PROJECT EXECUTIVE SUMMARY

Title: Approaching Exascale Models of Astrophysical Explosions
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Applying Institution/Organization: Stony Brook University
Number of Processor Hours Requested: 80 Mh (year 1), 111 Mh (year 2), 122 Mh (year 3)
Amount of Storage Requested: 800 TB (year 1), 900 TB (year 2), 1 PB (year 3)

Executive Summary: We propose to carry out a comprehensive study of two classes of thermonuclear-powered stellar explosions involving compact objects, Type Ia supernovae (SNe Ia) and X-ray bursts (XRBs), using the state-of-the-art multiphysics simulation codes Maestro and Castro. This work builds upon the successes of our current INCITE campaign while shifting the focus to exciting new problems.

SNe Ia are the thermonuclear explosion of a white dwarf (a compact stellar remnant up to 1.4 times more massive than the Sun but the size of the Earth). There are several progenitor systems proposed to meet the observational constraints on SNe Ia: the Chandrasekhar-mass white dwarf model; the sub-Chandrasekhar mass white dwarf model (sub-Ch); and the merger of two white dwarfs. In the three years of this proposal, we will focus on the latter two models, complementing the study of the Chandrasekhar-mass model undertaken during our current INCITE award. This shift in focus mirrors that of the field, responding to increasingly abundant observations showing the diversity of SNe Ia explosions.

The sub-Ch SNe Ia model involves the ignition of a surface helium layer and subsequent compression and explosion of the underlying white dwarf. Many open questions remain about the viability of this model. If too much surface He is ignited, then iron-group elements will be over produced at the surface, and the resulting explosion will not look like an SNe Ia. We also don't know under what conditions and in how many locations the ignition of the He begins. We will address these questions directly by modeling the final stages of convection before the explosion, the ignition, and the subsequent explosion. The unique capabilities of our two simulation codes, described below, allow us to seamlessly model these three stages of the event.

We will also consider the inspiral and merger of two white dwarfs as a model for SNe Ia. There is a lot of potential variability in this model, since the white dwarf masses are likely unequal. Our initial goal will be to explore a variety of initial configurations and understand the dynamics that ensues when the stars first make contact. We will determine whether the conditions that arise lead to an immediate detonation or whether the merged remnant needs to relax before the explosion occurs.

XRBs occur on the surfaces of neutron stars, compact stars more extreme than white dwarfs—more mass than the Sun is packed into a star just 10 km in radius. The extreme gravity at the surface compresses H/He fuel accreted from a companion to the point of thermonuclear runaway. The resulting X-ray burst releases a large amount of energy as H and He burn to heavier elements. These are repeating events, making them excellent probes of neutron stars. Most theoretical understanding of XRBs comes from 1D, spherically-symmetric models, but as convection dominates the onset of the burning, a proper treatment requires 3D simulation. We will perform the most detailed simulations of convective burning in XRBs, yielding a detailed picture of how the convection alters the nucleosynthesis and observables.

Our simulations codes, Maestro and Castro, were designed specifically for the efficient modeling of astrophysical explosions. They are running on titan—the target of this proposal. The codes make excellent use of the multi-core architecture by using a hybrid approach to parallelism (MPI and OpenMP), and we have made considerable progress in targeting the effective use of GPUs. We will build on the already strong parallel performance of these codes by implementing new efficient algorithms for core solvers, building on our close collaboration with the BoxLib group at LBNL. Our collaboration has been together more than 10 years and includes core developers of the simulation codes along with the scientific expertise to analyze the simulations. Finally, both codes are available to the public, and performance (or physics) improvements developed in the course of the proposed work will be made available to the community.

PROJECT NARRATIVE

1 SIGNIFICANCE OF RESEARCH

We propose a collaborative investigation of multiple types of stellar explosions and their precursors using a suite of state-of-the-art hydrodynamics codes. Several progenitor models of Type Ia supernovae will be explored, including their pre-explosion and explosive phases, using our codes Maestro, Castro, and Flash. X-ray bursts will also be studied in their pre-explosive and explosive phases, using Maestro and Castro. The curious radiation-dominated systems like the black widow pulsar will be explored with Castro, and core-collapse supernovae will be studied using Chimera. All calculations will be three-dimensional and face the challenges of capturing the effects of turbulence, instabilities, strong gravitational interactions, nuclear reactions, and radiation. These challenges make these problems INCITE-class, and only the resouces titan can provide will enable use to further our understanding. Despite the broad suite of codes, there are common links, namely in the microphysics (reactions, equations of state) and in our shared approach to utilitizing the GPUs on titan. This collaboration is an expansion of our existing INCITE proposal, but we believe that it represents the most efficient use of resources, allowing us to work together as a team to create portable solvers to effectively make use of this architecture and its successor. These GPU-enabled solvers will be made freely available.

Our publication record demonstrates that we have made productive use of our current INCITE award, and we expect similar productivity carrying forward. Furthermore, this INCITE time will be used to train the next generation of computational scientists—graduate students feature prominently in the proposed work plan.

1.1 Type Ia supernovae

Type Ia supernovae (SNe Ia) are the thermonuclear explosion of a carbon/oxygen white dwarf (WD) in a binary system. These are incredibly bright explosions that rival the light output of their host galaxy, making them visible at vast distances in the Universe. Furthermore, they have an interesting property: the brightest events take the longest to dim. This allows them to be used as distance indicators and led to the discovery of the acceleration of the expansion of the Universe [1, 2] (recently awarded the Nobel Prize).

A fundamental uncertainty in our understanding of SNe Ia is the nature of the progenitor—a single white dwarf accreting from a normal companion star (single degenerate scenario) or two white dwarfs that inspiral (or violently collide) and merge (the double degenerate scenario). No progenitor system of an SN Ia has ever been identified, so astronomers must look for indirect clues. Regardless of the progenitor system, in every case the majority of the carbon and oxygen in the white dwarf(s) is converted into iron/nickel and intermediate-mass elements like silicon, and this nuclear energy release unbinds the star.

For many years, the Chandrasekhar-mass single degenerate model (henceforth called the Chandra model) saw the most attention. The Chandrasekhar mass is the maximum possible mass of a white dwarf—beyond this mass, the degenerate electrons that provide the pressure support against gravity in a white dwarf succumb to the weight of the star and it will collapse into an even more dense object: a neutron star. By always exploding near the Chandrasekhar mass, the same amount of fuel will be involved in every event and to first-order all SNe Ia would be alike. Many groups (e.g. [3, 4, 5], including us [6, 7]) have modeled the explosion (and also the convective stage preceding it [8]; again including us [9]) and have shown that it can reproduce the spectra and lightcurves of the observations (e.g. [10]). However, it is not clear if nature makes SNe Ia this way—massive carbon/oxygen white dwarfs in binary systems are rare. An additional complication is that the successful models rely on a deflagration-to-detonation transition (subsonic to supersonic burning), the physics of which is not completely understood. Buoyed by observations that showed SNe Ia are more diverse than previously thought, and evidence that there may be two populations [11, 12, 13], two alternative models, the double degenerate and sub-Chandra models for SNe Ia, have become more scientifically interesting. Theoretically, these both have challenges.

The standard picture for double degenerate SN Ia (henceforth WDWD) has the two white dwarfs spiraling toward each other as gravitational radiation removes orbital energy from the system. Here the white dwarfs can be more moderate in mass, but the sum of their masses may exceed the Chandrasekhar mass. As the stars inspiral, the less massive star will become tidally disrupted and the more massive star will accrete this material. A longstanding concern is that when this mass transfer begins, thermonuclear burning can ignite at the edge of the star, converting it to oxygen/neon/magnesium, and leading to the collapse of the white dwarf into a neutron star [14, 15], instead of an SNe Ia. This system is inherently three-dimensional, and only through detailed simulation can we understand the dynamics of the mass transfer, and thereby assess the feasibility of this model. Alternatives involving (nearly) head-on collisions of white dwarfs may account for a few events, but are unlikely to explain the majority.

