulations

Max P. Katz\(^1\) and Michael Zingale\(^2\)

\(^1\) NVIDIA Corporation, 2788 San Tomas Expressway, Santa Clara, CA 95051, USA
\(^2\) Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY 11794-3800, USA

Received 2019 February 5; revised 2019 February 27; accepted 2019 February 28; published 2019 April 4

Abstract

Some simulations of SNe Ia feature self-consistent thermonuclear detonations. However, these detonations are not meaningful if the simulations are not resolved, so it is important to establish the requirements for achieving a numerically converged detonation. In this study we examine a test detonation problem inspired by collisions of white dwarfs. This test problem demonstrates that achieving a converged thermonuclear ignition requires a spatial resolution much finer than 1 km in the burning region. Current computational resource constraints place this stringent resolution requirement out of reach for multidimensional supernova simulations. Consequently, contemporary simulations that self-consistently demonstrate detonations are possibly not converged and should be treated with caution.

Key words: supernovae: general – white dwarfs

1. Introduction

Thermonuclear detonations are common to all current likely models of SNe Ia, but how they are actually generated in progenitor systems is still an open question. Different models predict different locations for the detonation and different mechanisms for initiating the event. Common to all of the cases is a severe lack of numerical resolution in the location where the detonation is expected to occur. The length and timescale at which a detonation forms is orders of magnitude smaller than the resolution that typical multidimensional hydrodynamic simulations can achieve. The mere presence of a detonation (or lack thereof) in a simulation is therefore only weak evidence regarding whether a detonation would truly occur.

In this study we examine the challenges associated with simulating thermonuclear detonations. The inspiration for this work comes from the literature on head-on collisions of WDs, which can occur, for example, in certain triple star systems (Thompson 2011; Hamers et al. 2013). WD collisions rapidly convert a significant amount of kinetic energy into thermal energy and thus set up conditions ripe for a thermonuclear detonation. Since they are easy to set up in a simulation, they are a useful vehicle for studying the properties of detonations.

Early studies on WD collisions (Rosswog et al. 2009; Lorén-Aguilar et al. 2010; Raskin et al. 2010; Hawley et al. 2012; García-Senz et al. 2013) typically had effective spatial resolutions in the burning region of 100–500 km for the grid codes, and 10–100 km for the SPH codes, and observed detonations that convert a large amount of carbon/oxygen material into iron-group elements. These studies varied in methodology (Lagrangian versus Eulerian evolution, nuclear network used) and did not closely agree on the final result of the event (see Table 4 of García-Senz et al. 2013 for a summary).

There is mixed evidence for simulation convergence presented in these studies. Raskin et al. (2010) claim that their simulations are converged in nickel yield up to 2 million (constant mass) particles, but the nickel yield still appears to be trending slightly upward with particle count. The earlier simulations of Raskin et al. (2009) are not converged up to 800,000 particles, where the smoothing length was kept constant instead of the particle mass. Hawley et al. (2012) do not achieve convergence over a factor of 2 in spatial resolution. García-Senz et al. (2013) claim at least qualitative (though not strict absolute) convergence, but their convergence test is only over a factor of 2 in particle count, which is a factor of \(2^{5/3} = 1.3\) in spatial resolution (for constant mass particles).

Kushnir et al. (2013) test convergence over an order of magnitude in spatial resolution, and find results that appear to be reasonably well converged for one of the two codes used (VULCAN2D), and results that are not converged for the other code used (FLASH). Papish & Perets (2016) claim convergence in nuclear burning up to 10% at a resolution of 5–10 km, but do not present specific data demonstrating this claim or precisely define what is being measured. Lorén-Aguilar et al. (2010) and Rosswog et al. (2009) do not present convergence studies for their work.

Kushnir et al. (2013) argued that many of these simulations featured numerically unstable evolution, ultimately caused by the zone size being significantly larger than the length scale over which detonations form. The detonation length scale can vary widely based on physical conditions (Seitenzahl et al. 2009; Garg & Chang 2017) but is generally not larger than 10 km. Kushnir et al. argue that this numerically unstable evolution is the primary cause of convergence difficulties. They further argue that it is possible to apply a burning limiter to achieve converged results, which was used in their work and later the simulations of Papish & Perets (2016). We investigate this hypothesis in Section 3.

