Ash-detonation interactions in multi-dimensional simulation of Type Ia supernovae

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Abstract. Thermonuclear supernovae (Type Ia SNe) are believed to result from the complete disruption of a near-Chandrasekhar-mass white dwarf (WD) by explosive thermonuclear runaway. Their role in galactic chemical evolution ultimately depends on a reliable and robust understanding of the explosion mechanism. We have undertaken a study of turbulent thermonuclear combustion in these events, focusing on the effects of increased physical fidelity in simulations, through improved resolution and increased dimensionality. We begin with a series of detonation simulations at low WD densities that we will use for baseline metrics against which subsequent simulations will be measured. We have performed these simulations using a version of the FLASH code[1]. We show progress on a set of simulations in one, two, and three spatial dimensions designed to explore the impact of dimensionality on the evolution of the detonations, and thereby clearly delineate the role of the nuclear kinetics. By performing a suite of simulations incorporating an alpha network at several levels of maximum mesh refinement, we will be able to quantify the effects of resolution and network size on future results.

1. Introduction
Driven by the need to explain the physical mechanism that generates the one of the Universe’s brightest standard candles, Type Ia supernovae, considerable effort has been expended to understand the physics of burning degenerate carbon and oxygen in exploding white dwarf stars. For Type Ia supernovae it is believed that the detonation, which drives the explosion, is preceded by a sub-sonic burning phase that pre-expands the white dwarf and, due to turbulence driven by that burning, leaves the carbon and oxygen in the interior of the white dwarf riddled with more evolved pockets of ash. The ash presents a likely damping obstacle to a subsequent detonation.

Maier & Niemeyer (2006), here after M&N, carried out a small number of 1-D and 2-D simulations in order to test the ability of detonations to pass through ash restrictions and thin funnels of fuel separating neighboring regions of ash [2]. Limited computational resources restricted the resolution of their 2-D study to 0.50 cm, which is not sufficient to fully resolve the detonation at the appropriate densities. We build on their preliminary studies, reproducing their results and running simulations at higher resolutions and in 3-D.
We begin with initial conditions similar to those of M&N [2]. Using the FLASH adaptive mesh hydrodynamics code [1], we set up a system of length 1024 cm and width of 128 cm with a reflecting boundary at 0 cm and an outflow boundary condition at 1024 cm. The long sides of the box have periodic boundary conditions. Our 3-D setup has a height of 128 cm. This setup allows the resolution to be equal in all dimensions. The FLASH code refines the mesh based on temperature and density differences between grid cells. In regions where there are small gradients between cells the code de-refines the mesh.

As initial conditions we choose a composition of 50% $^{12}$C and 50% $^{16}$O by mass at a temperature of $10^7$ K and a material velocity of 0 cm s$^{-1}$. To ignite the detonation we set the initial conditions in a 25.6 cm “match head” to a temperature of $10^{10}$K and a material velocity of $10^9$ cm s$^{-1}$. Halfway down the tube, fuel funnels are formed by two opposing semi-circles of ash with a composition near NSE. The narrowest constriction formed by the two semi-circles will be referred to as the width of the fuel funnel. For the 3-D case we used “soup cans” of ash where two semi-cylinders formed the constriction for the fuel funnel so the constriction had the same width along the third dimension. For all simulations described here, we use a fuel density of $5.0 \times 10^7$ g cm$^{-3}$. In all cases nuclear burning is turned off in the shock itself.

2. Resolution in 1-D

We ran 1-D simulations without ash to study the formation of the detonation. Figure 1 is in agreement with M&N and shows that the behavior of the maximum nuclear energy generation associated with the detonation is erratic for resolutions courser than 0.125 cm [2]. Though it is less erratic using 0.125 cm resolution, true convergence to a steady energy generation rate does not occur until the resolution is set to 0.031 cm. Thus the burning associated with the detonation, excluding the shock, is fully resolved at 0.031 cm resolution. The burning must be sufficiently resolved to conclusively determine the fate of the detonation.

![Figure 1](image-url)  
**Figure 1.** Maximum energy generation rate plotted over time for a detonation in 1-D at three resolutions. The behavior of energy generation rate associated with the detonation is erratic until the resolution is fine enough to resolve the burning.
3. Resolution Studies in 2-D and 3-D

![Figure 2](image1.png)

**Figure 2.** The survival of an under-resolved detonation shown in carbon abundance. Resolution is 0.5 cm.

![Figure 3](image2.png)