The other alternative mechanism, sub-Chandra mass single degenerate SNe Ia [16, 17, 18] (henceforth called the sub-Ch model), has the advantage that systems with a moderate mass white dwarf (0.8–1.0 solar masses) are known and abundant. In addition, they are able to reproduce what we know of delay-time distributions and SNe Ia rates—something the Chandra model struggles with [19]. The core idea of this model is that the white dwarf accretes a layer of helium on its surface and a detonation ignites in this helium layer. This surface detonation can send a compression wave into the underlying carbon/oxygen white dwarf, compressing the core to the point of igniting a detonation that unbinds the star. The main problem with this "double detonation" model is that it is easier to ignite a detonation in a more massive helium layer than a low mass helium layer, but too much helium will lead to excessive production of iron-group elements when compared to observations. Also, models have difficulty reproducing the intermediate mass elements (i.e. Si) seen in the spectra on standard SNe Ia [20, 21, 22]. Investigations into so-called ".Ia" explosions suggest the mass of the helium shell need not be as large as previously assumed to trigger runaway [23]. Inspired by this, it has been suggested that a detonation in a very thin He layer can trigger the detonation of the core without over-producing surface iron-group elements [16], although detailed 1D stellar evolution calculations suggest that these smallest mass He shells may ignite as deflagrations or novae instead of as detonations, depending on the properties of the system [24]. If it can ignite as a detonation, synthetic lightcurves can match observations [22]. The challenge now becomes understanding whether and under what conditions ignition can take place in these thin shells when a realistic 3D convective field is realized, as well as the subsequent evolution and character of that ignition—this is what we will answer.

In past INCITE awards, we focused on the last hours of convection, ignition, and the explosion in the Chandra model. There is an aspect of the Chandra model that we have not explored in detail—this is the earliest stages of the convection in the white dwarf, when neutrino losses in the reaction can alter the dynamics of the convection (called the URCA process). The only multi-dimensional simulations of URCA [25] to date have been 2D, with only a portion of the star modeled. We can apply the same methodology we used for the ignition calculations in the Chandra model during our current INCITE award to study this problem in 3D. This will be a small focus of the proposed work.

1.2 Type I X-ray bursts

Type I X-ray bursts (XRBs) are the thermonuclear runaway of a thin layer of hydrogen and/or helium on the surface of a neutron star. This fuel layer accretes from a binary companion star and the immense gravitational acceleration on the surface of the neutron star compresses it, increasing the temperature and density to the point of explosion. One-dimensional hydrodynamic studies have been able to reproduce many of the observable features of XRBs such as burst energies ($\sim 10^{39}$ erg), rise times (seconds), durations (10's – 100's of seconds) and recurrence times (hours to days) (see [26] for an overview of XRBs). By construction, however, 1D models assume that the fuel is burned uniformly over the surface of the star which is unlikely if the accretion is not spherically symmetric [27]. Furthermore, the *Rossi X-ray Timing Explorer* satellite has observed coherent oscillations in the lightcurves of $\gtrsim 20$ outbursts from low-mass X-ray binary systems (first by [28]; more recently by [29] and references therein). The asymptotic evolution of the frequency

of such oscillations suggests they are modulated by the neutron star spin frequency [30] and are therefore indicative of a spreading burning front being brought in and out of view by stellar rotation.

Before the actual outburst, the burning at the base of the ignition column will drive convection throughout the overlying layers and set the state of the material in which the burning front will propagate. One-dimensional simulations of XRBs usually attempt to parametrize the convective overturn and mixing using astrophysical mixing-length theory or through various diffusive processes (e.g. [31]). A proper treatment of the convection in these extreme conditions, free from parameterizations, requires 3D simulations. We completed the most detailed (2D) studies of convection in pure He bursts [32] and mixed H/He bursts [33], and have just begun 3D simulations. 3D is expensive, restricting us to small domains to resolve the burning processes and small reaction networks (10-isotopes currently) to fit the model in memory. In small domains, the convection "senses" the boundaries, which can alter the dynamics. Ultimately we want to model a wide domain with many convective plumes side-by-side and a more realistic reaction network—this is what we will accomplish with our proposed simulations.

1.3 Maestro and Castro

The workhorses of the proposed work will be our state-of-the-art simulation codes Maestro [34] and Castro [35], developed over the past 8 years in collaboration with Lawrence Berkeley Lab. Maestro is tuned to efficiently model the highly subsonic convective flows that often precede stellar explosions. It accomplishes this by reformulating the equations of hydrodynamics, filtering the soundwaves from the equations of hydrodynamics, while keeping the compressibility effects due to stratification and local heat release. Maestro has been used successfully to model the convection leading to ignition in the Chandra model for SNe Ia (a focus of our current INCITE allocation) and will continue to be used for the XRB and sub-Ch convection simulations proposed here. Castro solves the fully compressible equations of hydrodynamics, allowing it to model shocks and explosive phenomena. It will be the simulation code for the white dwarf merger simulations, and in later years, for the explosions following the convection phases modeled by Maestro. Maestro and Castro share the underlying microphysics e.g., equation of state (EOS) and nuclear reaction networks, as well as the underlying BoxLib library that manages their adaptive mesh refinement (AMR) grid hierarchy. This makes it straightforward to transition a problem from Maestro to Castro, as was done during our current INCITE allocation when studying flame propagation in Chandra model SNe Ia [36]. Both codes are already up and running on our target platform, titan (OLCF). Additionally, both codes are publicly available[1,2]—any performance or physics improvements developed under this INCITE award will become part of the public releases, benefiting the community at large.

1.4 Core-collapse supernovae

1.5 Work under previous INCITE awards

We are currently in the last year of a 2-year INCITE award (AST106; PI: Zingale; allocation on OLCF/titan) that focused on XRBs and SNe Ia. Many of the current investigators have also collaborated on other previous INCITE awards.

number of papers

Maestro convection models: We completed our initial study of sub-Ch SNe Ia simulations [37] with Maestro, and are currently writing up the results of our second study (led by graduate student co-I Jacobs). These are the only models in the world that have explored the dynamics of the convection in the accreted helium layer in a full-3D resolved simulation. This study showed that Maestro presents a robust simulation platform for investigating the physics of ignition in the accreted helium layer. Follow-on calculations have explored a range of WD and He-shell masses and what minimum mass is necessary for ignition. A paper describing these results is in preparation.

[1] Maestro: `http://bender.astro.sunysb.edu/Maestro/`

[2] Castro: `https://ccse.lbl.gov/Downloads/downloadCASTRO.html`

An original focus of our INCITE award was modeling the convection in Chandra mass white dwarfs leading up to an SNe Ia. This has been completed and published in a series of papers in the Astrophysical Journal [38, 9]. We used AMR to greatly increase the resolution of our ignition simulations—this allowed us to explore the resolution dependence of our results. We demonstrated that the ignition is most likely to take place off-center, around 50 km from the center of the white dwarf, and by following hotspots as they develop in the flow, we showed that ignition is likely only at a single point. We characterized the turbulence in the convective region and showed that it follows Kolmogorov statistics. Further, we measured its intensity and integral length scale and argued that it is unlikely to affect the flame propagation.

Finally, we did the first simulation using Maestro convection results for a Chandra model SN Ia as initial conditions in Castro to model the subsequent explosion [36]. This "end-to-end" capability is facilitated by the fact that the two codes share the same underlying BoxLib library. This is the first 3D calculation of the explosion phase in the literature to begin with a self-consistent convective field. This capability added to our understanding of how the convection affects the evolution of the explosion. One of the results from this study was that the flame is unhindered by turbulent convection for typical ignition locations ($\sim$ 40 km off-center), but is strongly distorted for more centrally-located ignition. Even a perfect sphere ignited at the center of the star will be carried off-center by the turbulent convection. This results in asymmetric explosions for all Chandra models, which should be accounted for when matching to observations.