In this paper, we attempt to find what simulation length scale is required to achieve converged thermonuclear ignitions. The inspiration for this work comes from our simulations of WD collisions using the reactive hydrodynamics code CAS-TRO (Almgren et al. 2010; Zingale et al. 2018). We have done both 2D axisymmetric and 3D simulations of collisions of 0.64 \(M_\odot\) carbon/oxygen WDs, and were unable to achieve converged simulations at any resolution we could afford to run (the best was an effective zone size of 0.25 km, using AMR, for the 2D case). We were therefore forced to turn to 1D simulations, where we can achieve much higher resolution (at the cost, of course, of not being able to do a test that can be directly compared to multidimensional simulations).
believe the simulations presented below help show why we and others had difficulty achieving convergence at the resolutions achievable in multidimensional WD collision simulations.

2. Test Problem

Our test problem is inspired by Kushnir et al. (2013), and very loosely approximates the conditions of two 0.64 $M_\odot$ WDs colliding head-on. The simulation domain is 1D with a reflecting boundary at $x = 0$. For $x > 0$ there is a uniform fluid composed (by mass) of 50% $^{12}$C, 45% $^{16}$O, and 5% $^4$He. The fluid is relatively cold, $T = 10^7$ K, has density $\rho = 5 \times 10^6$ g cm$^{-3}$, and is traveling toward the origin with velocity $-2 \times 10^8$ m s$^{-1}$. A uniform constant gravitational acceleration is applied, $g = -1.1 \times 10^8$ m s$^{-2}$. This setup causes a sharp initial release of energy at $x = 0$, and the primary question is whether a detonation occurs promptly near this contact point, or occurs later (possibly at a distance from the contact point). The simulated domain has width 1.6384 $\times$ 10$^7$ cm, and we apply inflow boundary conditions that keep feeding the domain with material that has the same conditions as the initial fluid. Simulations are performed with the adaptive mesh refinement (AMR) code CASTRO. For the burning we use the alpha-chain nuclear network aprox13. Release 18.12 of the CASTRO code was used. The AMReX and Microphysics repositories that CASTRO depends on were also on release 18.12. The problem is located in the Exec/science/Detonation directory, and we used the inputs-collision setup.

The simulation is terminated when the peak temperature on the domain first reaches $4 \times 10^8$ K, which we call a thermo-nuclear ignition (for reference, the density at the location where the ignition occurs is approximately $1.4 \times 10^7$ g cm$^{-3}$). This stopping criterion is a proxy for the beginning of a detonation. Reaching this temperature does not guarantee that a detonation will begin, and in this study we do not directly address the question of whether an ignition of this kind always leads to a detonation. Nor are we commenting on the physics of the ignition process itself. Rather, the main question we investigate here is whether this ignition is numerically converged, and for this purpose this arbitrary stopping point is sufficient, since in a converged simulation the stopping point should be reached at the same time independent of resolution. A converged ignition is a prerequisite to having a converged detonation. We measure two diagnostic quantities: the time since the beginning of the simulation required to reach this ignition criterion, and the distance from the contact point of the peak temperature.

The only parameter we vary in this study is the spatial resolution used for this problem. For low resolutions we vary only the base resolution of the grid, up to a resolution of 0.25 km. For resolutions finer than this, we fix the base grid at a resolution of 0.25 km, and use AMR applied on gradients of the temperature. We tag zones for refinement if the temperature varies by more than 50% between two zones. Timesteps are limited only by the hydrodynamic stability constraint, with CFL number 0.5. Although this leads to Strang splitting error in the coupling of the burning and hydrodynamics for low resolution, we have verified that the incorrect results seen at low resolution do not meaningfully depend on the timestep constraint (both by applying a timestep limiter based on nuclear burning, and by using the spectral deferred corrections driver in CASTRO, which directly couples the burning and hydrodynamics). At very high resolution, the splitting error tends to zero as the CFL criterion decreases the timestep.

