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I am submitting herewith a dissertation written by Christopher Ryan Smith entitled Application of the Explicit Asymptotic Method to Nuclear Burning in Type Ia Supernova. I have examined the final electronic copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Physics.

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Application of the Explicit Asymptotic Method to Nuclear Burning in Type Ia Supernova

A Thesis

Presented for the
Master of Science

Degree

The University of Tennessee, Knoxville

Christopher Ryan Smith

August 2009

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Acknowledgments

I would first like to thank my advisor Dr. Michael Guidry for accepting me as a Master's student. Without his knowledge and insight, this project could not have happened. For his frequent assistance dealing with the intricacies of FLASH, I must thank Dr. Otis Messer. He was able to provide insight into the workings of the code that allowed problems to be overcome in hours or days instead of weeks. Dr. Viktor Chupryna, whose work laid the foundation for my own, was of much help in my understanding of how FLASH and our burner were organized. Elisha Feger, with whom I shared an office for the later part of my work, was always willing to lend his knowledge of FLASH and coding in general. I must also thank Rachel Ainsworth who was kind enough to lend her time in assisting me with the visualization of my data. Finally, I would like to thank the entire Department of Physics and Astronomy, of which I have been a part for the last seven years, for all the help and support over during my time here.

Abstract

Modern problems in astrophysics tend to require large, complex computational frameworks to solve many aspects of the system simultaneously. Calculation of the energy production through nuclear reactions is typically one of those aspects. The use of standard nuclear burning algorithms will take up the majority of the computational time with all but the smallest of networks. The explicit asymptotic method has shown promise in computing large networks faster than existing methods in various environments while retaining accuracy. The purpose of this thesis is to show that this method can be successfully used to solve complex systems using a network of realistic size in a reasonable amount of time, and to investigate some problems in the flame propagation for a Type Ia, which have never been investigated with a realistic network.

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Chapter 1

Introduction

Supernovae are some of the most energetic objects in the universe. A typical one will emit as much light as an entire galaxy during its short lifetime. They are also the primary source for elements up to the iron group. In addition, modern cosmology relies on Type Ia supernovae in particular for the accurate measurements of distance that are so important in that field. Therefore, it is only natural that they would be of much interest to the field of astrophysics. However, they are also some of the most complex systems that exist and require knowledge from most branches of physics and advanced computational methods in order to study them.

Because of their complexity, it has only been recently that computational power and numerical algorithms have developed sufficiently to allow the study of many of the details of the supernova problem. The research discussed in this thesis has been focused on the implementation of a new method of studying the nuclear burning that takes places within all stars. This has become particularly important in the study of Type Ia supernova which are believed to occur when a white dwarf is consumed in a thermonuclear runaway. Historically, the problem was investigated in a very limited form using at most the first 13 elements in the alpha chain. Often even smaller networks, or in some cases no network at all, were used due to the complexity of the reactions involved. This study aims to demonstrate a method for calculating the nuclear reactions that allows for the use of a realistically sized network, and show that the results agree with those obtained using more conventional methods.

Chapter 2

Supernova Type Ia

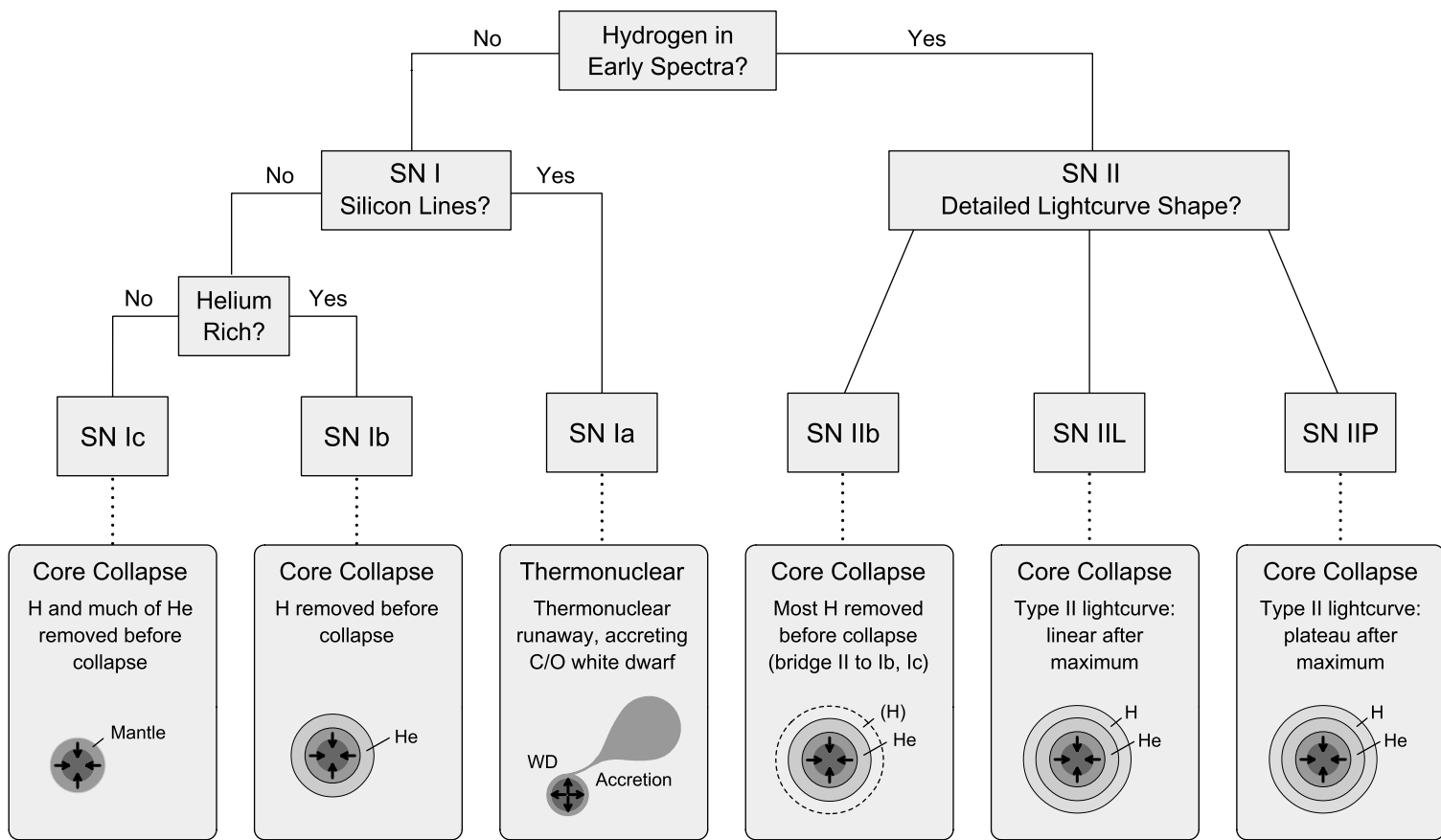
2.1 Classification

Supernovae are classified into two main types each with several subtypes based on the spectral properties they display (Figure 2.1). This is done by careful measurement of the intensity and the spectra throughout the evolution of the supernova. Type I supernovae all display weak hydrogen lines at early times, while the spectra for a Type II is dominated by the H_α lines. Type I supernovae are divided into three sub-groups, again based on their spectral properties at different times. Type Ib and Ic are characterized by a lack of Si II at early times, a feature which is prominent in Type Ia. Types Ib and Ic are then differentiated by the strength of the helium lines. Type Ib are rich in helium, while Type Ic supernovae are not.

In contrast to the Type I's, Type II supernovae are classified by the shape of the light curve rather than their spectra, specifically how the curve behaves after the maximum (Figure 2.2). Type IIL and IIP supernovae have light curves that become linear or plateau, respectively, after the maximum intensity. The third Type II, Type IIf, has a light curve that resembles Types Ib and Ic except for the lack of hydrogen. As such, they are considered to be an intermediate between the other Type II's and the Type I's. There is a fourth Type II that is not shown on the figure, Type IIn. These supernovae are characterised by the narrow hydrogen lines that appear in their spectra.

All supernovae other than Type Ia are believed to be caused by a similar mechanism called a core collapse. That is they occur when the core of a massive star ($> 8 M_\odot$) collapses in on itself and forms a neutron star or black hole, with the primary difference between the types being the composition of their

Figure 2.1: The current classification of supernovae



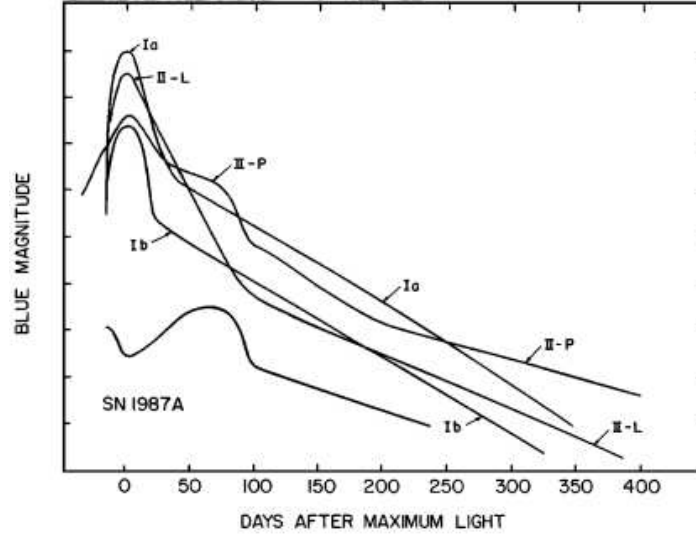


Figure 2.2: Typical light curves from each sub-type of supernova. [3]

outer layers. Type Ib and Ic supernovae have had parts of their outer layers removed by strong stellar winds or by overflow of their Roche lobe.