Castro WD merger models: A final focus of research under our current INCITE award, begun only recently, are the initial simulations of the WDWD problem. Castro had not yet been deployed for problems of this type, and therefore required a number of algorithmic improvements, including new boundary conditions for the gravity solver and better treatment of the temperature in the hydrodynamics module. Titan was used for verification purposes by running simulations of the early part of a merger scenario, when the two WDs are orbiting each other at a large distance. In this case, the motion should remain stable, and as with all hydrodynamics codes, conservation of energy and angular momentum was paramount. We performed several large-scale simulations of these, checking various parts of the parameter space to ensure that we can robustly simulate these events. This helped us fix a number of underlying issues, and we are beginning production runs. We note that these calculations are different than those lead by the UCSC/UCB group above—they started with a merged remnant and then modeled the subsequent explosion. In the work proposed here, we will model the merger process itself. This project is led by graduate student co-I Katz.

1.6 Significance of our proposed work

To advance the state of the knowledge of SNe Ia and XRBs, we will carry out the following sets of simulations (all in 3D):

- Full star Maestro sub-Ch models with detailed nucleosynthesis and realistic initial models.
- Castro sub-Ch explosion models beginning with the Maestro initial conditions.
- The largest-domain-to-date 3D resolved Maestro XRB convection calculations.
- The first XRB convection calculations with a burning sub-grid model.
- Highly-resolved Castro WDWD models capturing multiple orbits and the inspiral.

We are the only group in the world modeling the detailed convection with realistic nuclear physics in XRBs and the sub-Ch SNe Ia. In all simulations we will push the size of the nuclear reaction networks to accurately capture the nucleosynthesis (as discussed later, GPUs will be used for this task).

XRBs are important probes of the nuclear equation of state [39, 40], and the nucleosynthesis that takes place will involve the nuclei that are a target of the DOE FRIB experiment. Our simulations will advance our understanding on the burning dynamics and tell us (1) whether any burning products can be carried to the photosphere, altering the interpretation of observations; (2) how the full 3D treatment of convection modifies the nucleosythesis, allowing us to provide feedback to the 1D modelers; (3) how to create a sub-grid model to enable larger scale simulations; and (4) ultimately, in year 3 when we are able to implement a sub-grid

model, start to learn how turbulence in the burning alters the spreading of the front across the neutron star. With Maestro, we are in the unique position to address each of these points.

While several groups are investigating explosions in the sub-Ch model, we are the only group that is modeling the 3D convective field and ignition that precedes the explosion. Much like our previous INCITE work in carrying Maestro convection calculations of the Chandra model into the explosion phase with Castro, our similar work here (proposed for year 3) for the sub-Ch model will be unmatched. Initially we will focus on using more realistic models of WDs generated from stellar evolution codes (we currently use simple parametrized models), and we will answer the question of which configurations (WD mass and He mass) lead to ignitions as well as the timing and geometry of this ignition. Along the way we will switch from our simplified 4-isotope network to a more general in-situ network to better understand the sensitivity of our results to the nuclear physics, metallicity, and trace abundances of other species. In addition, we will complete our implementation of nucleosynthetic post-processing using Lagrangian tracer particles to allow offline exploration. This is key, as the exact composition of the helium layer at detonation can have profound effects on the subsequent observations, impacting the model's viability as a SNe Ia progenitor [22]. All simulations will be 3D, and the vast majority will model the entire star. These results will provide the foundation for Castro simulations capable of determining if the ignition evolves as a detonation and that detonation's subsequent evolution with realistic 3D initial conditions.

Several groups are pursuing WDWD mergers [41, 42, 43, 44] or collisions [45, 46, 47]. The majority of these have used smoothed particle hydrodynamics (SPH), a gridless alternative to the methods we use here. SPH is known to have trouble capturing instabilities and has low resolution in regions of low density—precisely the regions where the stars make contact. Our grid–based simulations will provide an important counterpart to existing simulations. With the power of AMR, we can push far beyond the resolutions of the grid-based simulations in the current literature to levels necessary to assess whether an explosion upon contact is feasible. Castro is ready for these simulations—we have made the necessary changes for isolated gravity boundary conditions, and while we will start with simple WD models on the grid, we are nearly complete in implementing a self-consistent method to initialize a binary pair of WDs on our grid using the full stellar equation of state.

2 RESEARCH OBJECTIVES AND MILESTONES

As described above, we plan a suite of comprehensive simulations of XRBs and SNe Ia (both the sub-Ch and WDWD models) using our codes Maestro and Castro. All the problems we describe are inherently three-dimensional, requiring large resources. Our codes are running on titan today, and they perform and scale well. The starting point for all the simulations proposed are in place. We are ready to run.

The calculations we describe in further detail here are INCITE–class for two reasons. First, as is often the case in astrophysics, we can never capture all the length-scales that come into play in these stellar explosions, for example, the turbulent dissipation scale in the convective regions is often quite below our grid resolution. As a result, we need to push to higher-and-higher resolution to assess whether our results are converged. This high resolution demands a lot of computational resources—the type that only INCITE can provide. Second, the temporal scales we need to model are equally impressive. For the XRB simulations, we would like to model a second of evolution. At our current resolution (6 cm), we would need over a million timesteps (and that is with the large efficiency gain we get through the low Mach model). Since there is no parallel-in-time equivalent to domain decomposition, we need to run a big problem for long amounts of time on the machine—again, a feat only possible through INCITE. Finally, we want to push the realism of the physics, in particular, our reaction networks. This will only be feasible by offloading some of the reaction expense to the GPUs.

The basic motivation for our science problems was given in the previous section. Here we begin by discussing the milestones we hope to achieve in each year and then we give specific details about the number

and size of the simulations we plan to run. We note that because we have preliminary calculations of each of the problems we propose to run, we can base our time requests on existing simulations from titan (here Mh = mega-hours). Also, there is a pattern to our milestones: one milestone for each of the major topics per year (XRBs, sub-Ch, WDWD), the utilization of the GPU-enhanced reaction network becomes the norm in year 2, and the application of new features (rotation and sub-grid models in Maestro) and the transfer capability from Maestro to Castro. The Maestro calculations make up most of the time request in year 1, but by year 3, that proposed Castro and Maestro calculations reach parity.

- **Year 1: 80 Mh total**
  - *Full star, high-resolution Maestro models of convection in sub-Ch WDs*: Many simulations will be performed, with various initial models. Our experience shows that a moderately-high resolution simulation requires about 0.5 Mh and we imagine 20 runs. We would like to do 5 higher resolution runs, which we budget at 4 Mh each. *total: 30 Mh*
  - *Large domain Maestro XRB convection models*: Our current 3D XRB simulation (in a domain 15 m wide) will require about 2 Mh. On titan, we would like to run something that is 2× wider in the transverse directions, bring the cost of a single simulation to 8 Mh. We will do two of these in year 1 (with different initial models), as well as a number of smaller exploratory calculations to test the effects of bigger reaction networks (with GPUs). We budget 4 Mh for the exploratory calculations). *total: 20 Mh*
  - *Castro multi-orbit WDWD inspiral and merger*: We want to follow up to 5 orbits of the white dwarf pair to capture the tidal disruption and first contact. Three models will be done with various WD masses. Our estimates are 10 Mh per simulation (based on our initial runs on titan). *total: 30 Mh*
- **Year 2: 111 Mh total**
  - *Maestro sub-Chandra SNe Ia models with large reaction networks*: These calculations will be the follow-on to year 1, using more detailed initial models and larger (20-40 isotope) reaction networks. We expect that with the GPUs handling the reactions that we will see only a modest increase in cost despite the much larger network. We budget 2 Mh per simulation, with the goal of doing 10 simulations. *total: 20 Mh*
  - *Maestro XRB convection models with large reaction networks*: This will be the follow-on to year 1. Again, we hope to push the size of the domain and increase the size of the network. Since we are already using a moderate network, we expect that the GPUs can offset the size of the network. If we double the width of the domain again, we put the cost of a simulation at 32 Mh. We will do a single simulation at this scale, plus two more at the size from year 1. *total: 40 Mh*
  - *Castro WDWD models with nuclear physics*: These calculations will pick up where year 1 left off. We will now model the details of the merger event itself, with a reaction network to assess the potential for prompt ignition. The number of cells in the calculation is expected to increase with the complexity of the flow (through AMR), so we need to scale the time requirements accordingly. We budget 25 Mh for each calculation, and wish to perform 2 (different initial conditions). *total: 50 Mh*
  - *Exploratory Maestro URCA calculations*: As discussed above, this is a direct application of the methodology we used for the Chandra ignition calculations during our current award. We will budget 1 Mh for a single 3D calculation of the URCA convection. *total: 1 Mh*
- **Year 3: 122 Mh total**
  - *Maestro to Castro models of sub-Ch SNe Ia*: We will use one of our existing Maestro sub-Ch models from year 2 to initialize a Castro simulation. We have made this transfer before with the Chandra models. Our estimate for the time required for this simulation is based on pure Castro models of sub-Ch explosions, and we place it at 10 Mh. *total: 10 Mh*
  - *More realistic Maestro sub-Ch SNe Ia models*: These calculations will improve upon those from

