FINAL REPORT

UCSC

COMPUTATIONAL ASTROPHYSICS CONSORTIUM (2006 - 2013)

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Awarded to: The Regents of the University of California, Santa Cruz

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Personnel:

The Consortium was a collaborative proposal among researchers at nine institutions. The personnel directly involved at UCSC were:

- **Faculty:** Stan Woosley (PI), Gary Glatzmaier, and Enrico Ramirez-Ruiz Glatzmaier and Ramirez-Ruiz dropped after year 3
- **Postdocs and Senior Staff:** Sung Chul Yoon, Fritz Roepke (visitor from the MPA), Dan Kasen (also paid by a Hubble Fellowship), Haitao Ma, Chris Malone, Rainer Moll (paid by another grant), Ken Chen (also paid by a Gruber Fellowship from the IAU), Shawfeng Dong (staff)
- **Graduate Students:** Candace Joggerst (PhD), Haitao Ma (PhD), Luke Roberts (PhD, also supported by another grant), James Guillichon, Tabatha Hole, Elizabeth Lovegrove

Abstract

During the six year duration of the Computational Astrophysics Consortium, UCSC contributed by helping to train the next generation of computational scientists, develop new, highly scalable codes for radiation hydrodynamics, and make major advances in our understanding of supernovae of all types, especially Type Ia. At UCSC, 3 faculty, 4 postdocs, and 4 graduate students participated directly (i.e., salaries paid mostly by this grant) and another 3 postdocs and 1 graduate student were leveraged. A total of 85 publications report progress in modeling stellar evolution, nucleosynthesis, supernovae, and gamma-ray bursts. Important secondary advances in the field of nuclear astrophysics included a better understanding of the evolution of massive stars, especially first generation "Pop III" stars and x-ray bursts from accreting neutron stars.

1 Introduction

The Computational Astrophysics Consortium (CAC) was a Science Application project (SciAp) working jointly with a Strategic Application Partnership (SAP) during the period 2006 - 2012 (at UCSC there was a no-cost extension that allowed research to continue through 2013). Further details of the funding history are given in the Appendix which is the final report for the entire Consortium. This report covers only activities at UCSC.

1.1 Training the Next Generation

At UCSC, 4 faculty and permanent staff (half of them junior"), 4 postdocs and 4 graduate students were supported directly by the grant. An additional 3 postdocs (Roepke, Moll, and Chen), and 1 graduate student (Roberts) were "leveraged", i.e., worked on the project without receiving direct monetary support. The majority of the funds we received went to paying postdocs and graduate students. The people involved in the project are listed here:

- *Faculty and Permanent Staff*: Stan Woosley, Enrico Ramirez-Ruiz, Gary Glatzmaier, Shawfeng Dong
- *Postdocs*: Sung Chul Yoon, Fritz Roepke, Dan Kasen, Haitao Ma, Chris Malone, Rainer Moll, Ken Chen
- *Graduate Students*: Candace Joggerst, Haitao Ma, James Guillochon, Tabetha Hole, Elizabeth Lovegrove
- *Postdocs Leveraged*: Fritz Roepke, Rainer Moll
- *Graduate Students Leveraged*: Luke Roberts

2 Research Proposed and Accomplished

2.1 Summary

The bibliography at the end of the report lists 85 major publications *from UCSC* that cite support by this grant. Abstracts of talks less than 1 page in length are omitted. Of these papers, 66 were in refereed journals (3 of the articles in the bibliography, [43, 44, 49], report work begun under this grant, but finished under another that failed to cite this grant). Given the breadth of the work though, it is perhaps useful to highlight up front what we view as some of the major accomplishments.

- Major advances in our understanding of the Chandrasekhar mass (single-degenerate) model for Type Ia supernovae. Unresolved issues at the time the grant began were ignition, flame propagation and conditions for a transition to detonation. In a series of papers, using MAESTRO, we showed that ignition always happens off-center and only once. In other studies using CASTRO, the flame speed was shown to be inadequate to burn a large fraction of the white dwarf during the deflagration stage. The conditions for a transition to detonation were elucidated and it was shown that turbulent speeds greater than about one-third sonic were required. Taken together the results suggest that a spontaneous transition to detonation (DDT) is difficult to achieve, but that that the Chicago "Gravitationally Confined Detonation (GCD) Model" is viable. If the DDT does not occur, a weak faint supernova might result, but not a normal Ia.