2.2 Evolution

2.2.1 Progenitors

Unlike the others, Type Ia supernovae are believed to be the result of a thermonuclear runaway in a white dwarf composed mainly of carbon and oxygen. There are a few circumstances under which it is believed such a runaway could occur, the most likely of which is the accretion of matter onto the white dwarf by a companion star that has overflowed its Roche Lobe. A binary system is required as C+O white dwarfs form with a typical mass of between approximately $0.6\text{--}1.1 M_{\odot}$, while the conditions for the thermonuclear burn require a the mass to be near M_{Chan} ($1.4 M_{\odot}$). As the material, which is mainly H and He, accretes onto the white dwarf, burning of the new material to C and O is required to prevent a significant amount from showing up in the observed spectra. The precise accretion and burning rates necessary to transition from the initial low mass white dwarf to the final sub-Chandrasekhar mass one are not yet known as current models do not include important pieces of physics [1].

2.2.2 Pre-Ignition

As the mass approaches the Chandrasekhar limit, the increased pressure will cause the carbon in the core to begin to smolder. Since the matter in the white dwarf is degenerate, the energy release will not go into expanding the star and will instead cause the temperature in the core to increase. During the smoldering phase, convection sets up in the white dwarf involving the majority of the star and leads to a near uniform composition [15]. This lasts until the star reaches a temperatures of approximately 1×10^9 K, at which point the energy production by carbon burning exceeds the rate at which the convection can remove it [15]. This is the start of the thermonuclear runaway.

2.2.3 Explosion

The specifics of how the explosion progresses are still under debate, but the general mechanism seems to be understood. After reaching the critical temperature, a point near the core will ignite and begin to burn outward. This burning will raise the degeneracy of the matter slightly causing it to expand, after which buoyancy will cause the newly formed bubble to rise and expand (Fig. 2.3). The burn front as represented by the edge of the bubble continues to expand as it rises. The velocity of the burn tends to increase linearly with its area. As seen in the figure, the surface of the bubble tends to get more convoluted over time as a result of the development of instabilities such as Rayleigh-Taylor. So far, the burn has been in what is known as a deflagration phase: the burn front has been moving at less than the speed of sound. From observations of the relative amounts and energies of various isotopes, particularly ^{56}Ni and ^{28}Si , we know that at some point during the explosion the burn has to transition to a detonation where the burn front moves faster than the speed of sound in the material. There are various theories as to how this might happen, but this paper will assume that it is by gravitationally confined detonation (GCD). In the GCD case, the bubble will continue to expand until it eventually reaches the surface of the white dwarf. It will then break free, but the material will lack the velocity needed to escape the stars gravity and as such will proceed to expand outward above and around the surface in a wave. Eventually, the material will collide with itself at a point almost directly opposite that at which it originally broke out (Fig. 2.4). This collision will drive the material into the surface and spark the detonation that will consume the rest of the star [47].

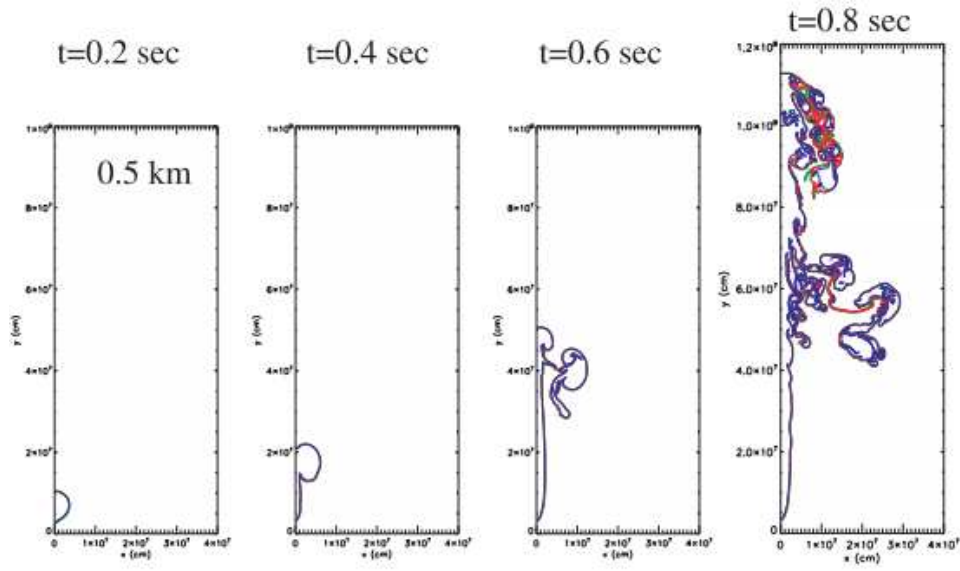


Figure 2.3: Development of a bubble. [47]

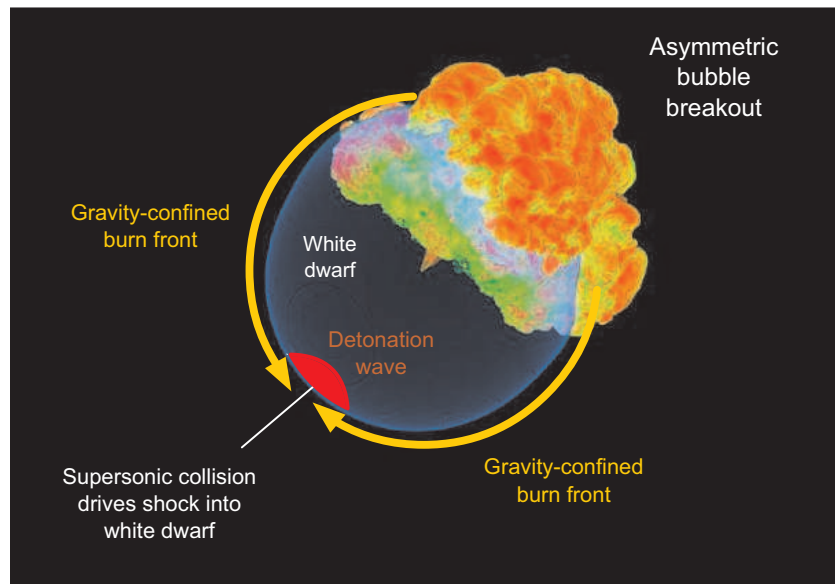


Figure 2.4: The Gravitationally Confined Detonation Mechanism [50]

2.3 Type Ia and Cosmology

As observational techniques have improved over the years, the ability to accurately gauge the distance an object is from Earth has become increasingly important. This is normally done by using what are called standard candles, classes of objects that have well defined luminosities that show little deviation between the members. Type Ia's show too much variation to be considered standard candles, however all Type Ia's display remarkably similar shapes in their light curves, absolute magnitudes, and spectra. The differences that are observed can be corrected for with a single parameter that describes the strength of the explosion [1]. They are therefore considered to be standardizable candles.

As measuring devices, the Type Ia supernova have served astronomers and cosmologists well, but there is still a significant amount of uncertainty inherent in their distance calculations. This is, of course, partially caused by imperfections in the observational data itself, but a significant amount of the uncertainty comes from a lack of understanding about the mechanism behind the supernova. With a better understanding of the explosion, the accuracy of Type Ia Supernova measurement should improve. This has become especially important in the last few decades as evidence has accumulated which indicates that the expansion of the universe is increasing. An accurate measurement of the rate of expansion is vital to understanding many fundamental questions currently faced, such as the nature of dark energy.

Chapter 3

Computational Modeling of Type Ia Supernova

3.1 Computational Difficulties

When modeling any astrophysical process, one of the most common difficulties that must be overcome is range of physical scales that must be considered, and the Type Ia supernova is no different (Fig. 3.1). The white dwarf itself is on the order of ten thousand kilometers in diameter while the flame itself is a centimeter or less in thickness [19] [20]. Fully resolving these disparate scales is out of the realm of possibility for modern computational resources, the size of a typical computational cell is one kilometer, so simpler models that approximate the correct results by statistical or other means must be employed. In addition to problems of scale, there is also the issue of stiffness. A stiff problem is one in which the timestep (Δt) needed to fully resolve the problem is limited by stability rather than accuracy considerations. An example of a stiff equation is [46]

$$y(t)' = -100y + 100t + 1 \quad y(0) = 1 \quad (3.1)$$

which has as an analytic solution

$$y = e^{-100t} + t \quad (3.2)$$

. When solved numerically, the result is dramatically different depending on the timestep used as seen in 3.2. With the smallest timestep, $h = 0.0166$, the solution is oscillatory in the exponential region, but

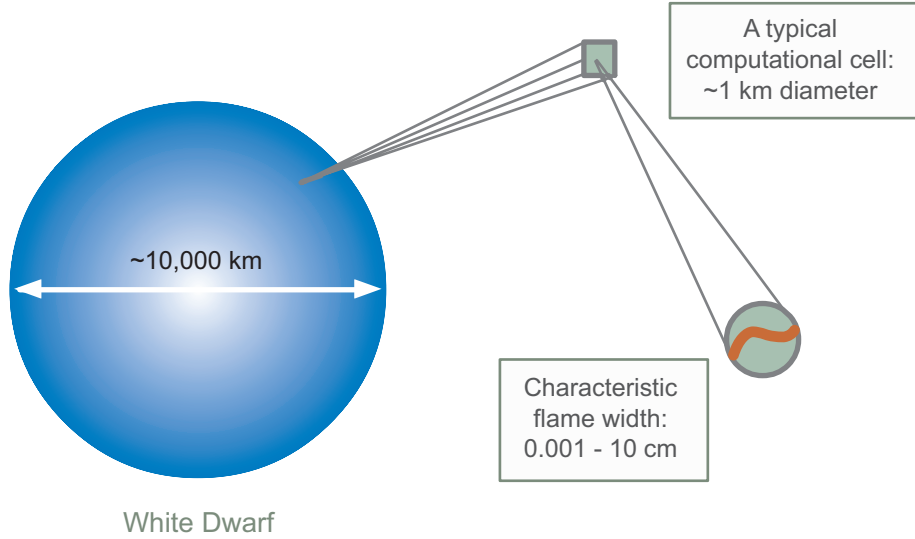


Figure 3.1: Difference in the scales that must be considered in a Type Ia. [45]

quickly approaches the analytic solution after the function becomes linear. The intermediate timestep, $h = 0.02$, oscillates about the solution throughout the entire extent. For the largest timestep, $h = 0.03$ the numerical solution is completely unstable and eventually goes to infinity [46].