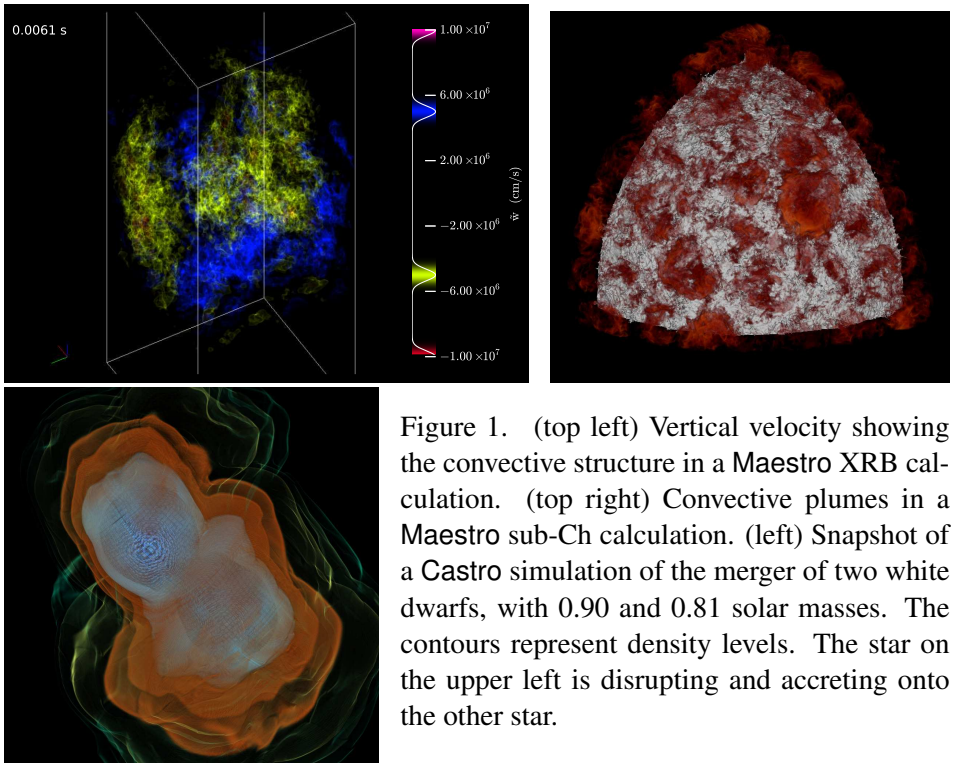


Figure 1. (top left) Vertical velocity showing the convective structure in a Maestro XRB calculation. (top right) Convective plumes in a Maestro sub-Ch calculation. (left) Snapshot of a Castro simulation of the merger of two white dwarfs, with 0.90 and 0.81 solar masses. The contours represent density levels. The star on the upper left is disrupting and accreting onto the other star.

year 2. We will use more realistic initial models from the MESA stellar evolution code and we will perform some simulations with rotation. The rotation simulations rely on expected development in Maestro. The overall cost of the calculations should be comparable to the year 2 models, and we budget 2 Mh per simulation and hope to repeat the same 10 models from year 2. *total: 20 Mh*

- *Sensitivity study of XRB simulations (Maestro)*: We will perform several more XRB convection models with different (and more realistic) initial models. We budget these as in year 1 at 8 Mh, and hope to do 4 calculations. *total: 32 Mh*
- *Large-scale XRB burning model with sub-grid burning*: This calculation relies on the development of a subgrid model using the simulations from years 1 and 2 as a basis. The time estimate depends on how much we are allowed to relax the resolution requirements, which is unknown at this time. We will be in a better position to estimate the time in mid-year 2, but we pick 10 Mh as a representative estimate for a big 3D convection problem with Maestro. *total: 10 Mh*
- *Castro WDWD models with realistic initial conditions*: These calculations will continue those from year 2, but we will incorporate models from stellar evolution codes to give us a more realistic composition and structure. In particular, we will explore some models with a think He layer on the surface. The cost should be the same as in year 2. *total: 50 Mh*

XRB simulations: Figure 1 shows a snapshot from a current Maestro XRB simulation. Our 2D study [33] showed us that in order to resolve the nuclear burning, we needed to use a model with 6 cm resolution. The current 3D simulation is done on a 256×256×768 grid. At this resolution, we achieve timesteps of about 0.3 μs, and this running this calculation to 0.1 s would require about 2 Mh on titan.

There two are primary goals for the XRB simulations. First, we want to run larger domains. When the domain is small, the boundaries confine the convective rolls, and an artificial flow is setup. We want the width of the domain to be several times larger than the scale height ($\sim$ 10 m). Keeping the resolution fixed at 6 cm, we will perform simulations in 30 m and 60 m wide domains. These will give a clear picture of the dynamics of the convection and allow us to answer the questions posed in the previous section: how does

the convection alter the nucleosynthesis? and are ashes brought up to the surface where they can change the observables?

Secondly, we want to enable even larger domains by relaxing the resolution requirements. Using the results from years 1 and 2, we will work on developing a sub-grid burning model that can be used to capture the dynamics of the convection at coarser resolution. We will then push the domain sizes to 100s m. At this point, we can find ourselves with burned regions in one part of the domain and unburned in others. Describing these different vertical structures is not currently possible in Maestro (the different temperatures and composition result in different hydrostatic structures, and Maestro is built on modeling the flow superposed on a hydrostatic background). Nevertheless, allowing for lateral gradients is in the plans for Maestro's development, and we hope to be in the position to capture this new dynamics by year 3.

For the year 1 and 2 calculations, the resolved nuclear burning will require us to use accurate reaction networks. At the moment, we use a 10-isotope network that captures the hot-CNO H burning, 3-α He burning, and some links to heavier elements and the rp-process. Our current study showed that approximations in the network introduce some artifacts in the convective flow, so we will push to larger networks. As described later, we will ultimately use the GPUs to offset the computational demands of these larger networks.

sub-Ch simulations: Maestro sub-Ch convection simulations are running on titan through our INCITE allocation right now (see Figure 1). Our goal in the proposed INCITE allocation is increased realism. This means better initial models, better nuclear physics, and following the event from convection to ignition to explosion. In [37], we modeled a single WD mass (1 solar mass) and single He layer mass (0.05 solar masses). Our current simulations are exploring an array of WD masses (0.8–1.2 solar masses) and He masses (0.025–0.1 solar masses). At the moment, we are relying on simple parameterized models, and many of our simulations are done in an octant, to reduce the computational cost.