- A better understanding of other previously "non-standard" models for SN Ia. During the course of the grant, several sets of observations that were highly constraining on the progenitors shifted the debate from how to make the "standard" Chandrasekhar mass model work to exploring alternatives, notably sub-Chandrasekhar mass models and merging white dwarfs. Sub-Chandra models were explored in 1d in a broad survey and interesting cases were followed up in multi-D with CASTRO. It was found that, for slow accretion, the thickness of the helium shell at the time of the runaway was restricted by hydrodynamics and spectroscopy to about 0.05 $M_\odot$. Mergers were studied both under this grant and in subsequent works by Kasen, Woosley, Moll and Raskin funded by DOE-HEP.

- SN Ia Light Curves. The physics behind the width luminosity relation was explored and illuminated using basic physics arguments (essentially a temperature dependent effective opacity from line blanketing and UV redistribution); surveys of 1D models and 2D models were carried out.

- Shock break out in supernovae of all types using SEDONA. As the shock wave erupts from the surface of the star a brief hard transient is produced that, in the case of Type Ib supernovae, has been observed in the x-ray spectrum. A paper on breakout in pair-instability supernovae was published [34] and calculations are underway for the other varieties using CASTRO.

- Models for first generation stars including their formation, light curves, and nucleosynthesis Most of these models were 1D though some employed advanced radiation transport.

- Pulsational-Pair-Instability Supernovae and Magnetar-powered Supernova and Pair supernova - These are among the brightest supernovae in the universe. The pulsational pair instability supernovae, which occur when the shell ejected by one nuclear-powered pulse runs into another at a large distance from the star are especially interesting and are being followed up in 2D studies using CASTRO.

- Models for Gamma-ray Bursts. These varieties of supernovae are certainly powered by rotation and magnetic fields and thus offer a counter-point to the traditional neutrino transport model in massive stars. Models based upon the formation of both neutron stars and black holes were considered.

- Nucleosynthesis in massive stars was studied using the KEPLER implicit hydrodynamics package. The resulting models became the standard set in the community for the study of supernova explosions, neutron star masses, and nucleosynthesis. The dependence of the outcome on key nuclear reaction rates and metallicity was explored.

2.2 Research That Was Proposed and Outcomes

The goals and deliverables of the Computational Astrophysics Consortium and its constituent sites were laid out in the 2006 proposal. In particular section 2 of that proposal specified research in seven areas. Those areas are listed below with the original proposal subsection on parentheses. Stated UCSC deliverables and achievements are listed.

- **Administration and Oversight of the Project:**

- **Models for Type Ia supernovae (2.1):** a) 1D and 2D parametric surveys - carried out and reported in publications [67, 28, 79]; b) small scale simulations of turbulent flames - carried out in 1D [69, 73, 74, 78] and in 3D [2, 3, 4, 5, 53]; c) multi-D calculations of the convection leading to explosion - most of this was done elsewhere with our participation [84, 85, 45], but we did some 3D simulations at UCSC that were reported in Haitao Ma's PhD thesis [40]; d) highly resolved calculations of centrally ignited explosions using CASTRO [39, 40, 41]; e) highly resolved 3D calculations of off-center ignited explosions using CASTRO [42] and other codes [52]. Work by Dong, Ma, and Malone on this last topic is still being written up for publication.

Additional SN Ia science accomplished that was not in the original proposal, but mandated by observational developments in the field included exploration of other models for SN Ia than the Chandrasekhar mass model originally proposed for study in 3D [55, 57, 43, 44, 49]

The following goals were not achieved because of diminished funding in the out years: a) MHD modifications to MAESTRO - work was to be done by Glatzmaier and members of the SAP. b) 3D nucleosynthesis studies using CASTRO and tracer particles. Both projects relied upon the SAP which had less funds than anticipated when the proposal was written and other higher priorities in years 4 and 5. MHD processes are not currently thought to be central to the explosion of SN Ia.