Figure 1 shows our main results. The lowest resolution we consider, 256 km, is typical of the early simulations of white dwarf collisions, and demonstrates a prompt ignition near the contact point. As the (uniform) resolution increases, the ignition tends to occur earlier and nearer to the contact point. This trend is not physically meaningful: all simulations with resolution worse than about 1 km represent the same prompt central ignition, and as the resolution increases, there are grid points physically closer to the center that can ignite. However, when the resolution is better than 1 km, the situation changes dramatically: the prompt central ignition does not occur, but rather the ignition is delayed and occurs further from the contact point. When we have finally reached the point where the curves start to flatten and perhaps begin to converge, the ignition occurs around 900 km from the contact point, about 1 second after contact (contrast to less than 0.05 seconds for the simulation with 1 km resolution). Even at this resolution, it is not clear if the simulation is converged. We were unable to perform higher resolution simulations to check convergence due to the length of time that would be required.

We also tested a similar configuration made of pure carbon/oxygen material (equal fraction by mass). This is closer to the configuration used in the 0.64 $M_\odot$ WD collision simulations that previous papers have focused on. However, for the setup described above, pure carbon/oxygen conditions do not detonate at all. This is not particularly surprising, since the 1D setup is a very imperfect representation of the real multidimensional case, and is missing multidimensional hydrodynamics that could substantially alter the dynamical evolution. So the small amount of helium we added above ensured that the setup ignited. (Of course, there will likely be a small amount of helium present in C/O white dwarfs as a remnant of the prior stellar evolution.) However, we can prompt the C/O setup to ignite by starting the initial temperature at $10^9$ K instead of $10^7$ K. This loosely mimics the effect from the first test where helium burning drives the temperature to the conditions necessary to begin substantial burning in C/O material. But since no helium is present in this case, it allows us to test whether it is easier to obtain convergence for pure C/O burning, even though the test itself
is artificial. The only other change relative to the prior test is that we refined on relative temperature gradients of 25% instead of 50%. The results for this case are shown in Figure 2. In this case, the ignition is central at all resolutions, but the simulation is still clearly unconverged at resolutions worse than 100 m, as the ignition becomes significantly delayed at high resolution.

This story contains two important lessons. First, the required resolution for even a qualitatively converged simulation, less than 100 m, is out of reach for an analogous simulation done in 3D. Second, the behavior for resolutions worse than 1 km qualitatively appears to be converged, and one could perhaps be misled into thinking that there was no reason to try higher resolutions, which is reason for caution in interpreting reacting hydrodynamics simulations. With that being said, our 1D tests are not directly comparable to previous multidimensional WD collision simulations. The 1D tests should not be substituted for understanding the actual convergence properties of the 2D/3D simulations, which may have different resolution requirements for convergence. Our tests suggest only that it is plausible that simulations at kilometer-scale (or worse) resolution are unconverged. This observation is, though, consistent with the situation described in Section 1, where our 2D WD collision simulations (not shown here) are unconverged, and many of the previous collision simulations presented in the literature have relatively weak evidence for convergence.

3. Numerically Unstable Burning

Kushnir et al. (2013) observe an important possible failure mode for reacting hydrodynamics simulations. Let us define $\tau_e = e/\dot{e}$ as the nuclear energy injection timescale, and $\tau_s = \Delta x/c_s$ as the sound-crossing time in a zone (where $\Delta x$ is the grid resolution and $c_s$ is the speed of sound). When the sound-crossing time is too long, energy is built up in a zone faster than it can be advected away by pressure waves. This effect generalizes to Langrangian simulations as well, where $\tau_e$ should be understood as the timescale for transport of energy to a neighboring fluid element. This is of course a problem inherent only to numerically discretized systems as the underlying fluid equations are continuous. This can lead to a numerically seeded detonation caused by the temperature building up too quickly in the zone. The detonation may be spurious in this case. If $\tau_s < \tau_e$, we can be confident that a numerically seeded detonation has not occurred. In practice, we quantify this requirement as:

$$\tau_s \leq f_\text{d} \tau_e$$

and require that $f_\text{d}$ is sufficiently smaller than one. Kushnir et al. (2013) state that $f_\text{d} = 0.1$ is a sufficient criterion for avoiding premature ignitions. Kushnir et al. enforced this criterion on their simulations by artificially limiting the magnitude of the energy release after a burn, and claimed that this resulted in more accurate WD collision simulations.