Our proposed models will all be full-star. When running in an octant, boundary effects can lead to heating at the walls, perhaps biasing the ignition. Full star models avoid this issue. These models rely on the AMR capability in Maestro to focus the resolution in the He layer (we model the entire star on a Cartesian grid). Our current simulations show that some mass configurations need increased resolution, so we will explore higher resolution models in year 1.

The current models include only the 3-α reaction and $^{12}\mathrm{C}(\alpha,\gamma)^{16}\mathrm{O}$. We will use more extensive networks in year 2. Again, the GPUs will be needed here to allow for this new physics. At the same time, we will begin to explore more realistic models from the MESA stellar evolution code. These models will continue into year 3. As development of Maestro continues, we aim to have the ability to do moderate rotation. The issue here is that rotation deforms the star and there is no longer a single 1D hydrostatic base state that describes the underlying star. We have ideas on how to improve this allowing for moderate rotation. This development will take place over the next few years and we hope to have the first applications of it in year 3 of this proposal.

A final effort will be to carry the convective calculations into the explosive phase by restarting a promising model in Castro. We have done this process for the Chandra models of SNe Ia [36]. This will be the first "end-to-end" simulation of the sub-Ch model for SNe Ia. It will be the most realistic such model to date and we expect to learn a lot about the feasibility of the sub-Ch paradigm through this calculation.

WDWD simulations: Our simulations of merging white dwarfs are just beginning. We have modified Castro to incorporate the necessary physics to allow for the simulation of the inspiral and merging. In particular, we extended the gravity Poisson solver to incorporate boundary conditions corresponding to an isolated potential. To conserve angular momentum, we perform the simulation in the co-rotating frame—the stars initially will appear motionless.

Our initial set of simulations map two WDs onto the computational domain. For simplicity, these WD models were constructed in isolation with a uniform composition. After a few orbits tidal forces deform the stars and when the stars are close enough, the lower mass star can be disrupted and the material will accrete

onto the more massive star (see Figure 1). In year 1, we will explore a variety of different mass ratios and focus on understanding what happens when the disruption occurs and material first hits the more massive star. In particular, we wish to see if the conditions necessary for the detonation of the carbon fuel are met.

In year 2 we will refine the simulations by incorporating a nuclear reaction network. This will allow for us to self-consistently model the merger event beyond the time when they first touch. We will also begin to use self-consistent initial conditions. These are equilibrium conditions that initialize the stars on the grid as a system, so the tidal-distortion effects are already in place. This reduces the cost of the simulation by allowing us to model fewer orbits before the merger.

There are a lot of unknowns in the WDWD system, and we will use the INCITE time to explore the parameter space. We will consider many different initial configurations and explore the resolution needs for these simulations. With AMR, we can focus the resolution on the conditions where the detonation may take place, saving on the computational cost. In year 3, we will explore models with initial conditions generated from a stellar evolution code like MESA. These may not have uniform composition and perhaps will have a thin helium layer on the surface, both of which can alter the nuclear burning.

Post processing and observables: For the SNe Ia models that we bring to explosion, we will use the Sedona radiation transfer code to produce synthetic observables (lightcurves and spectra)—the Sedona author Dan Kasen is a Co-I on this proposal. This post processing was done with many of the explosion models in the current INCITE allocation and the pieces are in place for this workflow. We do not expect Sedona to require a lot of compute time for these models.

Exploratory simulations: We are capable of modeling all phases of these explosive phenomena. As a result, when a new idea is promoted in the field, we will be in an excellent position to explore it through detailed high-resolution simulation. We will keep pace with the field and propose some add-on calculations in later year renewals. One example already placed in our milestones is the URCA calculation.

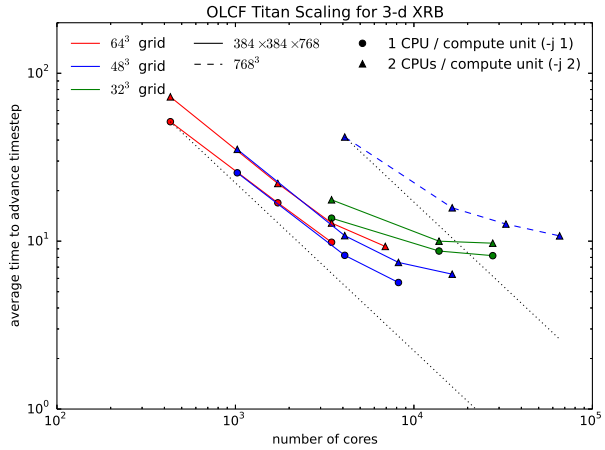
3 COMPUTATIONAL READINESS

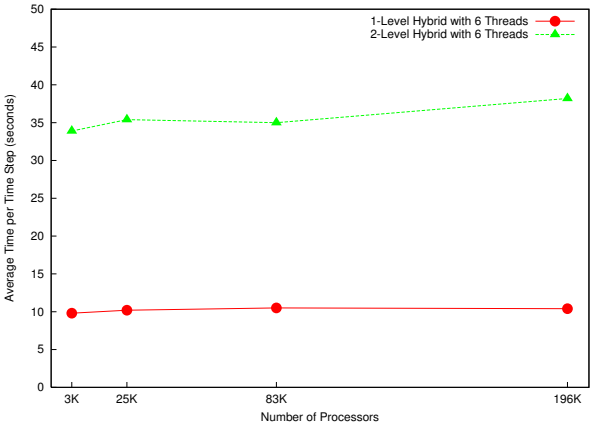
The proposed work uses two simulation codes: Maestro, a low Mach number hydrodynamics code suited to convective flows and Castro, a compressible hydrodynamics code designed for high Mach number flows. The two codes share a common framework, built around the BoxLib library. We note that both of these codes are freely available to the community and any improvements to their parallel performance based on the work proposed here will benefit all users of the codes. The unique features of titan, in particular the GPUs on each node, are of critical importance to meeting the science goals proposed here—GPUs, will allow us to consider bigger networks. We have proof-of-concept GPU results on titan already, and discuss our plans for finishing the implementation below.

3.1 Use of Resources Requested

Our list of large jobs to run along with detailed time estimates is given in the previous section. In each case, the time estimates were computed based on actual runs of the proposed problem on titan. The convection jobs all share something in common—the need for long time-integration. This means *many* trips through the queue (it's not uncommon to require 500 wallclock hours, broken up into may smaller segments). With 10,000 cores, this is 5 Mh—a number representative of many of our jobs. This will represent the typical job size for the base calculations. The addition of bigger networks will push the base calculations up to larger core counts in subsequent years.

There are several large calculations each year when that will need more processors. The biggest XRB runs will require 10,000s of cores. We scale well to that point now, and planned developments described below will make this a more typical size. For the WDWD simulations, as the stars merge, the number of AMR grids created will dramatically rise, as a result, the last 10% of the simulation may require 10× more processors. The same will be true of the Castro continuation of our Maestro sub-Ch model.





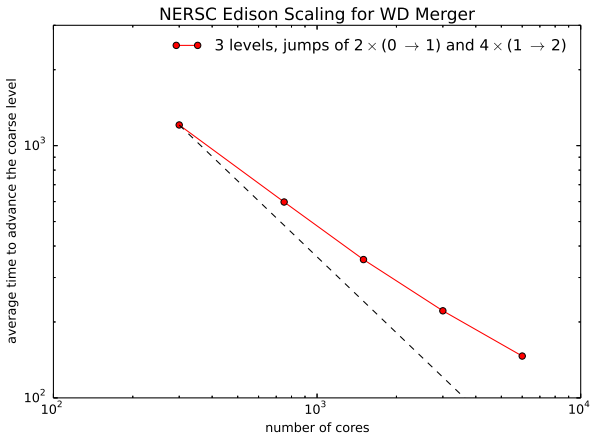


Figure 2. (top left) Maestro strong scaling for the XRB problem. Two problem sizes are shown, with different domain decompositions and OpenMP threads. In each case, the time to advance the solution is the average of 10 steps. Comparing the two problem sizes shows the weak scaling. (top right) Castro weak scaling on the titan-predecessor jaguarpf for a SNe Ia explosion. This has the same physics and solvers as will be used for the sub-Ch explosions. (left) Castro strong scaling for the initial (non-interacting) stage of the WDWD problem, run on the NERSC Edison machine. This solves the full Poisson problem using multigrid with isolated boundary conditions.