- **Supernova light curves and spectra (2.2:** a) Grids of 1D SN Ia model light curves and spectra - published for both Chandrasekhar [67, 79] and sub-Chandrasekhar massed models; b) Develop a physical understanding of the width luminosity relation to provide more confidence in their use as calibratable standard candles - published [23]; c) calculate light curves and spectra of supernovae other than SN Ia including IIp [29] and Ib [6, 7, 9] d) Calculate 2D and 3D spectra and light curves for a representative survey of SN Ia models SN Ia - published [24, 26, 27, 28, 59, 44, 49]

- **Core collapse supernovae (2.3):** Provide 1D presupernova models for core-collapse supernova simulations - published what is now the standard set in the community for Type IIp [67] and Ibc [81, 82] supernova progenitors. Also calculated the standard set of progenitors for first generation zero metallicity stars [13]; b) explore hydrodynamical mixing in core-collapse supernovae using the CASTRO code [16, 17, 18, 19, 20]. This was Candace Joggerst's PhD thesis and an early testbed for the CASTRO code. She thus was on the CASTRO development paper [1]; c) Study fallback in 1D to determine neutron star and black hole masses - published [83].

- **Models for gamma-ray bursts (2.4):** This was emphasized during the first three years of the grant, mostly at Berkeley and Stanford, but due to a review-mandated refocusing of the effort was not vigorously pursued in the out years. Some important work nevertheless went on at UCSC, primarily because it involved the application of the same tools and expertise we developed to study core-collapse supernovae :a) new models for common GRBs [48] b) study other varieties of GRBs produced by events related to neutron star formation including the tidal disruption of neutron stars [51], supernovae whose light curves are powered by magnetars [76, 31], and very long GRBs (hours to months) produced by envelope accretion in the collapsar model [80] c) use 3D relativistic hydrodynamical simulations to limit the lowest power a jet must have to break through the envelope of the progenitor star (about 10^{48} erg s^{-1}) [66]

- **Population III Stars (2.5):** The first generation of stars to be born after the Big Bang (aka Pop III") may have had unusual properties compared with stars nowadays. In particular, their birth masses may have been larger and their death masses were almost certainly greater due to reduced mass loss for stars with no heavy elements. Topics proposed and studied were a) new models for pulsational pair instability supernovae - the defining 1D paper [70] was published and multi-D studies [65] were carried out; b) new models for pair instability supernovae in 1D and 2D - these were calculated [20, 21]; c) break out and its observational characteristics at high redshift were examined [34, 35, 62]; d) the spectra and light curves of pair-instability supernovae were calculated [33, 25]; and e) mixing in Pop III stars and environs was studied [61, 63, 64].

- **X-ray bursts (2.6):** 1D multizone-models with realistic reaction rates and convective mixing were calculated and compared with observations [11, 12]. Woosley also assisted Fisker and Hoffman with their studies of x-ray bursts at LLNL.

- **Studies of nucleosynthesis (2.7):** UCSC and secondarily the University of Minnesota were responsible for computing the nucleosynthetic diagnostics for all models computed by the Consortium as well as carrying out 1D surveys using the KEPLER code. Hoffman at LLNL and Woosley, with input from the Joint Institute for Nuclear Astrophysics, maintained the standard nuclear physics library used for studies of nucleosynthesis. Specific tasks were: a) to provide the necessary nuclear reaction networks, tables, and rates for all CASTRO and MAESTRO studies of supernovae - this was done [e.g. 40, 41, 42, 43, 44]; b) use the KEPLER code to compute surveys of nucleosynthesis in massive stars and supernovae - we computed what are now the standard grids for solar metallicity [68], zero metallicity stars [13], and sub-Chandrasekhar mass SN Ia [79]; c) use KEPLER and the BURN to study the r-process and the p-process - we did so and published the results [14, 50]

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APPENDIX: FINAL REPORT FOR THE COMPUTATIONAL ASTROPHYSICS CONSORTIUM

FINAL REPORT

COMPUTATIONAL ASTROPHYSICS CONSORTIUM (2006 - 2013)

Grant number:DE-FC02-06ER41438

Subsidiary grants: DE-FG02-08ER41544 (Princeton), DE-FC02-01ER41176 (LLNL and LANL), DE-FC02-09ER41618 (Minnesota), DE-FG02-06ER06-04 (LBNL), DE-FG02-06ER41453, DE-FC02-06ER41438 (UCB)

Principal Award to: The Regents of the University of California, Santa Cruz

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Office of Science Program Office: Office of High Energy Physics

Science Program Office Technical Contact: Dr. Lali Chatterjee

Collaborators and co-I's:

This was a collaborative proposal among researchers at nine institutions: Though many senior researchers ultimately were involved in the research, the original co-I's on the proposal are given below. OASCR support ended two years into the grant and the number of collaborators was significantly reduced.