3.2 FLASH Code

The FLASH code, developed by the Center for Astrophysical Thermonuclear Flashes at the University of Chicago, is a multi-dimensional hydrodynamics code using Adaptive Mesh Refinement (AMR) designed to solve problems involving thermonuclear burning. It is written mainly in Fortran 90 using the Message-Passing Interface (MPI) for parallelism and portability. FLASH is written in a modular form to allow for quick swapping of physics solvers. The software package comes with many modules already included which can be combined to solve a large selection of problems. The modular nature of the software allows for the implementation of new physics without a substantial rewriting of the entirety of the code. FLASH also utilizes a shared datastructure that all modules can access to store any variables that may be needed by multiple parts of the code without the need to pass variables explicitly. Due to the modular nature, our changes were able to be implemented through two modules: Composition and Burn (submodules of the Equation of State and Source Terms respectively) [45].

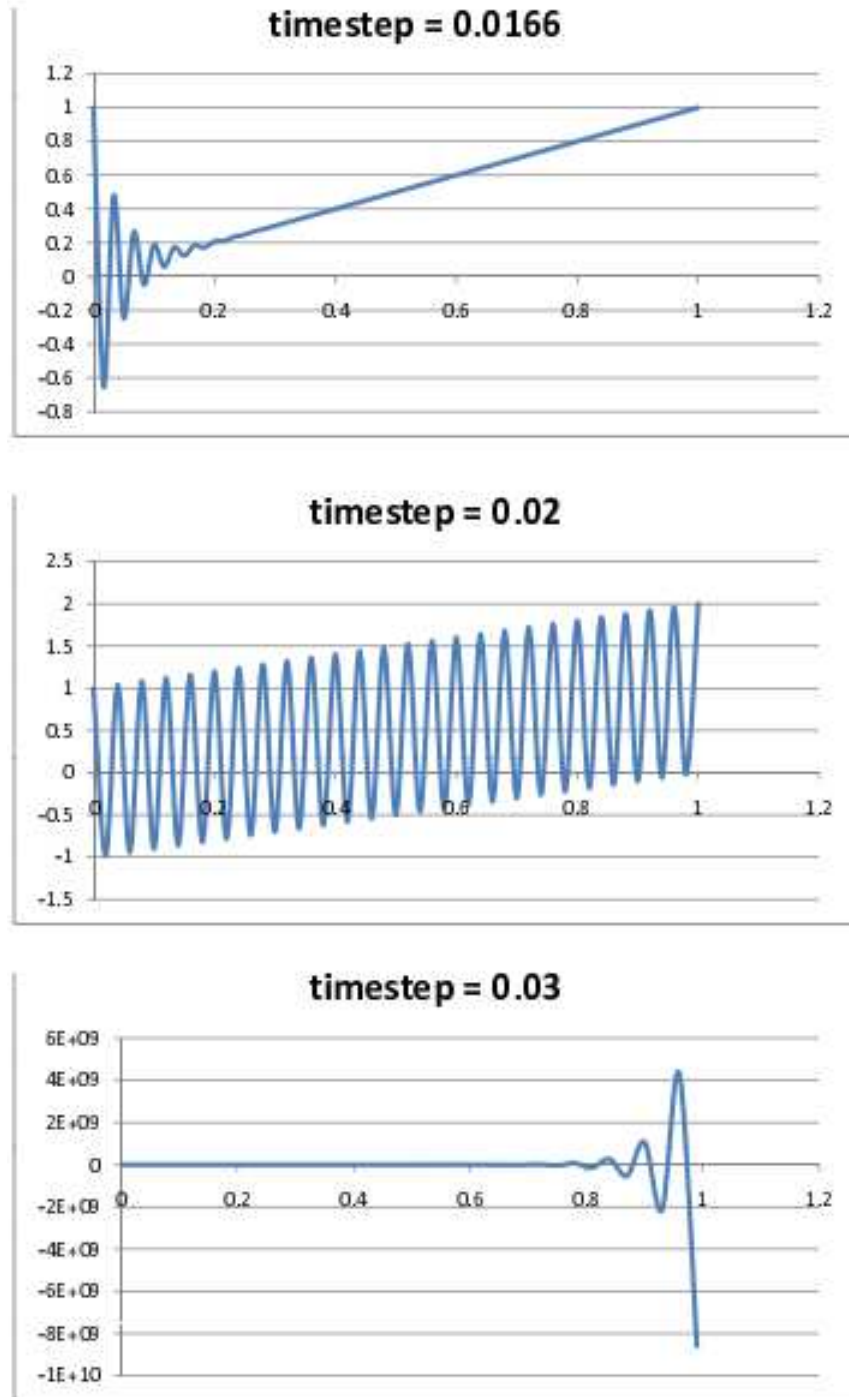


Figure 3.2: Numerical solutions to Equation 3.1 using different timesteps. [46]

3.2.1 Hydrodynamics

As mentioned earlier, the FLASH code allows for the linking of the multi-dimensional hydrodynamics with the nuclear burning. On the hydrodynamics end, FLASH employs an AMR routine, which can increase the resolution of the grid by, in 2D, creating 4 smaller blocks to replace a larger one when a given condition is met, such as a gradient becoming too steep, and decrease the resolution by merging the four blocks back into one when the flux goes back below a threshold. This allows FLASH to scale the current resolution between a given maximum and minimum as needed as the problem progresses. This is highly desirable in a supernova problem as in the majority of the star, FLASH would only need to be able to resolve the hydrodynamics of the problem and the nuclear burning would only be resolved in the regions where burning is taking place, leading to a substantial decrease in the computational resources required. Another necessary component is the equation of state, which determines the thermodynamic properties of the fluids. In our case, the Helmholtz equation of state was used [24]. This EOS uses an interpolated table to solve the differential equations for an electron-positron plasma. This still yields correct results with other materials since a simple multiplication of the result by Y_e , the number of electrons per baryon, will give the answer for the desired fluid. The Helmholtz EOS is desirable primarily because it is valid for a degenerate gas, unlike the other EOSs that are available in FLASH.

3.3 Explicit Asymptotic Method

The thermonuclear burning module used in this paper is an implementation of an explicit asymptotic method [46]. The algorithm used in the Flux Limited Forward Differencing (FLFD) method was originally developed by M.W. Guidry [49] and added to the FLASH software by V. Chupryna [45]. It is an explicit stochastic method for modeling systems with large numbers of particles. It uses Forward Euler differencing to solve for the abundance at the next time given the current abundance, the number of test particles changing from one isotope to another (the flux), and the timestep. An additional restriction must be put on the values of the fluxes to prevent the propagation of a negative population. To ensure that this does not occur, the fluxes are constrained such that $F_{ij} \geq 0$, where F_{ij} is the flux of particles from isotope i into isotope j . This allows the algorithm to take much larger timesteps than it would normally as the slight negative populations introduced by numerical errors are a major limiter on the size of the timestep in many explicit methods.

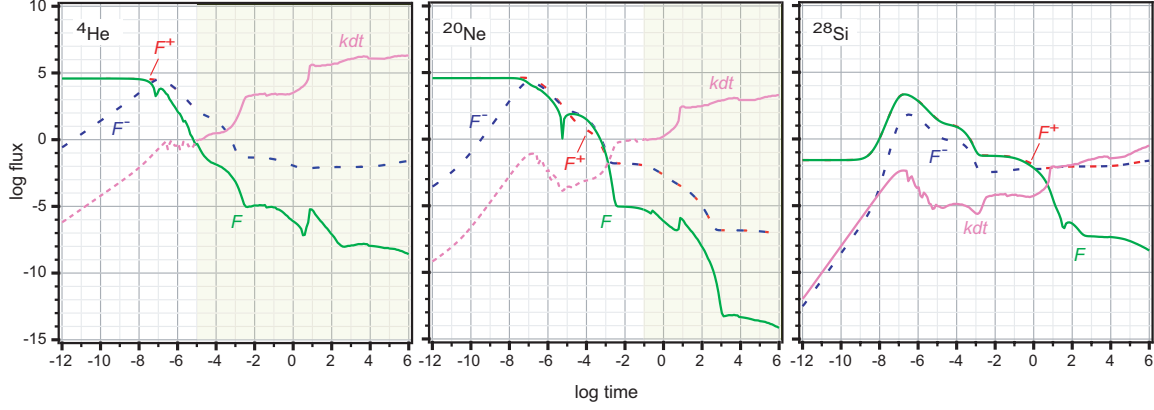


Figure 3.3: Fluxes and the asymptotic approximation. Three isotopes are shown from an alpha network run under constant conditions $T = 3 \times 10^9 \text{K}$ and $\rho = 1 \times 10^7 \text{gcm}^{-3}$ [49]

The FLFD method works well as long as the fluxes are not in the asymptotic region. In this region the incoming and outgoing fluxes are both very large, and the differences between them are many orders of magnitude less than the fluxes themselves. Once the calculation enters the asymptotic region, a small numerical error in the flux can lead to a large error in the actual rate, and therefore the timesteps tend to crash. The rates for some isotopes can become asymptotic very early in the calculation, while some may never, as shown in Fig 3.3. An explicit asymptotic method was then developed to deal with this situation as detailed in [45]. The derivation discussed eventually yields the new equation for for the population

$$y_n^{(2)} \simeq \frac{F_n^+}{k_n} - \frac{1}{k_n \Delta t} \left(\frac{F_n^+}{k_n} - \frac{F_{n-1}^+}{k_{n-1}} \right) \quad (3.3)$$

$$k^i \equiv \frac{F_i^-}{y_i} \quad (3.4)$$

Where y_n is the abundance of isotope n , F^- is the sum of the rates that deplete isotope n , F^+ is the sum of the rates that increase n , and $F/eqF^+ + F^-$. The method that is used in a given situation is decided for each isotope as follows

1. If $k^i \Delta t < 1$, use the flux-limiting explicit algorithm.
2. Otherwise, update the population using the approximation given in Equation 3.3.