**Figure 3.** The death of a well resolved detonation shown in carbon abundance. Resolution is 0.031 cm.

We explored cases with ash constrictions in 2-D and in 3-D, with a number of different resolutions and configurations as shown in the table. Our results confirm the 2-D results of
Table 1. Resolution Study

| Case Number | Resolution cm | Dimensions for Flame | Ash position cm | Fuel funnel width cm | Cellular Structure | Detonation Survived? |
|-------------|----------------|----------------------|-----------------|----------------------|--------------------|---------------------|
| 1           | 0.5            | 2                    | 512             | 16                   | No                 | Yes                 |
| 2           | 0.5            | 2                    | 786             | 16                   | No                 | No                  |
| 3           | 0.5            | 2                    | 786             | 20                   | No                 | Yes                 |
| 4           | 0.25           | 3                    | 786             | 20                   | No                 | Yes                 |
| 5           | 0.25           | 2                    | 786             | 20                   | No                 | No                  |
| 6           | 0.125          | 2                    | 786             | 20                   | Yes                | No                  |
| 7           | 0.125          | 3                    | 786             | 20                   |                    |                     |
| 8           | 0.031          | 2                    | 786             | 20                   | Yes                | No                  |

M&N, at the insufficient resolutions they report [2]. For example, Figure 2, case 1 in the table, shows conditions similar to those reported by M&N with 0.5 cm resolution, where the detonation survives passing through the ash constriction. However, if the ash was located further from the match head as in case 2, the detonation did not survive unless the width of fuel funnel was extended to 20 cm, as in case 3. Based on their 1-D results, M&N expected that no conclusions could be drawn from under-resolved numerical experiments. Our preliminary study indicates that the detonation will not survive passing through the ash constriction if the resolution is sufficient to resolve the detonation. Figure 3 shows a time series of a case with 0.031 cm resolution. In this case the burning front becomes detached from the pressure front soon after the flame emerges from the ash and the detonation dies.

Figure 4 shows the setup and end state of a 3-D trial, case 4 in the table, run at 0.5 cm resolution. The gross behavior in 3-D is similar to that of its 2-D analog, in that the detonation survives. Figure 5, which shows a comparison of a slice of the 3-D case with its 2-D analog, demonstrates that the smaller scale structure in the two simulations differs. The 3-D flame front is slightly slower than that of the 2-D after it emerges from the ash. Both of these observations are consistent with more efficient turbulent cascade in the 3-D case.

![Figure 4](image_url)

**Figure 4.** Initial setup and end state of a 3-D case at 0.05 resolution. The detonation survives the ash, but this resolution is insufficient to resolve the detonation.
Figure 5. Slices of the 3-D case share the gross features of their 2-D analogs.

Future work will include a systematic study of the effects of resolution on this problem in 2 and 3 dimensions. We are also planning to investigate more complicated ash geometries for the 3-D cases.

4. Cell Structure

Figure 6. The carbon burning cells at 0.125 cm resolution, a, and 0.031 cm resolution, b. All distances given in cm.

Multi-D simulations allow the formation of cellular detonation structures that were first observed in terrestrial gaseous explosions and have since been studied theoretically and numerically for nuclear burning [3][4][5][6].

The cellular structure results from transverse instabilities in the detonation. This instability could impact Type Ia supernova models, by increasing the effective reaction length of the detonation compared to that predicted by 1-D models, thereby altering the detonation speed and final composition of the resulting ash. The transverse waves and the resulting unreacted pockets of fuel could also change the conditions for detonation failure due to the incomplete energy release [4][6].

Cell formation occurs in all of our trials with resolutions finer than 0.125 cm, consistent with the results of [5] and [4]. Figure 6 uses the magnitude of the pressure gradient to display the cellular structure that results from carbon burning for resolutions of 0.125 cm and 0.03 cm.
Figure 7 shows the oxygen cells burning cells which form on a longer timescale and are an order of magnitude larger than the carbon cells. Gamezo et al. (1999) found that the size of the cells as well as the time needed for them to form is greatly impacted by resolution [4]. However, Timmes et al. (2000) found that the size was independent of the spatial resolution once the cells were fully resolved [5]. Consistent with Timmes et al., we do not notice a large difference in the size of the oxygen burning cells between the different resolutions. However, the smaller carbon burning cells appear to be markedly larger in the 0.125 cm resolution case than in the 0.031 cm resolution case, likely indicating that we are not fully resolving carbon burning at 0.125 cm resolution.

5. Conclusions
Though this work is still ongoing, we have learned several important lessons. Our higher resolution study supports the conjecture of M&N [2], that a detonation front can not survive passage through ash or fuel constrictions caused by ash if the width of the constriction is close to the detonation thickness. This is an important lesson because the burning must be sufficiently resolved to conclusively determine the fate of the detonation. This study also implies that the 2-D models for this problem are reasonable predictors of the behavior of the analogous 3-D models, though the influence of dimensionality is apparent in the size of the ash structures. This work supports the conjecture of Timmes et al. (2000) that the size of cellular structures that results from the transverse instability in the flame is independent of the resolution once the structures are sufficiently resolved [5]. In the absence of any additional data, for models that attempt to study the development of the thermonuclear runaway in Type Ia supernovae, this study suggests that detonation fronts are likely to be quenched when they encounter regions of ash.

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