- Stan Woosley (PI), Gary Glatzmaier, Enrico Ramirez-Ruiz - UCSC - Glatzmaier and Ramirez-Ruiz dropped after year 2
- John Bell, Ann Almgren, and Peter Nugent - LBNL
- Alex Heger - LANL then moved to Univ. Minnesota
- Louis Howell, Rob Falgout, Rob Hoffman - LLNL - Falgout and Hoffman dropped after year 2
- Dan Kasen - initially a postdoc at John Hoplins and UCSC; later a co-I at UC Berkeley
- Adam Burrows - initially at the University of Arizona, later at Princeton
- Mike Zingale - a co-I at SUNYSB that received all his support from a separate grant from DOE-NP
- Chris McKee - UC Berkeley (dropped after year 2)
- Roger Blandford - Stanford (dropped after year 2)

Abstract

During its six year duration the Computational Astrophysics Consortium helped to train the next generation of computational scientists, developed new, highly scalable codes for radiation hydrodynamics, and made major advances in our understanding supernovae of all types, especially Type Ia. The eight institution Consortium eventually involved the participation of 75 faculty, scientific staff, graduate students and postdocs, including 15 faculty and senior staff, 21 postdocs and 17 graduate students paid directly by the grant. A total of 231 publications report progress in observing and modeling thermonuclear supernovae (Type Ia and pair instability), core-collapse supernovae, and gamma-ray bursts. The three codes developed demonstrated that useful science could be done efficiently on over 100,000 CPU. Two of these codes, CASTRO and MAESTRO, are now available to the public. Important secondary advances in the field of nuclear astrophysics included a better understanding of the evolution of massive stars, the origin of the elements, and x-ray bursts from accreting neutron stars.

1 Introduction

1.1 overview

The Computational Astrophysics Consortium (CAC) was a Science Application project (SciAp) working jointly with a Strategic Application Partnership (SAP) during the period 2006 - 2012 (at UCSC there was a no-cost extension that allowed research to continue through 2013). The funding history was complicated by the fact that the Consortium was funding by four DOE Programs - OASCR, NNSA, NP and HEP - during its first three years, but by only three during the last two (OASCR funding expired in 2009). During the first three years, level of support was greater and the Consortium addressed a broad range of problems in computational astrophysics related to supernovae. These included: a) the development of highly scalable codes for astrophysics and other applications; b) modeling of supernovae of all types, but especially Type Ia; c) theoretical studies of models for gamma-ray bursts and x-ray bursts; d) studies of stellar evolution and nucleosynthesis; and e) observations of supernovae. Topic a) was of interest to OASCR and the NNSA. Topics b), c) and d) were of interest to NP and topics a), b), and e) were of interest to HEP. Faculty, postdocs and graduate students at eight institutions were initially involved: UCSC, LBNL, LLNL, LANL, Stanford, UC Berkeley, U Arizona, and Johns Hopkins U.

Following the end of OASCR funding in 2009, it was recognized that code development and optimization needed to continue, and that the science was best done with the continued involvement of the code developers (applied mathematicians), who by then had become skilled astrophysicists themselves. As a result, there continued to be substantial support directed to LBNL, but at the expense of the broader science application. Work was refocused and some institutions and collaborators were dropped. Participation by Stanford, UC Berkeley, and LLNL was curtailed and research into gamma-ray bursts, x-ray bursts, supernova observations, stellar evolution, and stellar nucleosynthesis was greatly cut back. The prime focus during the out years was then on: a) the continued development of three codes for computational astrophysics (in particular, supernovae) - CASTRO, MAESTRO, and SEDONA - as was necessary for all other aspects of the research and still of interest to the NNSA; b) Models for Type Ia supernovae because of DOE HEP's interest in dark energy; c) Models for core-collapse supernovae (carried out at Princeton only), because of DOE NP's interest to these objects and the application of CASTRO with radiation transport to an important test case. During the last two years, additional funds were provided by DOE-HEP and they became our chief sponsor. Type Ia supernova thus became our highest priority.