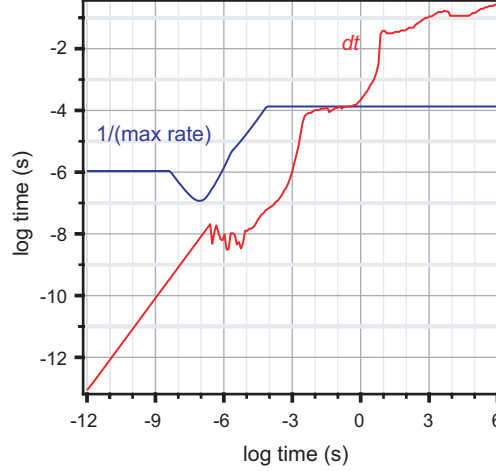


Figure 3.4: Network timesteps dt and maximum explicit timestep $1/(\text{max rate})$ for the calculation illustrated in Fig. 3.3 [49]

Through the use of the asymptotic approximation, we are able to take increasing larger timesteps as more and more of the rates become asymptotic. The speed increase over an explicit method limited by the maximum rate is clearly shown in Fig. 3.4 for a simple integration of the CNO cycle. Also, it should be noted that the region in which the timestep for the asymptotic method is greater than that for a normal explicit method is also the region that takes most of the calculation time due to the plot being log/log in time. An extreme example of this is given in figure 3.5 for the CNO cycle where a calculation that would take the explicit asymptotic method one second would take a standard method longer than the age of the universe.

3.3.1 Recent Progress

There have been several changes that have been incorporated into the FLASH code since the publication of [45]. They are mainly corrections to the way the code had been implemented at the time, along with a few slight improvements in performance, the most important of which is the change to a realistic equation of state which is better suited to the conditions encountered during a Type Ia simulation than the polytropic EOs used in earlier tests. The changes lead to the calculation yielding qualitatively different results as can be seen by comparing Fig. 3.6 and Fig. 3.7. Both calculations were made using an 150-isotope nuclear network and only calculated a single computational zone. The initial conditions were a composition of 50/50 carbon and oxygen with a temperature of $T_9=3\text{K}$ and $\rho = 1 \times 10^7 \text{ g cm}^{-3}$. Most notably the oxygen burn occurs much

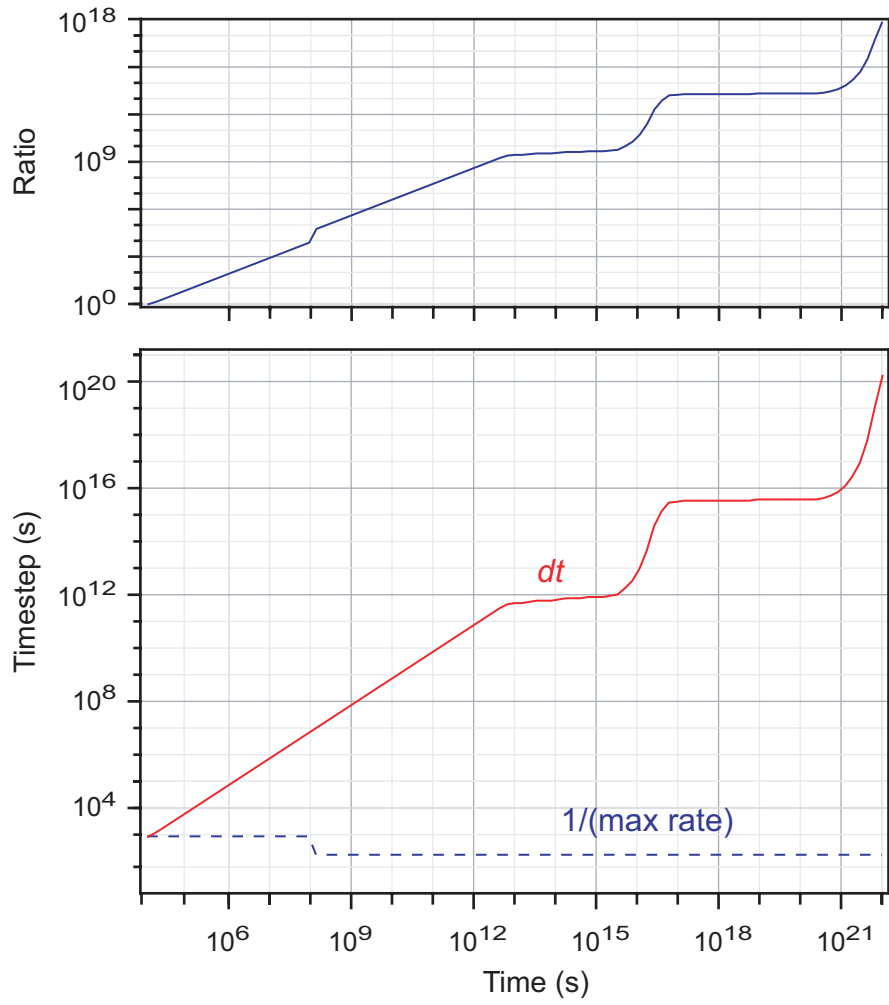


Figure 3.5: Integration timesteps in the CNO cycle for the explicit asymptotic integrator. The upper plot shows the ratio of the actual timestep to the maximum expected to be stable for a normal explicit method, estimated as $1/(\text{max rate})$. [49]

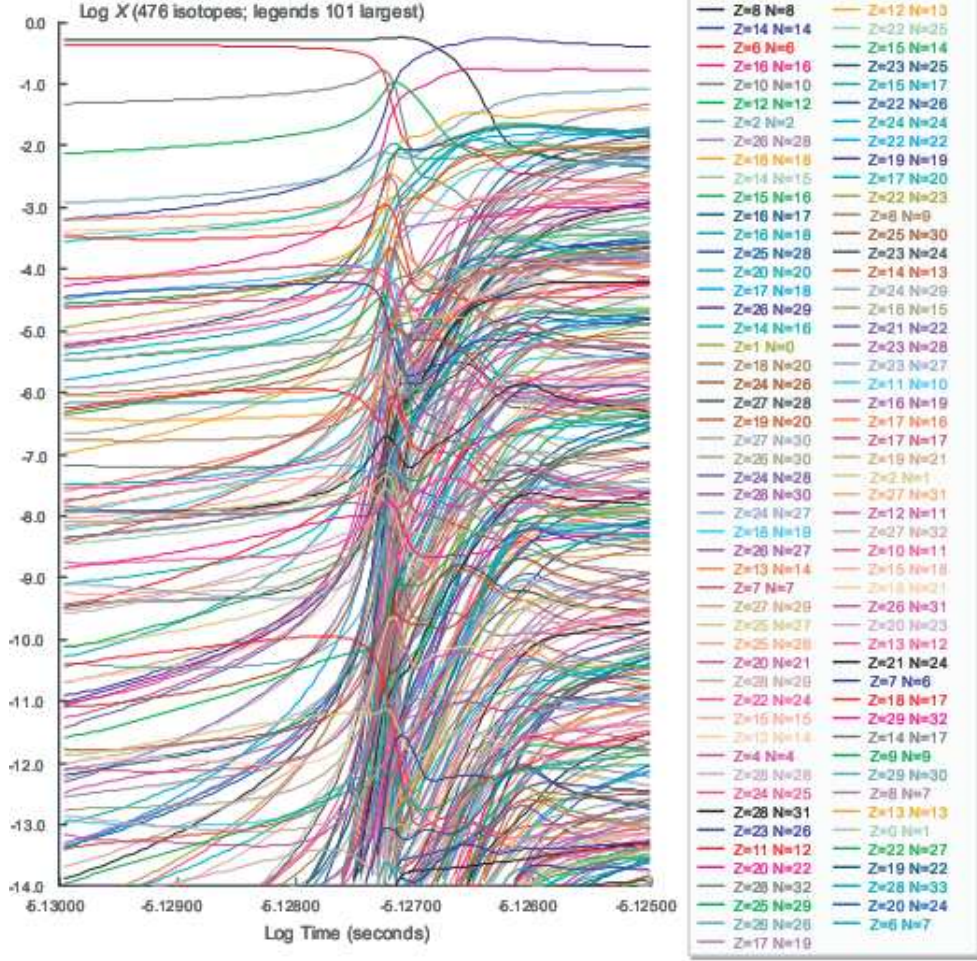


Figure 3.6: Results: 150-Isotope Network as of December, 2008. [45]

later than the carbon in the current results, rather than immediately following it. Also while the carbon flash still occurs in a narrow region, it no longer resembles a delta function. While the speed has also increased by a factor on the order of 100 since December (the original calculation took approximately 9hrs to run, while the newer case ran in 35min, both on a single processor), there are still many improvements to be made to the code in the way of optimization, both through improvements of the algorithm and standard numerical optimization.