We find that for our test problem (and also the WD collisions we have simulated) we do observe $\tau_s > \tau_e$; typically the ratio is a factor of 2–5 at low resolution (see Figure 3). This means that an ignition is very likely to occur for numerical reasons, regardless of whether it would occur for physical reasons. At low resolution, adding more resolution does not meaningfully improve the ratio of $\tau_s$ to $\tau_e$ at the point of ignition. The ignition timescale is so short that almost all of the energy release occurs in a single timestep even though the timestep gets shorter due to the CFL limiter. It is only when the resolution gets sufficiently high that we can simultaneously resolve the energy release over multiple timesteps and the advection of energy across multiple zones. Even at the highest resolution we could achieve for the test including helium, about 50 cm, $\tau_s/\tau_e$ was 0.8 at ignition, which is not sufficiently small to be confident of numerical stability. Note that merely decreasing the timestep (at fixed resolution) does not help here either, as the instability criterion is, to first order, independent of the size of the timestep.

We thus investigate whether limiting the energy release of the burn (we will term this “supressing” the burn), as proposed by Kushnir et al., is a useful technique for avoiding the prompt detonation. Since the limiter ensures the inequality in Equation (1) holds by construction, the specific question to ask is whether the limiter achieves the correct answer and is converged in cases where the simulation would otherwise be incorrect or unconverged.

Before we examine the results, consider a flaw in the application of the limiter: a physical detonation may also occur...
with the property that, in the detonating zone, \( \tau_e > \tau_s \). For example, consider a region of WD material at uniformly high temperature, say \( 5 \times 10^9 \) K, with an arbitrarily large size, say a cube with side length 100 km. This region will very likely ignite, even if it is surrounded by much cooler material. By the time the material on the edges can advect heat away, the material in the center will have long since started burning carbon, as the sound-crossing timescale is sufficiently large compared to the energy injection timescale. This is true regardless of whether the size of this cube corresponds to the spatial resolution in a simulation. Suppression of the burn in this case is unphysical: if we have a zone matching these characteristics, the zone should ignite.

When the resolution is low enough, there is a floor on the size of a hotspot, possibly making such a detonation more likely. This is an unavoidable consequence of the low resolution; yet, it may be the correct result of the simulation that was performed. That is, even if large hotspots are unphysical because in reality the temperature distribution would be smoother, if such a large hotspot were to develop (which is the implicit assumption of a low resolution simulation), then it would likely ignite. If the results do not match what occurs at higher resolution, then the simulation is not converged and the results are not reliable. However, it may also be the case that a higher resolution simulation will yield similar results, for example, because even at higher resolution, the physical size of the hotspot stays the same. For this reason, an appeal to the numerical instability criterion alone is insufficient to understand whether a given ignition is real.

Figure 4 shows the results we obtain for our implementation of a “suppressed” burning mode. In a suppressed burn, we limit the changes to the state so that Equation (1) is always satisfied. This is done by rescaling the energy release and species changes from a burn by a common factor such that the equality in Equation (1) is satisfied. (If the inequality is already satisfied, then the integration vector is not modified.) We find that the suppressed burn generally does not yield correct results for low resolutions. The 64 km resolution simulation happens to yield approximately the correct ignition distance, but it does not occur at the right time, and in any case the incorrectness of the results at neighboring resolutions suggests that this is not a robust finding. The suppressed burning simulation reaches qualitative convergence at around the same 100 m resolution as the normal self-heating burn. Because of both the theoretical reasons discussed above, and this empirical finding that the burning suppression does not make low-resolution simulations any more accurate, we do not believe that the suppressed burning limiter should be applied in production simulations.

4. Conclusion

Our example detonation problem demonstrates, at least for this class of hydrodynamical burning problem, a grid resolution requirement much more stringent than 1 km. This test does not, of course, represent all possible WD burning conditions. However, the fact that it is even possible for burning in white dwarf material to require a resolution better than 100 m should suggest that stronger demonstrations of convergence are required for simulations that do not meet this resolution. This is especially true bearing in mind our observation that the numerical instability can result in simulations that appear qualitatively converged when the resolution is increased by a factor of one or two orders of magnitude but not three orders of magnitude.