Our usage throughout the year will have periods of intense usage—when we have decided on our initial conditions and are running a suite of calculations for a paper. Many of us teach, and will be less active during the semester, but the graduate students will be running steadily throughout the year.

3.2 Leadership Classification

The job characteristics as described above are hundreds of hours on 10k cores for our standard jobs and several 10,000s of cores (again for hundreds of hours) for our biggest jobs. We are proposing 10s of jobs per year, with an average cost of a few Mh, and the biggest jobs requiring 25 Mh. These numbers cannot be met by any facility other than through INCITE. We can run at this scale today. Any larger, and it becomes difficult to get the runtime needed to complete our jobs. Our largest jobs will be on the leadership class by themselves, requiring $\sim$ 20% of the machine, and our wide range of concurrent moderately-sized studies for the proposed simulations will utilize more than 20% of the total machine. Finally, we have been investing our time in porting our microphysics to the GPUs. This is essential to implementing the physics we require. A proof-of-concept running on titan is shown below. This will speed up some of the more time-intensive parts of our simulations and enable new science (in particular, bigger reaction networks). For this investment to payoff, we need a machine with GPUs on all of the nodes—titan has been our target. Only INCITE resources meet these needs.

3.3 Parallel Performance

Maestro: Figure 2 (top-left) shows the strong scaling behavior for our Maestro XRB problem on titan. A subset of this same information is shown in a speedup plot as well (Figure 3). For Maestro strong scaling,

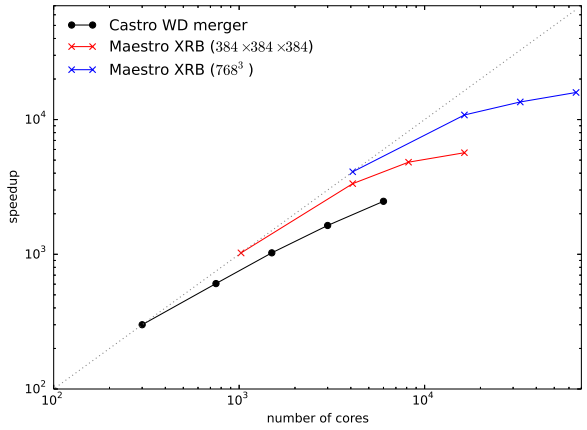


Figure 3. Speed-up plot for the Maestro and Castro strong scaling data. For the Maestro runs, we only show the 48^3 grid case using all CPUs on a compute unit (-j 2)

we explored two problem sizes (a 3D XRB with a domain of 384×384×768 zones, and one that is twice as wide in each lateral direction, 768^3). For the smaller size, we did three different domain decompositions—breaking it up into 432 64^3 sub-grids, 1024 48^3 sub-grids, or 3456 32^3 sub-grids (the different color lines show these different decompositions). We always assigned one grid per MPI task and experimented with 1, 4, 8, or 16 OpenMP threads per MPI task. We also explored the number of CPUs per compute unit (since two titan CPUs share a single floating point unit in the compute unit). We find that only using one CPU per compute unit results in about a 30% performance gain, but it does not affect the scalability. We see that we get the best scaling with the larger sub-grids (64^3 and 48^3), and that 32^3 does not thread well for our application. Furthermore, we see that with the large grid sizes, we get good strong scaling over a decade increase in processor count. Note, we did not explore assigning tasks to specific NUMA nodes in this test. Finally, it seems that using 16 threads incurs a slight performance penalty over lower thread counts.

For the bigger job, we only did a single decomposition (48^3 grids) using all CPUs on the compute units. This run has 4× as much work and is run on 4× the number of processors as the corresponding smaller job. Looking at the first point in the curve and comparing to the corresponding point in the smaller-job-size curve, we see that we have excellent weak scaling as we increase the job size. The strong scaling curve for this larger problem shows that Maestro is reaching up to effective use of 20% of the machine. Some of the XRB runs in year 2 will be larger domains still.

The low Mach number constraint in imposed through a divergence constraint on the velocity field. Maestro uses two different multigrid solvers in the algorithm to enforce this constraint. At the half-time, a cell-centered multigrid solver enforces the low Mach divergence constraint on the velocities that go into the fluxes. At the final time, a node-centered (nodal) multigrid solver enforces this constraint on the final velocity field. Finer-grained timers tell us that the main scaling bottleneck is in the nodal multigrid solver. We have a plan to improve this scaling that we expect to implement in the near future—we discuss it in section 3.5 below. We note that this test corresponds to the proposed XRB simulations, which will run in exactly the fashion tested here. The sub-Ch and URCA Maestro simulations will exercise the same parts of Maestro and we would expect similar scaling. For both problems, our plans have us increasing the reaction network in later years—this will only improve scaling since the network is purely local physics.

Castro: For Castro, Figure 2 (top-right) shows a weak scaling study where we put a WD on the adaptive grid and simulated hydrodynamics with self-gravity using a monopole approximation—this is representative of the sub-Ch Castro simulations proposed. This was run on the pre-titan hardware (jaguarpf). We considered both a single level and a two-level case where the coarse resolution is equivalent to the single level case. Both scale well to approximately 200K processors. We note that the 2-level case does approximately three times the work of the single level case. The data shows an overhead of approximately 15-20% for AMR; however, achieving the same resolution as the two-level simulation with a uniform grid would be a factor of

16 more than the single level example treated here.

Our scaling numbers for the WDWD problem consider the initial stage, when the stars are not yet interacting. This is shown in the bottom left panel of Figure 2 and in the speedup plot, Figure 3. The calculations were run on the NERSC Edison platform, a Cray machine that shares many characteristics with titan. This problem uses 3 levels in the grid hierarchy, level 0 is 480^3, level 1 is $2\times$ finer than level 0, and level 2 is $4\times$ finer than level 1, giving us an effective grid of 3840^3. This is typical of the size problem we will want to run. Gravity is done using a full Poisson solve with multigrid, with the isolated boundary conditions constructed by doing a multipole expansion (up to $l = 6$) on the coarsest grid. Castro and Maestro share the same cell-centered multigrid solver from BoxLib, and our early numbers show that the gravity solve with isolated boundary conditions takes approximately 25% of the runtime for a WDWD problem where the stars have not yet begun interacting. We scale for over a decade in core count. At high core counts, we become work starved—there are too few grids at the fine level to redistribute equally. As the stars interact, many more grids will be created (about an order-of-magnitude increase is expected), and this will improve the scaling and allow us to move to higher core counts. Our plan is therefore to start this problem on a moderate number of cores and move to larger core counts as it evolves. The addition of burning in year 2 will greatly increase the local physics, further improving the scaling.

I/O: We directly measured the time to output from Maestro on titan, writing a 50 GB plotfile at a data rate ranging from 4–12 GB/s. We note that I/O takes less than 1% of our runtime, and it will not be an issue for the proposed runs. As Castro uses a similar I/O strategy, we expect it to attain the same performance. All of our codes have checkpoint/restart capability to make effective use of titan's queue system.

3.4 Computational Approach

Maestro decomposes the fluid state into a 1D radial hydrostatic base state and a perturbational Cartesian state. A divergence constraint on the velocity field captures the compressibility due to background stratification and local heating/diffusion sources. The resulting system allows for much larger time steps to be taken compared to corresponding compressible codes ($\sim 1/M$ larger), where M is the Mach number. The algorithm [34] utilizes a second-order accurate approximate projection method, developed first for incompressible flows. Fluid quantities are advected using an unsplit Godunov method, with reactions incorporated via operator splitting. The provisional velocities are then projected onto the space that satisfies the divergence constraint. The projections involve elliptic solves, solving a variable-coefficient Poisson problem, computed using a multigrid algorithm. AMR is used to achieve high spatial resolution. Maestro is written primarily in Fortran 95 and is parallelized using MPI and OpenMP. It is highly portable, and regularly runs at the OLCF, NERSC, and NCSA.