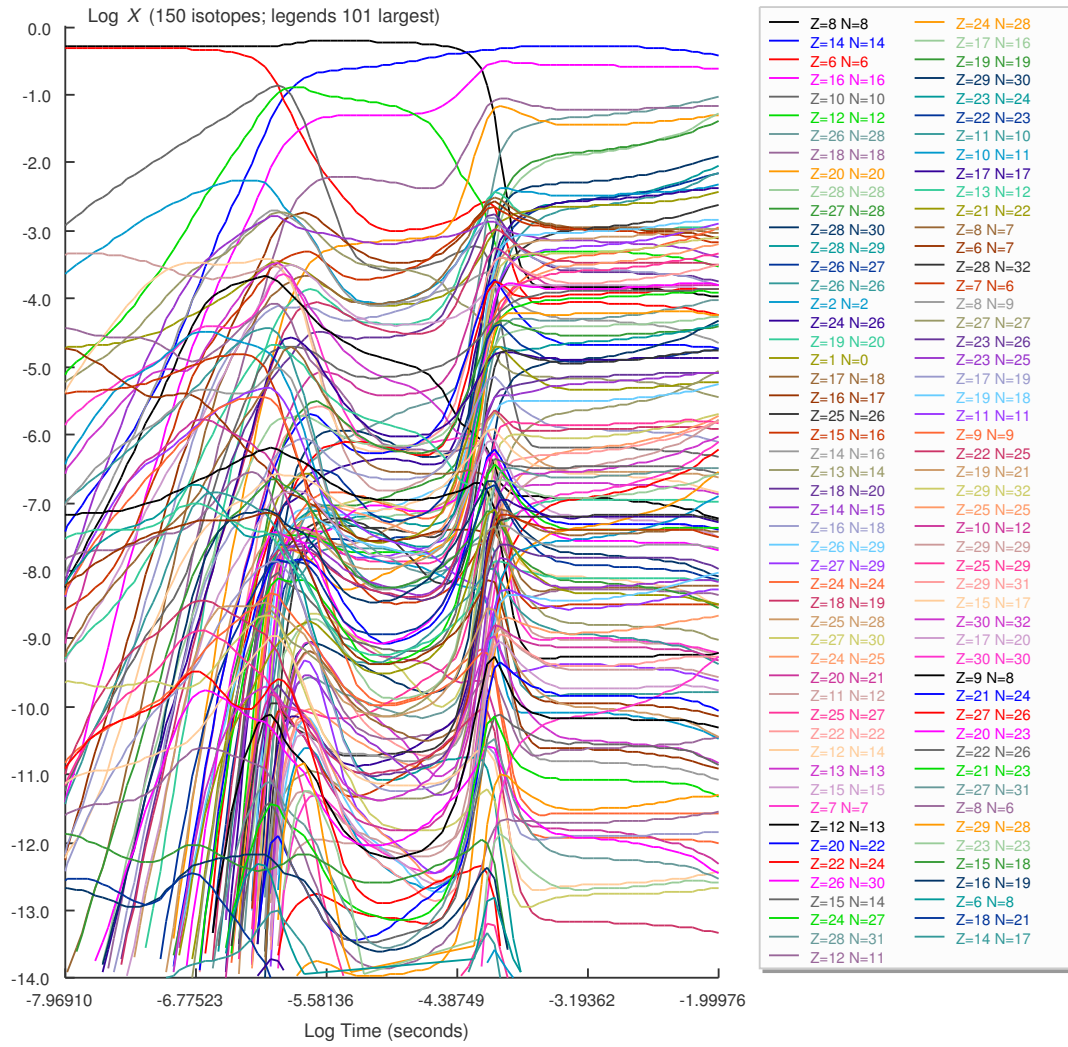


Figure 3.7: Results: 150-Isotope Network as of July, 2009.

Chapter 4

Results

As a test of the explicit asymptotic method, a comparison will be made of results from this burner and the results obtained in the paper by Maier and Neimeyer [48]. Their paper reported on the ability of a detonation shock within a Type Ia supernova to survive crossing an area of previously burned material. Due to constraints on time and computational resources, it was only possible to recreate one of the cases that they examined. A variation of the problem is also looked at in which the ash has been replaced by reflecting boundaries as define in the FLASH code. The final calculation was a repeat of the first, but with a larger nuclear network consisting of 150 isotopes instead of 13. The initial conditions for all of the calculations were taken directly from Reference [48], and are summarized in Table 4.1. The columns Fuel, Ash, and Burn refer to the regions of the initial setup. The experimental region is a 2D area that extends 1024 cm in the x direction and 128 cm in the y . In my calculations, I started th burn at 400cm in an effort to cut down on the computational time required. This was deemed acceptable as the burn front is unchanged during the propagation through the removed region. The Ash region consists of two hemispheres of radii 56 cm that are centered at the top and bottom, $y = 0$ cm and $y = 128$ cm respectively, of the region at $x = 500$ cm. This yields a gap between the two regions of ash that is 16 cm wide. The Burn conditions are defined in the first 20 cm in the x direction, and describe the detonation that will be propagating through the material. The Fuel is everything else. The boundary conditions of the problem were set so that the left x boundary is reflective while the right x boundary is outflow. The y boundaries are both set to be periodic.

Table 4.1: Initial Conditions, Approx13

	Fuel	Ash	Burn
C12	0.5	0.0	0.5
O16	0.5	0.0	0.5
Ni56	0.0	1.0	0.0
$T/10^9$ K	0.1	4.823	10
$\rho/10^7$ g cm ⁻³	5.0	1.103	5.0
$\frac{dx}{dt}/10^9$ cm s ⁻¹	0.0	0.0	1.0

4.1 Results Using an Explicit 13 Isotope Alpha Network

4.1.1 Hard Barriers in FLASH

The first test that was done used the reflecting barriers defined with FLASH rather than ash as the obstruction. The computational grid consisted of three regions which from left to right were a square region consisting of 9 blocks, a horizontal line of 3 blocks that lies in the middle of the y domain, and a rectangular region measuring 3 blocks in the y direction and 6 blocks in the x . The size of the domain is such that each block is 8 cm on a side giving a resolution of 1 cm. The entire region has a if filled with Fuel as described in the above table, except for the region of $x \leq 2$ cm, which is initialized to Burn (Fig. 4.2). All the boundaries except the right x edge are set to be reflecting. The $x+$ boundary is set as outflow.

4.1.2 Ash hemispheres

In this test, the setup from the Maier paper was recreated as closely as possible with the time and computational resources available. The initial conditions are listed in Table 4.1. The left edge of the region was placed at 420 cm and the initial thickness of the Burn region was 20 cm. This was done so that the properties of the burn front would be as similar to that of the Maier paper as possible when the flame encounters the ash. A test was made in which the flame was started at $x = 0 - 20$ cm. By the time the flame had reached the ash, it had cooled to temperature of approximately $T = 7 \times 10^9$ K. Also, the temperature of the fuel was raised from $T = 1 \times 10^7$ K in the Maier paper to $T = 1 \times 10^8$ K here. This was done as an attempt to alleviate an as yet unresolved error. FLASH was allowed to refine a total of 3 times in this case, giving a final resolution of 3.8 cm.

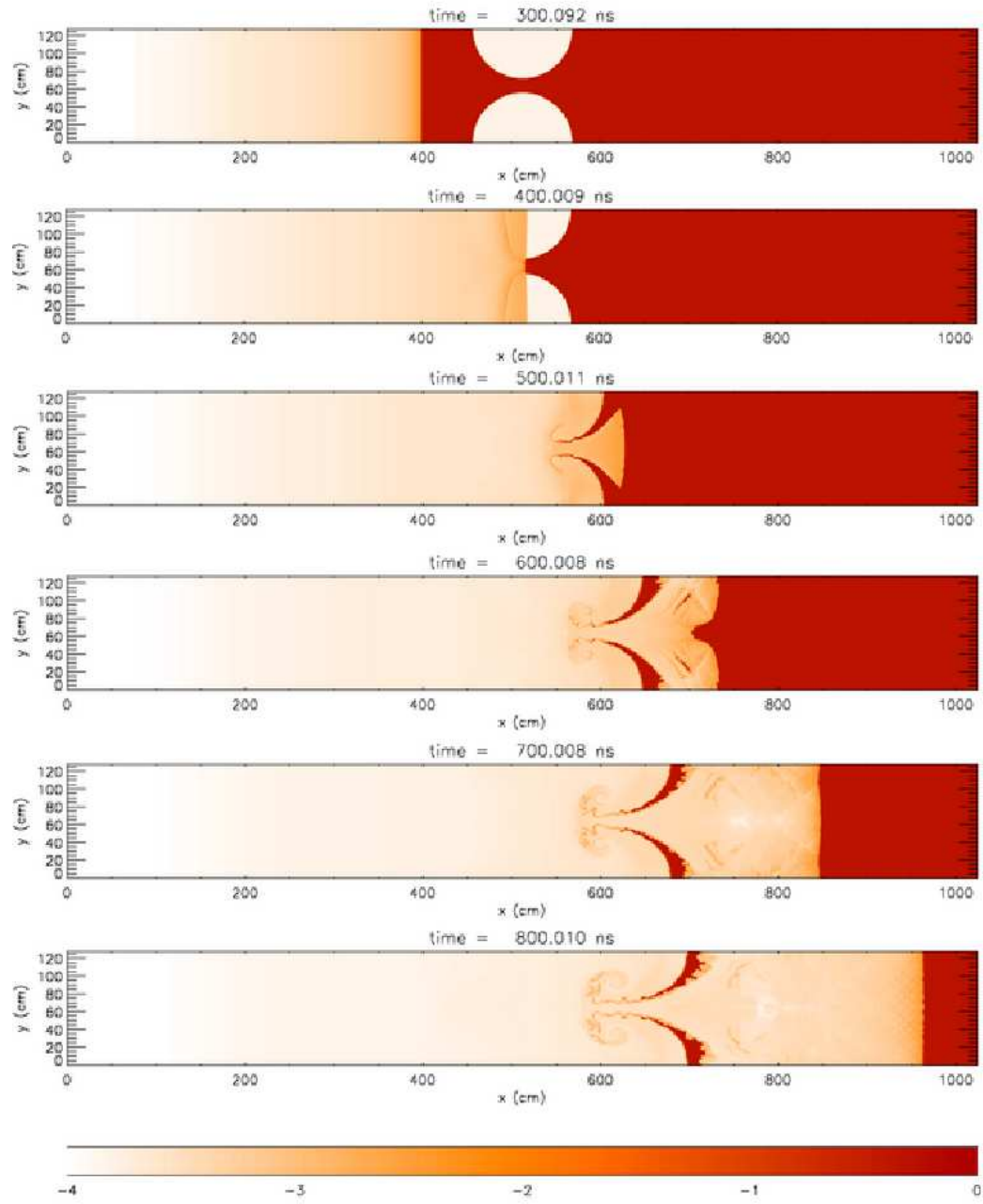


Figure 4.1: ^{12}C mass fraction at various times on a log scale from [48].