This study does not directly address the problem of how, in the detailed microphysical sense, a detonation wave actually begins to propagate, as we cannot resolve this length scale even in our highest resolution simulations. Rather, we are making the point that for simulations in which a macroscopic detonation wave appears self-consistently, this is only a valid numerical result if the resolution is sufficiently high. This convergence requirement does not imply that the detonation itself is physically realistic; but, it does imply that we are not even correctly solving the fluid equations we intend to solve when the convergence requirement is not met. We believe that our test case can be useful in the future for testing algorithmic innovations that hope to improve the realism of burning at low resolutions.

This research was supported by NSF award AST-1211563 and DOE/Office of Nuclear Physics grant DE-FG02-87ER40317 to Stony Brook. An award of computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. This research used resources of the Oak Ridge Leadership Computing Facility located in the Oak Ridge National Laboratory, which is supported by the Office of Science of the Department of Energy under Contract DE-AC05-00OR22725. Project AST106 supported use of the ORNL/Titan resource. This research used resources of the National Energy Research Scientific Computing Center, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. The authors would like to thank Stony Brook Research Computing and Cyberinfrastructure, and the Institute for Advanced Computational Science at Stony Brook University for access to the high-performance LRed and SeaWulf computing systems, the latter of which was made possible by a $1.4M National Science Foundation grant (#1531492).

The authors thank Chris Malone and Don Wilcox for useful discussions on the nature of explosive burning, and Doron Kushnir for providing clarification on the nature of the burning limiter used in Kushnir et al. (2013).

This research has made use of NASA’s Astrophysics Data System Bibliographic Services.

Figure 4. Similar to Figure 1, but for simulations with the suppressed burning limiter applied (Equation (1)).
Facilities: OLCF, NERSC.

Software: CASTRO (Almgren et al. 2010; Zingale et al. 2018), AMReX (Zhang et al. 2016), yt (Turk et al. 2011), matplotlib (Hunter 2007).

ORCID iDs
Max P. Katz @ https://orcid.org/0000-0003-0439-4556
Michael Zingale @ https://orcid.org/0000-0001-8401-030X

References
Almgren, A. S., Beckner, V. E., Bell, J. B., et al. 2010, ApJ, 715, 1221
García-Senz, D., Cabezón, R. M., Arcones, A., Relaño, A., & Thielemann, F. K. 2013, MNRAS, 436, 3413
Garg, U., & Chang, P. 2017, ApJ, 836, 189
Hamers, A. S., Pols, O. R., Claeys, J. S. W., & Nelemans, G. 2013, MNRAS, 430, 2262
Hawley, W. P., Athanassiadou, T., & Timmes, F. X. 2012, ApJ, 759, 39
Hunter, J. D. 2007, CSE, 9, 90
Kushnir, D., Katz, B., Dong, S., Livne, E., & Fernández, R. 2013, ApJL, 778, L37
Lorén-Aguilar, P., Isern, J., & García-Berro, E. 2010, MNRAS, 406, 2749
Papish, O., & Perets, H. B. 2016, ApJ, 822, 19
Raskin, C., Scannapieco, E., Rockefeller, G., et al. 2010, ApJ, 724, 111
Raskin, C., Timmes, F. X., Scannapieco, E., Diehl, S., & Fryer, C. 2009, MNRAS, 399, L156
Rosswog, S., Kasen, D., Guillochon, J., & Ramirez-Ruiz, E. 2009, ApJL, 705, L128
Seitenzahl, I. R., Meakin, C. A., Townsley, D. M., Lamb, D. Q., & Truran, J. W. 2009, ApJ, 696, 515
Thompson, T. A. 2011, ApJ, 741, 82
Turk, M. J., Smith, B. D., Oishi, J. S., et al. 2011, ApJS, 192, 9
Zhang, W., Almgren, A., Day, M., et al. 2016, SIAM Journal on Scientific Computing, 38, S156
Zingale, M., Almgren, A. S., Sazo, M. G. B., et al. 2018, Journal of Physics: Conference Series, 1031, 012024