There was also some movement of co-I's during the last several years. Alex Heger, who had been at LANL moved to U Minnesota; Dan Kasen moved from JHU to UCSC and then to UC Berkeley where he is now on the faculty; Adam Burrows moved from Arizona to Princeton.

1.2 Principal Accomplishments

1.2.1 Training the Next Generation

Before turning to more objective measures of productivity like publications and codes developed, we would like to mention what we feel was our greatest accomplishment: the training of a new generation of computational astrophysicists. In all, 15 faculty and permanent staff (about half of them junior"), 21 postdocs and 17 graduate students were supported. An additional 5 faculty, 11 postdocs, and 6 graduate students were "leveraged", i.e., worked on the project without receiving direct monetary support. The majority of the funds we received, especially at the universities, went to paying postdocs and graduate students. Secondarily we demonstrated that a sizable collective of applied mathematicians and astrophysicists at many locations could work together to train students and do good science. The people involved in the project are listed here:

- *Faculty and Permanent Staff*: (UCSC) Stan Woosley, Enrico Ramirez-Ruiz, Gary Glatzmaier, Shawfeng Dong; (LBNL) Ann Almgren, John Bell, Weiqun Zhang; (UCB) Peter Nugent, Jon Arons, Chris McKee, (Dan Kasen); (LANL-U Minn) Alex Heger; (Arizona-Princeton) Adam Burrows; (LLNL) Rob Hoffman, Louis Howell; (Stanford) Roger Blandford

- *Postdocs*: (UCSC) Sung Chul Yoon, (Dan Kasen), (Haitao Ma), Chris Malone; (LBNL) Andy Nonaka; (UCB) Sebastien Bongard, Dovi Poznanski, Antonino Cucchiarra, Jeffrey Oishi, Bradley Cenko, Eric Hsiao, Jason Dexter; (LANL-U Minn) Sanjib Gupta; (Arizona-Princeton) Luc Dessart, Jason Nordhaus, Rolf Walder, Christian Ott, Emmanouela Rantsiou; (LLNL) Jacob Fisker, Mike Singer; (Stanford) Jonathon McKinney, Shizuka Akiyama; (JHU) Dan Kasen

- *Graduate Students*: (UCSC) Candace Joggerst, Haitao Ma, James Guillocon, Tabetha Hole, Elizabeth Lovegrove; (LBNL) Candice Gilet; (UCB-LBNL) Michael Childress, Siva Dharba, Andrew Myers, Janos Botyanszki, Jeffery Silverman; (LANL-U Minn) (Candace Joggerst) Pamela Vo, Chris West, Charles McEachern, Ken Chen; (Arizona-Princeton) J. Murphy, T. Brandt

- *Faculty Leveraged*: (SUNYSB) Mike Zingale, Eric Myra, Doug Swesty, Alan Calder; (Stanford) Tom Abel

- *Postdocs Leveraged*: (UCSC) Fritz Roepke, Rainer Moll, (Ken Chen); (LBNL) Andy Aspden; (Ariz-Princeton) T. Thompson, Erik Schnetter, Ernazar Abdikamalov; (LANL-U Minn) Falk Herwig, Dan Whalen, Brian O'Shea, Laurens Keek; (SUNYSB) Brendon Kreuger

- *Graduate Students Leveraged*: (UCSC) Luke Roberts; (LANL-U Minn) Allan Straub James Anderson, (Dan Whalen), (Brian O'Shea), Fang Peng; (U Arizona-Princeton) Evan O'Connor; (SUNYSB) (Chris Malone); (Stanford) Pen Wang

In this list, a name in parenthesis means that the person worked at more than one institution within the Consortium or that the person was both a postdoc and a graduate student at the same institution. Such people were only counted once in the summary numbers given previously.