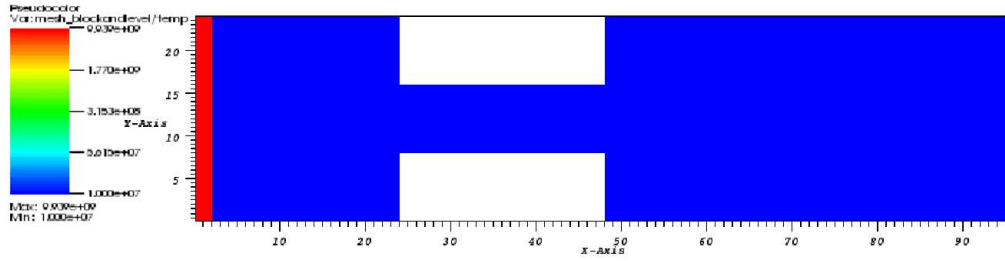


Figure 4.2: Initial temperature distribution using a logarithmic scale for the case with barriers.

In this case, the instability forms as the burn front is passing through the constriction (Fig. 4.3-4.5).. There are pockets of unburned material present well behind the burnfront which appears to be mixing with the ash. Also, the shape of burn front appears to be somewhat different from what was seen in the Maier paper, though this could be an effect of the lower resolution which was used, in the present study. In the later plots, the burn front has begun to reform into a plane wave. This is still well within the timeframe of the Maier results, though the spatial region that is covered during this time is somewhat larger. Most likely this is a result of starting the flame closer to the ash. Early tests showed that when started from zero, the flame had slowed significantly relative to the initial value, though it was still moving at a velocity well above the speed of sound in the fuel (Fig. 4.6).

In a slightly different test, this one done with the same conditions on the Ash and Burn, but with the Fuel at a $T = 3 \times 10^9$ K and $\rho = 1 \times 10^7 \text{gcm}^{-3}$, the effects of interacting with ash that is slightly denser than the fuel is observed. This run was also started slightly further from the ash than the previous one. The left edge here was defined as being at 300 cm with the Burn region again being 20 cm thick. The resolution of the run was 7.5 cm. As can be seen from Fig. 4.8, the detonation front is compressed somewhat by the ash, but not nearly to the extent seen in Fig. 4.1. The turbulence that is seen in the Maier paper is almost completely absent in these results, though that is to be expected: the Richtmeyer-Meshcov instability forms when the detonation shock encounters a discontinuity in density [48]. The presence of the previously burned material seems to have very little effect on the burn front. This is partially the result of the low resolution at which the computation was run artificially smoothing out the system.

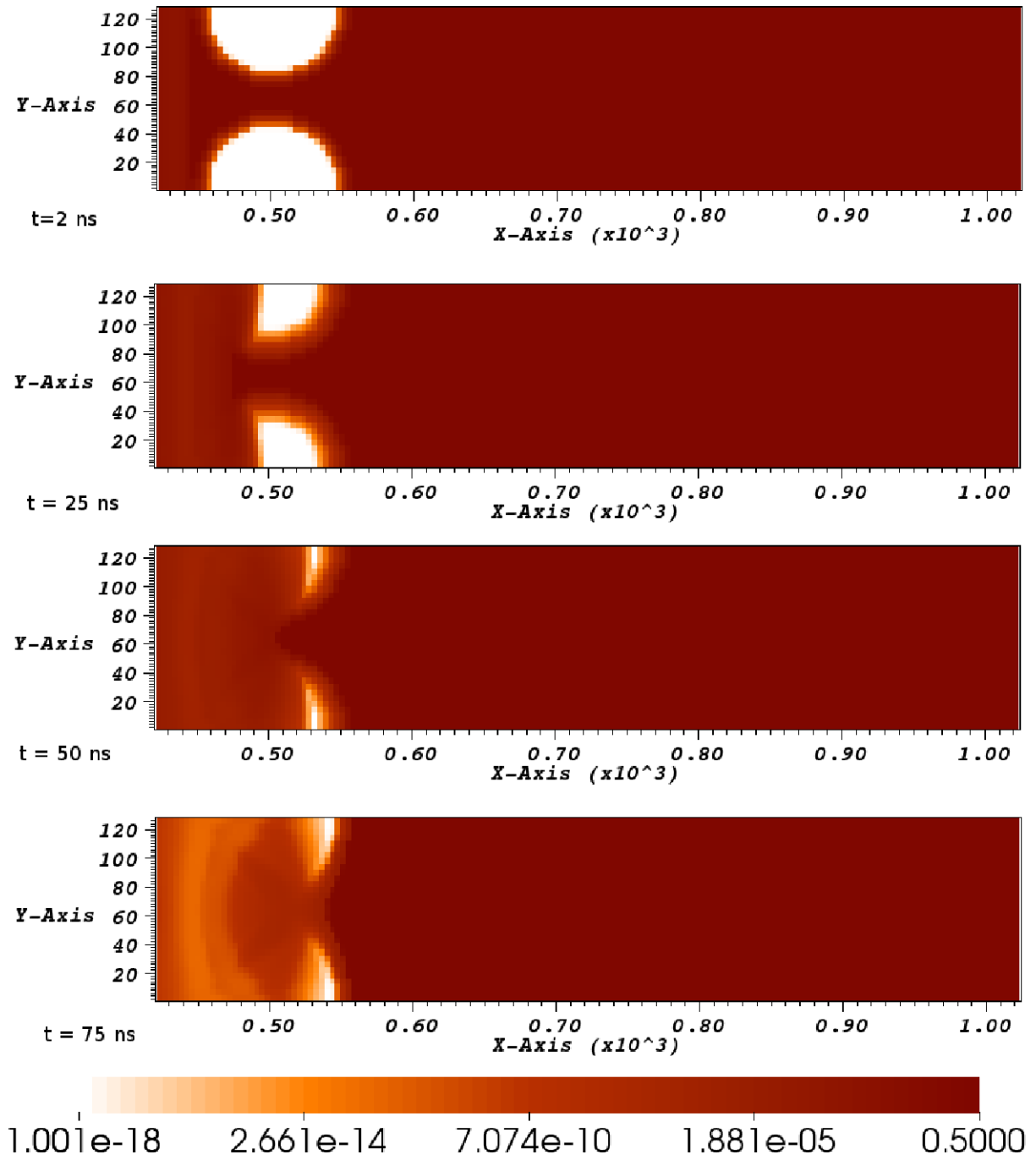


Figure 4.3: ^{12}C mass fraction at various times on a log scale.

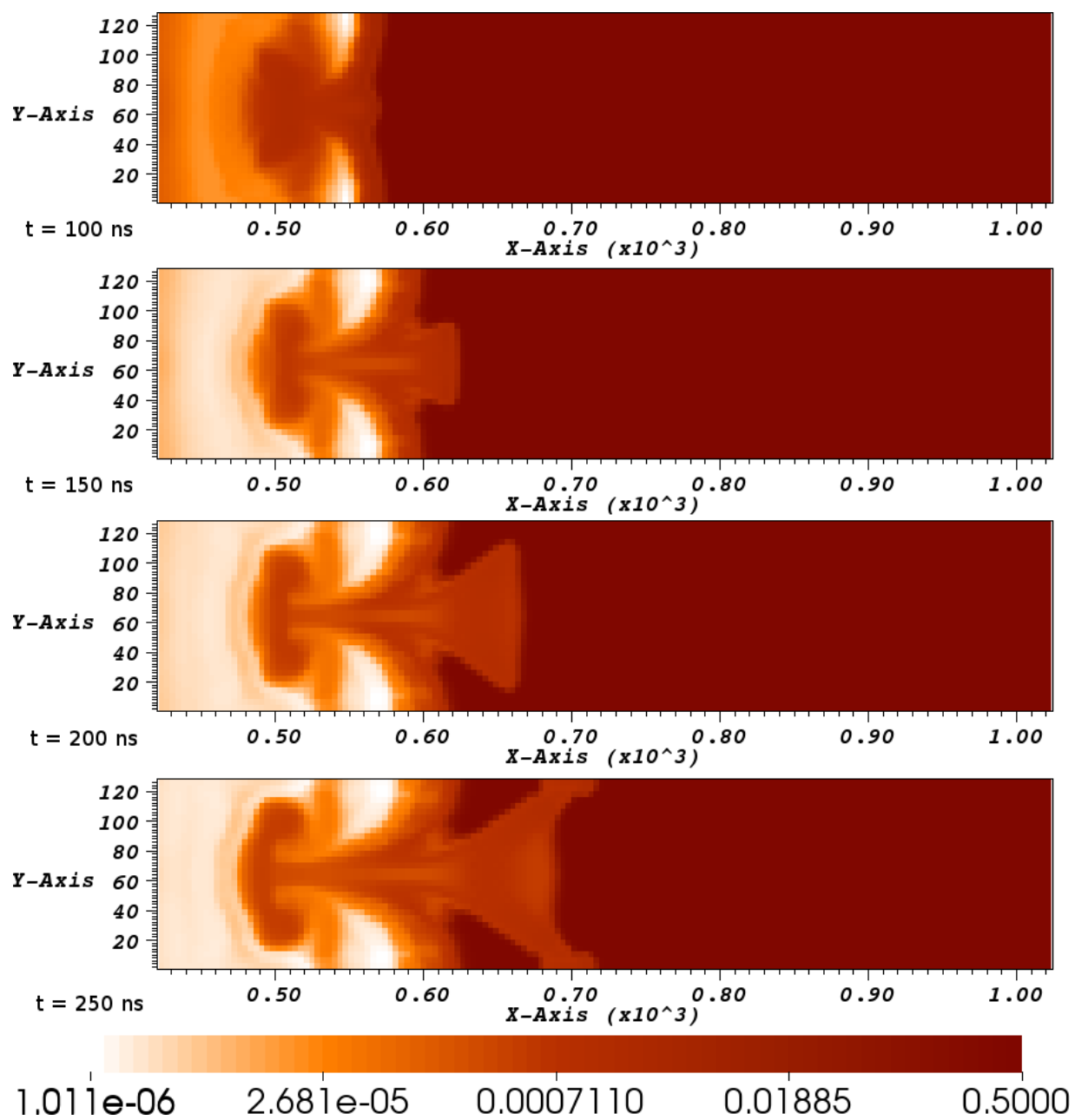


Figure 4.4: ^{12}C mass fraction at various times on a log scale.