Castro [48] is based on a compressible flow formulation in Eulerian coordinates and includes self-gravity and reaction networks. All Castro calculations will use AMR on a 3D Cartesian grid. The hydrodynamics in Castro is based on the either unsplit piecewise linear (PLM) or piecewise parabolic method (PPM) [49] and is designed to work with a general convex equation of state. Castro supports Newtonian self-gravitational forces through either a simple monopole approximation or a full solution of the Poisson equation using geometric multigrid techniques. The approach to AMR in Castro uses a nested hierarchy of logically-rectangular grids with simultaneous refinement of the grids in both space and time. The integration algorithm on the grid hierarchy is a recursive procedure in which coarse grids are advanced in time, fine grids are advanced multiple steps to reach the same time as the coarse grids and the data at different levels are then synchronized. The synchronization for self-gravity is similar to the algorithm introduced by [50].

Both Maestro and Castro uses a hybrid programming model based on MPI and OpenMP. Distribution of grid patches to nodes using MPI provides a natural coarse-grained approach to distributing the computational work, while threading of loops over zones in a grid using OpenMP provides effective fine-grained parallelization. Both codes use the same interface to the EOS and thermonuclear reaction networks. This

enables us to switch from a low Mach number simulation with Maestro to a fully compressible simulation using Castro without changing the underlying physics.

For analysis, Maestro and Castro dump out global diagnostics at each time step and plotfiles at regular intervals. The visualization packages VisIt and yt have native support for the BoxLib file format. We expect the largest simulations to output about 100–200 TB each in plotfiles, putting the storage needs at about 800 TB in year 1, rising to 1 PB in year 3. We will save plotfiles for as long as needed to finish the analysis and publication of the results. Only a minimal set of checkpoint files will be archived. Where possible, we will store output in single precision to conserve space.

3.5 Developmental Work

Both Maestro and Castro already scale well on titan and are capable of running the proposed science. Nevertheless, we are continually working on the performance of these codes, and in particular, in the last year have been actively targeting titan and its GPUs. Our graduate students have been the lead on this effort.

Our codes use multigrid algorithms that iterate across a hierarchy of grids of different resolution. At coarser levels of the multigrid hierarchy, the relaxation schemes that form the core of the multigrid algorithm may not be able to effectively utilize high thread counts because communication costs will dominate floating point work. Furthermore, standard relaxation schemes for denser stencils such as the nodal solver in Maestro are not well suited to high thread counts. We are pursuing a number of possible strategies for dealing with this issue including relaxation schemes with higher floating point intensity but good thread performance, communication avoiding algorithms and hybrid strategies that limit the amount of coarsening to address these issues. This effort is led by the BoxLib group.

With the advent of OpenACC 2.0 (in particular, its ability to support function calls), we have begun porting the microphysics (EOS, reactions) in our codes to the GPUs on titan. The EOS is the most time-consuming standalone physics module for the WDWD problem. Both codes use the publicly available Helmholtz stellar EOS, which although itself can take a vector, it was originally structured in our codes to work on a single zone at a time. We converted the EOS to operate in vectorized fashion, and moved almost all of the logic inside the main EOS routine, to maximize the work done in one place. This EOS calculates the relevant thermodynamic quantities by interpolating from a table that is read into memory at the beginning of the calculation. We used the OpenACC 2.0 `enter data` construct to move this table onto the GPU at the beginning of the simulation, and have it reside there for the remainder. Then we implemented a parallel loop over the input vector for the main EOS routine. To check the performance gain, we wrote a driver routine that loads the table into memory and then executes a number of EOS calls. We compared this to an OpenMP parallelization of the same loop. We chose a vector size of 32^3—representative of the size of a typical AMR grid that will enter the EOS routine. For low numbers of calls, the time of execution is dominated by the table read, but for large numbers of calls (approaching what we would see in a production run), the loop parallelized by OpenACC is significantly faster than OpenMP, as in Figure 4. We have run some actual Castro exploratory WDWD calculations using the OpenACC EOS. For a 256^3 uniform grid on 512 nodes, running for 10 timesteps, the case with the OpenACC EOS runs 60% faster than an unthreaded implementation of the EOS. We are still optimizing, but this shows that the EOS is a large factor in this problem's runtime, and we are able to run a Castro simulation using the GPUs on titan today.

We are applying similar techniques to put our reaction networks on the GPUs. For our XRB simulations, the reactions can represent a significant fraction of the runtime (up to 25% with our current, small network). Furthermore, we wish to use much larger networks to better capture the nucleosynthesis and energetics of the burning. To facilitate this, we are in the process of changing the ODE integrator in Maestro from VODE to a vectorized implicit ODE integrator written by our colleagues at LBNL. This will allow us to call the reaction network for a vector of zones and to put this entire operation onto the GPUs, much as we did for the EOS. We expect to finish this work in the next month or two. We note that a similar procedure of offloading

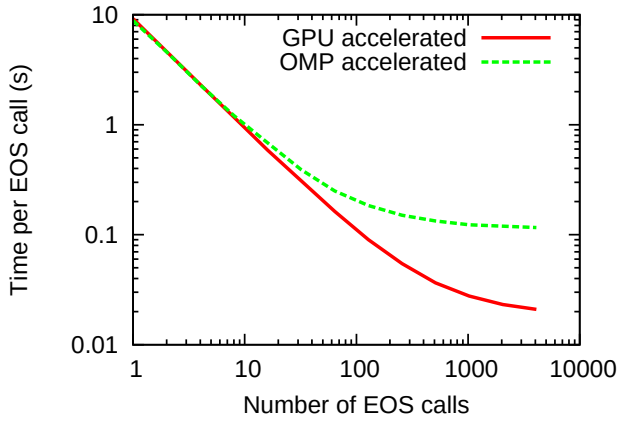


Figure 4. Comparison of OpenACC (solid, red) and OpenMP (dashed, green) parallelizations of the EOS. Each calculation involves reading the EOS table into memory and then calling the EOS a certain number of times. The vertical axis shows the average time per call. With few calls the execution time is dominated by reading the table into memory, but this is amortized out as we call the EOS more. The OpenACC-threaded calls are significantly faster than the OpenMP-threaded calls, even when taking data movement to the GPU into account.

the reactions to GPUs has been taken by other codes running on titan (the Chimera core-collapse code [51] and the S3D combustion code [52]) and we have begun to make contact with our OLCF liaison about the strategies needed here.

Finally we note that the porting of the microphysics to GPUs described here applies to both Maestro and Castro, and furthermore, we will make all of the resulting improvements available to the community. Importantly, accelerated microphysics opens the door to new physics. The network modifications will allow us to use larger, more realistic reaction networks. The GPU version of the EOS will allow us to "undo" some of the common approximations used in hydrodynamics codes to avoid expensive EOS calls [53], and improve our thermodynamic consistency.