1.2.2 Major Science Accomplishments

The bibliography at the end of the report lists 231 major publications that cite support by this grant. Abstracts of talks less than 1 page in length are omitted. Of these papers, 192 were in refereed journals (3 of the articles in the bibliography, [127, 128, 167], report work begun under this grant, but finished under another that failed to cite this grant). Some details of the work on Type Ia supernovae and code development are given in subsequent sections (§2 and §3). Given the breadth of the work though, it is perhaps useful to highlight up front what we view as some of the major accomplishments.

- The development of three major codes for computational astrophysics. These are major advances in computational science as well. See §3 for details. CASTRO [5, 226, 227] is a compressible (unsplit) hydrodynamics code with adaptive mesh refinement, multi-group radiation hydrodynamics, and general equation of state and nuclear physics modules. MAESTRO [141] is an equivalent low-Mach-number code which in its power and capability is unique in astrophysics. SEDONA [108] is a multi-dimensional Monte Carlo radiation transport package. MAESTRO and CASTRO (without radiation) are now publicly available (https://ccse.lbl.gov/Downloads/index.html). CASTRO (without radiation) and MAESTRO have demonstrated scaling on relevant problems up to 200,000 and 100,000 CPU respectively.

- Major advances in our understanding of the Chandrasekhar mass (single-degenerate) model for Type Ia supernovae (see §2). Unresolved issues at the time the grant began were ignition, flame propagation and conditions for a transition to detonation. In a series of papers, using MAESTRO, we showed that ignition always happens off-center and only once [2, 229, 230, 142]. In other studies using CASTRO, the flame speed was shown to be inadequate to burn a large fraction of the white dwarf during the deflagration stage [122, 124]. The conditions for a transition to detonation were elucidated and it was shown that turbulent speeds greater than about one-third sonic were required [9, 10, 11, 12, 171, 211, 216, 220]. Taken together the results suggest that a spontaneous transition to detonation (DDT) is difficult to achieve, but that that the Chicago "Gravitationally Confined Detonation (GCD) Model" is viable. If the DDT does not occur, a weak faint supernova might result, but not a normal Ia.

- A better understanding of other previously "non-standard" models for SN Ia. During the course of the grant, several sets of observations that were highly constraining on the progenitors shifted the debate from how to make the "standard" Chandrasekhar mass model work to exploring alternatives, notably sub-Chandrasekhar mass models and merging white dwarfs. Sub-Chandra models were explored in 1d in a broad survey [221] and interesting cases were followed up in multi-D with CASTRO [127]. It was found that, for slow accretion, the thickness of the helium shell at the time of the runaway was restricted by hydrodynamics and spectroscopy to about 0.05 $M_{\odot}$. Mergers were studied both under this grant [174, 69, 178, 183] and in subsequent works by Kasen, Woosley, Moll and Raskin funded by DOE-HEP.

- To test the radiation transport implemented in CASTRO, state of the art models of core-collapse in massive stars were calculated. The character of 2D and 3D turbulence pumped by neutrino deposition was explored and diagnostics were developed for distinguishing the two cases. We found that neutrino-driven explosions in 3D are driven by the growth of one or a few large bubbles built up from the merger of many smaller ones, and that the explosion may be roughly dipolar in nature [30, 31, 140, 53]. The radiation transport in CASTRO is multi-group, contains velocity-dependent terms, and fully multi-dimensional. We used these capabilities to model core collapse for a suite of progenitor models [54]. Other interesting studies led up to the later works [165, 189, 150, 86, 137, 138, 139, 143, 144, 145].

- SN Ia Light Curves. The physics behind the width luminosity relation was explored and illuminated using basic physics arguments (essentially a temperature dependent effective opacity from line blanketing and UV redistribution) [98]; surveys of 1D models [209]; and surveys of 2D models [103].

- A large variety of supernova observations were carried out, mostly in a (successful) attempt to limit the nature of common SN Ia progenitors [18, 60, 72, 84, 112, 147, 182] and improve their utility as distance indicators [16, 39, 55, 60, 85, 116, 191, 192]. Core collapse and ultraluminous supernovae were also studied [62, 63, 83, 115, 148, 184]. We also explored the use of Type II supernovae as distance indicators[158, 159, 160].