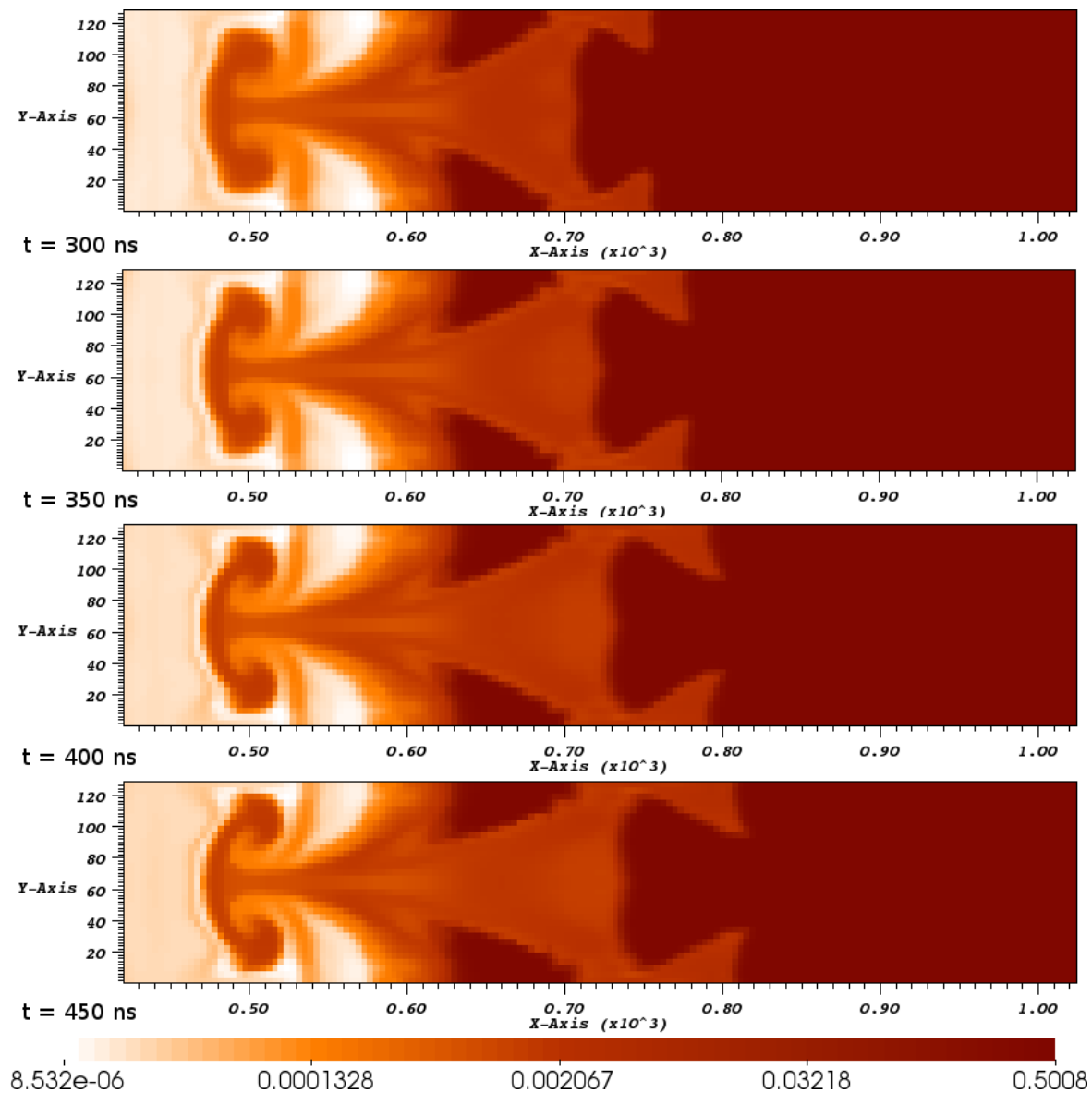


Figure 4.5: ^{12}C mass fraction at various times on a log scale.

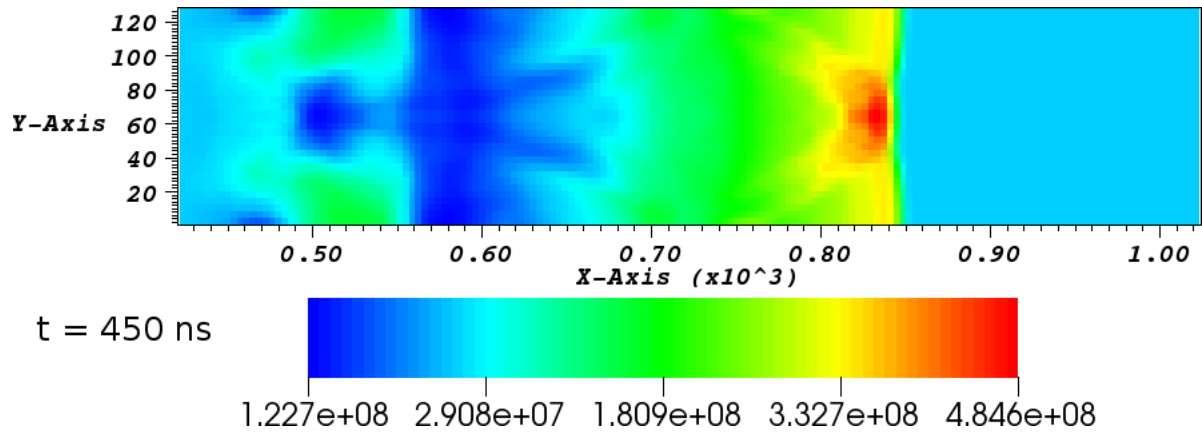


Figure 4.6: Velocity in the x direction in units of cm s^{-1}

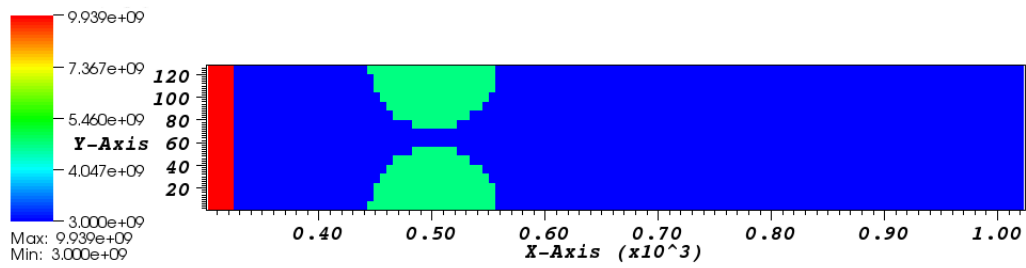


Figure 4.7: Initial temperature distribution using a logarithmic scale for the case with hemispheres of ash.

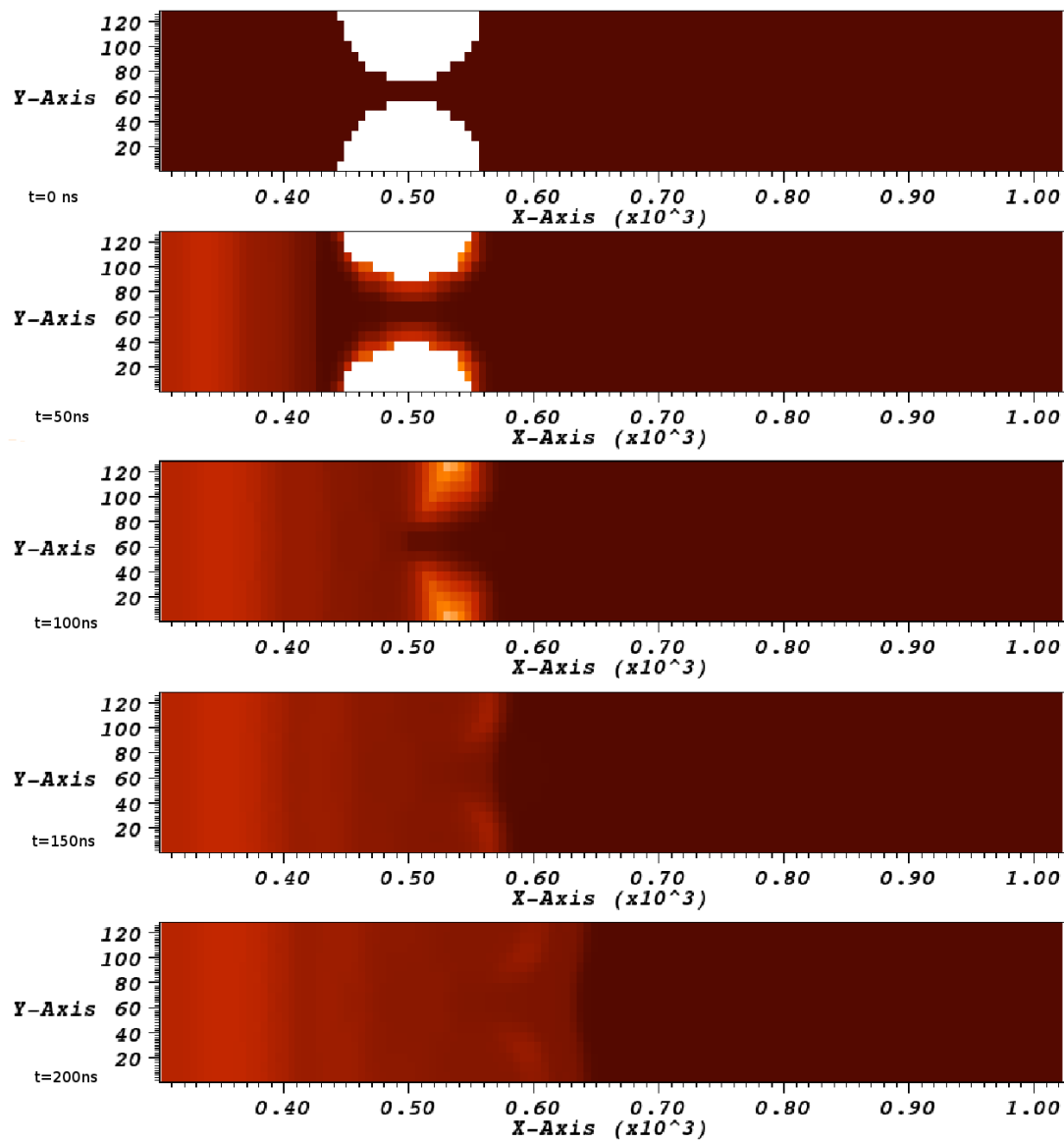


Figure 4.8: ^{12}C mass fraction at various times on a log scale.