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Proposal Title: Approaching Exascale Models of Astrophysical Explosions

Year 1		
Milestone	**Details**	**Date and Status**
Full star, high-resolution Maestro convection models in sub-Chandra WDs	20 moderate resolution runs + 5 high resolution runs exploring different initial conditions; all full star.	Summer 2015
Large domain Maestro XRB convection models	2 wide domain (30 m) models and several exploratory calculations looking at different initial models and nuclear physics.	Fall 2015
Castro multi-orbit inspiral and merger calculations of double degenerates	2 calculations with different initial conditions of WD orbit and inspiral.	End of 2015
Year 2		
Maestro sub-Chandra SNe Ia models with large reaction networks	Follow-on calculations to year 1, but with much larger reaction networks on the GPUs.	Spring 2016
Maestro XRB convection models with large reaction networks	Follow-on calculations to year 1, but some with larger domain (60 m wide), and all with bigger networks (run on GPUs)	End of 2016
Castro double degenerate mergers with nuclear physics	Model the merged beyond first contact and incorporate nuclear burning.	Summer 2016
Exploratory Maestro URCA calculations	Full star calculations of URCA convection in a white dwarf.	Fall 2016
Year 3		
Maestro to Castro models of sub-Chandra SNe Ia	Follow the explosion of a sub-Ch event in Castro beginning with a Maestro model constructed in earlier years.	Summer 2017
More realistic Maestro sub-Chandra SNe Ia models	sub-Ch convection models using initial models from a stellar evolution code.	Spring 2017
Sensitivity study of XRB simulations (Maestro)	Explorations of different XRB initial models.	throughout 2017
Largescale XRB burning model with sub-grid burning	The first XRB models using a sub-grid model for the burning, enabling larger domains	End of 2017
Castro white dwarf merger simulations with realistic initial conditions	WD merger calculations using realistic initial models from a stellar evolution code.	Summer 2017

PERSONNEL JUSTIFICATION AND MANAGEMENT PLAN

1 PERSONNEL JUSTIFICATION

All personnel are in place. Our team spans 4 institutions (Stony Brook, Los Alamos National Laboratory, Lawrence Berkeley National Laboratory, and UC Santa Cruz). We have been collaborating together for more than 10 years on problems related to those proposed here. Furthermore, we (together will additional collaborators at these same institutions) represent the principal authors of the two simulation codes used here, Maestro and Castro.

- **Michael Zingale** will act as the lead for this project. He will collaborate on all of the science applications, work on development and maintenance of the two simulation codes as needed for this project, and run simulations of the XRB.
- **Ann Almgren** will work on code development of both Maestro and Castro in support of the proposed problems. She will also be involved in the scientific analysis of the simulations proposed here.
- **John Bell** will be the main contact with the BoxLib group at LBNL. We will work with John to incorporate performance improvements into Maestro and Castro. John will also directly be involved in the scientific analysis of the simulations proposed here.
- **Alan Calder** will work primarily on the analysis and simulation design of the Castro white dwarf merger simulations. Alan will also be a lead on the "extra" exploratory applications proposed here, particularly the URCA calculations.
- **Adam Jacobs** is a SBU graduate student doing his thesis on the sub-Chandra SNe Ia convection. Adam will be the lead scientist on this problem. Adam is also the lead developer of the GPU version of the reaction networks.
- **Dan Kasen** will perform post-processing radiation transfer calculations on the explosion results with Sedona, generating lightcurves and spectra.
- **Max Katz** is a SBU graduate student doing his thesis on the white dwarf merger problem with Castro. Max will be the lead scientist on this problem. Max is also the lead developer of the GPU version of the equation of state.
- **Chris Malone** will be the lead scientist on the XRB problem with Maestro (Chris did his PhD thesis on Maestro XRB simulations in 2D). Chris will also assist in the reaction network development.
- **Stan Woosley** will collaborate on all of the science applications here and provide initial models and microphysics needed for the proposed simulations and assist in the analysis.

2 MANAGEMENT PLAN

We have been working together for over 10 years (you'll find many of the names here on the list of publications under the current INCITE award). Although we identified leads for each of the science problems above, we will all be involved in the science analysis and we expect many of the CoIs here to be co-authors on the publications that result from the proposed simulations. Allocation of computing resources will primarily follow the breakdown of time estimated in the narrative. As we work closely together and are in frequent contact, we do not expect any tensions or issues with the distribution of this time.

For the code development, the SBU group travels to LBNL several times a year to plan the development path of Maestro and Castro, and we make frequent contact with each other through e-mail and phone conferencing. All of the codes are managed by the git version control system and we use regular regression testing to ensure that the code continues to perform as expected while undergoing development. PI Zingale will be the primary contact dealing with the management of the award and preparing reports. We expect that the graduate students here will take a lead role in presenting the results to the community at conferences, and to be the lead authors in the publications that result.

PUBLICATIONS RESULTING FROM INCITE AWARDS
(last three years only)

- *Type Ia Supernovae from Merging White Dwarfs. II. Post-merger Detonations*, Raskin, C., Kasen, D., Moll, R., Schwab, J., & Woosley, S. E., 2014, ApJ, 788, 75
- *Type Ia Supernovae from Merging White Dwarfs. I. Prompt Detonations*, Moll, R., Raskin, C., Kasen, D., & Woosley, S. E., 2014, ApJ, 785, 105
- *Power-law Wrinkling Turbulence-Flame Interaction Model for Astrophysical Flames*, Jackson, A. P., Townsley, D. M., & Calder, A. C., ApJ, 784, 174
- *The Deflagration Stage of Chandrasekhar Mass Models for Type Ia Supernovae. I. Early Evolution*, Malone, C. M., Nonaka, A., Woosley, S. E., Almgren, A. S., Bell, J. B., Dong, S., & Zingale, M., 2014, ApJ, 782, 11
- *Multi-dimensional Models for Double Detonation in Sub-Chandrasekhar Mass White Dwarfs*, Moll, R. & Woosley, S. E., 2013, ApJ, 774, 137
- *Carbon Deflagration in Type Ia Supernova. I. Centrally Ignited Models*, Ma, H., Woosley, S. E., Malone, C. M., Almgren, A., & Bell, J., 2013, ApJ, 771, 58
- *Low Mach Number Modeling of Convection in Helium Shells on Sub-Chandrasekhar White Dwarfs. I. Methodology*, Zingale, M., Nonaka, A., Almgren, A. S., Bell, J. B., Malone, C. M., & Orvedahl, R. J., 2013, ApJ, 764, 97
- *High-resolution Simulations of Convection Preceding Ignition in Type Ia Supernovae Using Adaptive Mesh Refinement*, Nonaka, A., Aspden, A. J., Zingale, M., Almgren, A. S., Bell, J. B., & Woosley, S. E., 2012, ApJ, 745, 73
- *The Convective Phase Preceding Type Ia Supernovae*, Zingale, M., Nonaka, A., Almgren, A. S., Bell, J. B., Malone, C. M., & Woosley, S. E., 2011, ApJ, 740, 8

DATA MANAGEMENT

Each simulation can output 100s of TB of data. We need the ability to process all of this data at the end of a simulation, so we store the plotfiles to HPSS as they are created. A single scientific study involves several simulations, and factoring in queue times on the machines, it can take a year to complete a study. At that point we finish the analysis and write up a paper describing the results. Once we get done with the refereeing process, it can be 1.5 years since a simulation began. This defines the minimum timescale over which we need access to the data.

To reduce our data footprint, we can store the plotfile data in single precision, and we keep only a minimum set of checkpoint files archived. All of the analysis is done remotely, as the dataset is to large to transfer. In addition to homegrown analysis tools and basic runtime diagnostics (global quantities at each timestep), we use VisIt and, increasingly, yt for our visualization. This methodology has served well during our current INCITE allocation.

There is another important aspect to our data management. All of our codes are managed by version control (git) and we use regular regression testing to ensure that the code continues to give the same answers as it is developed. Furthermore, our codes are publicly available and our output files store all the information needed to reproduce a simulation (the git hashes for all code, the build machine and directory, the build and run dates, number of processors and threads, the compiler versions and flags, and the values of all runtime parameters). This gives us strong reproducibility of our results—in the event of data loss or if we wish to revisit a problem, all the information needed to reproduce a result is at hand.

We have not encountered any requests for data from a simulation, but we do make available all of the setup files needed for the various simulations once the primary science papers are published (typically this is to allow for the graduate student whose project it is to complete their thesis). For example, al the setup, inputs, microphysics, and model files for the Chandra WD convection problem that was a focus of our current INCITE are part of the standard Maestro code distribution.