Table 4.2: Initial Conditions, 150 Isotope Network

	Fuel	Ash	Burn
C12	0.5	0.0	0.5
O16	0.5	0.0	0.5
Ni56	0.0	1.0	0.0
$T/10^9$ K	0.01	5.505	10
$\rho/10^7$ g cm $^{-3}$	5.0	1.919	5.0
$\frac{dx}{dt}/10^9$ cm s $^{-1}$	0.0	0.0	1.0

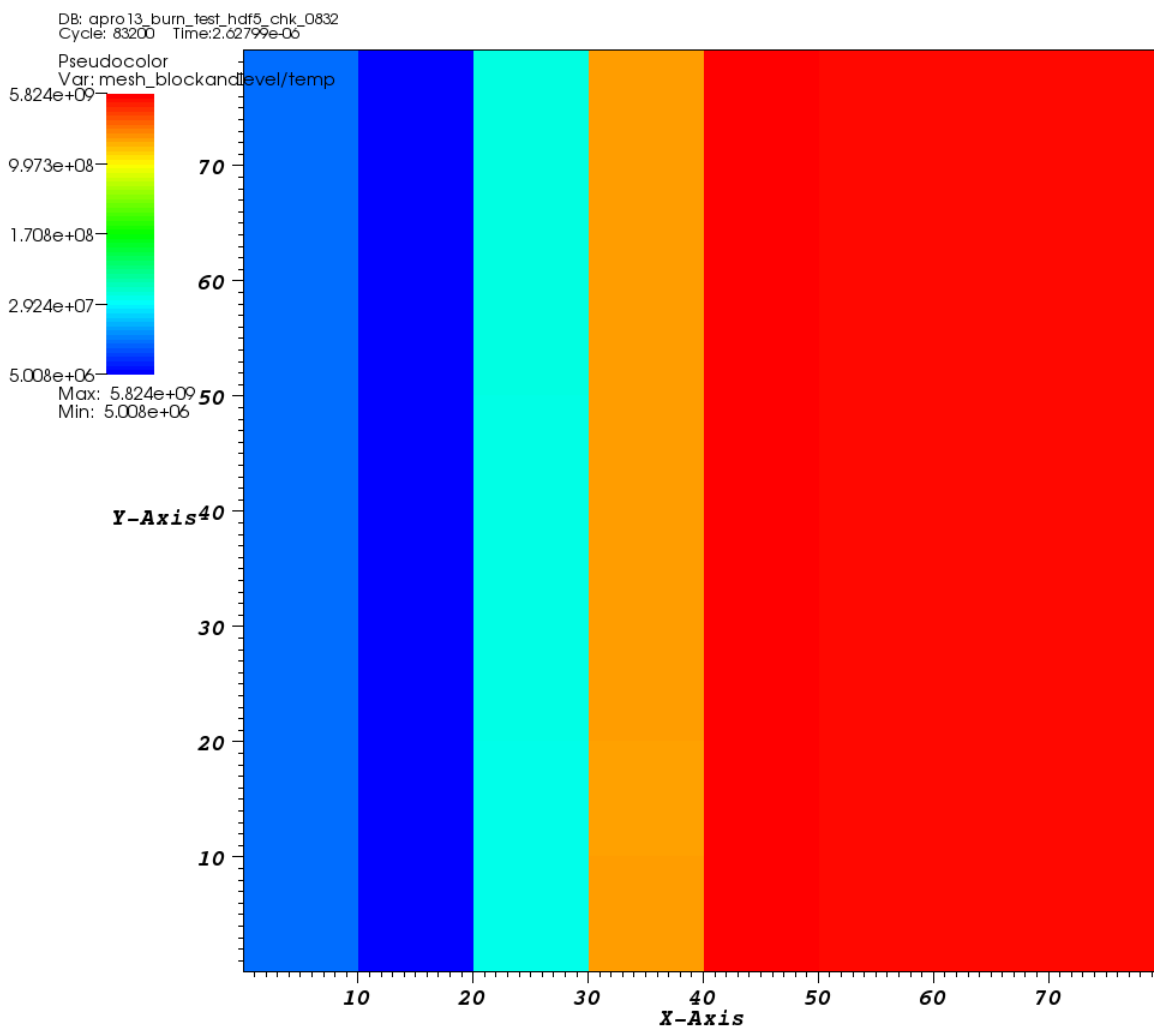
4.2 Results using 150-Isotope Network

After completing the low resolution test with the alpha network, we repeated the calculation with a larger network. The run was done with the same resolution, but with slightly different parameters given in Table 4.2. The left edge was again set to be 420 cm and the width of the burn area 20 cm. It was originally intended that the results of this run would be included in this thesis. Unfortunately, those computations have not yet been completed.

In preparation for running the 150-isotope network for a situation more complicated than a single computational cell, the FLASH code needed to be able to run on a massively parallel system. In this case, the target machine was Eugene at the Oak Ridge National Laboratory (ORNL), an IBM BG/P. The basic FLASH framework was able to run with only a few slight modifications that mainly involved finding the correct compiler flags for the architecture. The additions which had been made by our group required more work, as the code had to be updated to the Fortran 2003 standard which is used by the IBM XL compilers on Eugene. After these corrections were made, FLASH was able to run on Eugene. However, it was soon discovered that the nuclear network which was being used was behaving incorrectly due to a fundamental problem with the I/O routine. In our code, the nuclear network is read in from a text file that contains the name, atomic mass, proton number, and neutron number for all the isotopes to be used in a white space delimited list. Due to an unresolved I/O bug on Eugene, the C-code that reads this file correctly stores the proton and neutron number, but stores the wrong atomic mass. As one would expect, this results in serious errors later on in the calculation, especially with the isotopes that are assigned a mass of zero. Because of the problems that were encountered, it was decided to defer further work on the Eugene I/O problem until after the completion of this thesis and, for the time being, to instead run on the multiple processor workstation

that was available. This lack of processing power was also the reason to run at a much lower resolution in all of our cases.

The problem was setup and a run was started on the smaller machine (dual 3GHz processors). It was at this point that the problem with the EOS that was mentioned during the discussion of the approx13 runs began to manifest itself. This problem results in the EOS routine being unable to correctly calculate the internal energy for a zone. In the runs using the 150-isotope network, there were no obvious indications in the data that was output that a problem existed. The approx13 data did show that in certain zones on the boundary between the ash and fuel the temperature would suddenly fall by several orders of magnitude. This error did not occur when the initial temperature of the fuel was raised to $T = 1 \times 10^9$ K in the approx13 runs, but was still present in the 150-isotope calculations. Output from the code that deals with the nuclear burning in bad zones indicates that the nuclear network is behaving in such a way that no obvious problem could be found. This led to the conclusion that the error is with the equation of state itself, and is caused by sharp discontinuities in the composition, since the temperature and densities present in the problem are within the stated limits. Further tests have indicated that the error only occurs when a sharp discontinuity in the composition occurs along with low temperatures. It is possible that the problem is in fact related to the resolution, and that the gradient in the composition is too large across those blocks. If higher levels of refinement are allowed, the gradient would be less steep and the problem may be solved. This should be possible once the I/O problem present on Eugene is resolved. Tests have been done on a single block that is divided into two halves of the with the parameters for the fuel and ash as in the actual problem, but they have been inconclusive (See Fig. 4.9).



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Figure 4.9: Temperature plot from single block EOS test using the 150-isotope network.
The left half is fuel and the right ash.

Chapter 5

Conclusions

At the end of any endeavor it is vital to take stock in what has been accomplished and what is still left to be done.

5.1 Current Progress

- The calculations made with the approx13 network and ash hemispheres show that the behavior of the detonation wave is qualitatively the same whether the algorithm used is the explicit asymptotic method or the prescription used in the Maier & Niemeyer paper. This suggests that, the energies being provided to the hydrodynamics code by our nuclear burning algorithm are similar to those in the Maier and Niemeyer paper.
- Many of the changes necessary for running on larger computers such as the Eugene machine at Oak Ridge National Labs have already been completed.
- While the calculation using the 150-isotope network has failed to run far enough to make any reasonable conclusions as of the time this thesis was written, the problem has been defined and set up in such a way that it could be easily run as soon as the problem with the EOS is resolved.

5.2 Future Work

- Currently, there has been little done in the way of optimizing the code. As much as a factor of ten improvement may still be possible through numerical optimization and reorganization of the code. Some preliminary tests suggest that larger increases in speed may be possible by the implementation of newer explicit algorithms that are being developed to exploit the simplification that is implied by the approach to equilibrium.
- It should be possible to have FLASH running with the explicit asymptotic burner on the Eugene computer in a short amount of time. The only known problem currently preventing this is the error with the code that reads in the nuclear network which is surely solvable.
- The EOS issue which was mentioned in the results section still needs to be resolved. More testing should be done on small systems. So far the tests have all been done with the ash being 100% ^{56}Ni . The tests should be repeated with the ash at a composition that approximates nuclear statistical equilibrium (NSE). Also, different boundary shapes need to be tested, as well as the effect, if any, that a change in resolution will have on the error.
- After FLASH coupled to the explicit asymptotic burner is working on Eugene, larger scale computations can then be carried out, an example being a run using the initial conditions from the Maier paper at full resolution (.4 cm) using the 150-isotope network. The ultimate goal is to be able to run the simulation of a full star using a large network.
- Though many improvements remain to be made, current tests indicate that it should be possible to run full scale simulations using a realistic network with the current version of the code in a reasonable amount of time. The current barrier preventing this being the I/O problems that have been encountered.

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Vita

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