Other interesting results, mostly from the first three years of the grant, and perhaps of greater interest specifically to DOE NP were:

- X-ray bursts on neutron stars. These are interesting laboratories for nuclear physics along the proton drip line. The cutting edge calculations were carried out in 1D [73, 74, 58, 71, 89, 113, 114] and the first 2D studies were done using MAESTRO [123, 125].

- Shock break out in supernovae of all types using SEDONA. As the shock wave erupts from the surface of the star a brief hard transient is produced that, in the case of Type Ib supernovae, has been observed in the x-ray spectrum. A paper on breakout in pair-instability supernovae was published [110] and calculations are underway for the other varieties using CASTRO.

- Models for first generation stars including their formation, light curves, and nucleosynthesis [130, 110, 153, 154, 96, 201, 203, 204, 205, 206, 207]. Most of these models were 1D though some employed advanced radiation transport.

- Pulsational-Pair-Instability Supernovae [212] and Magnetar-powered Supernova [156, 218, 162] Pair SN [36]. These are among the brightest supernovae in the universe. The pulsational pair instability supernovae, which occur when the shell ejected by one nuclear-powered pulse runs into another at a large distance from the star are especially interesting and are being followed up in 2D studies using CASTRO.

- Models for Gamma-ray Bursts. These varieties of supernovae are certainly powered by rotation and magnetic fields and thus offer a counter-point to the traditional neutrino transport model in massive stars. Models based upon the formation of both neutron stars [21, 22, 34, 163, 164, 7, 8, 186, 187, 131, 132, 47, 152] and black holes [208, 222, 129] were considered.

- Nucleosynthesis in massive stars was studied using the KEPLER implicit hydrodynamics package. The resulting models became the standard set in the community for the study of supernova explosions, neutron star masses, and nucleosynthesis [210, 117]. The dependence of the outcome on key nuclear reaction rates [59, 168, 32, 80, 195, 196, 82, 40, 198, 14, 13] and metallicity [76] was explored.

2 TYPE Ia SUPERNOVA

As noted in the introduction, a major topic of investigation by the Computational Astrophysics Consortium was the multi-dimensional modeling of Type Ia supernovae (SN Ia). A SN Ia occurs when a critical mass of degenerate carbon and oxygen, i.e., a white dwarf, reaches a flash point and explodes. The progenitor star is in a binary system and the critical point is when enough matter accumulates that compressional heating ignites a thermonuclear runaway in the carbon. There is considerable uncertainty and debate, however, regarding just how the white dwarf ignites and burns and what sort of binary system it is situated in.

2.1 The Chandrasekhar Mass Model - aka the "Standard Model"

In the most popular model at the time the grant began, the star that exploded and made a SN Ia added mass slowly and almost reached the maximum mass a white dwarf could have, the Chandrasekhar mass (1.38 $M_\odot$), before starting to burn. Ignition occurred deep within the star, somewhere near the center, and the burning turned most of the star, which was initially carbon and oxygen, into radioactive ^{56}Ni. The energy released by this burning completely disrupted the star with a kinetic energy $\sim 10^{51}$ erg and the decay of the ^{56}Ni to ^{56}Co ($\tau_{1/2}$ = 6.1 d) and of ^{56}Co to ^{56}Fe ($\tau_{1/2}$ = 77.2 d) powered the light curve of the supernova, making it almost as bright as a galaxy for weeks. Since the mass of ^{56}Ni determined the brightness and didn't vary greatly from event to event, most SN Ia had quite regular light curves. The variation in brightness that did exist could be largely corrected for, since there is a relation between the ^{56}Ni mass and the effective opacity. More ^{56}Ni makes the expanding debris hotter, which increases its opacity making the light curve broader [98]. More radioactive decay also made the supernova brighter at peak. Hence the "width-luminosity relation" or WLR, brighter supernovae have broader light curves, i.e., stay brighter longer.

From the perspective of a model builder, there were three separable stages to the explosion of a standard Chandrasekhar mass supernova, starting with ignition, continuing with the propagation of burning through the star that results in its explosion, and finally, the spectrum of the resulting supernovae. Each stage had its

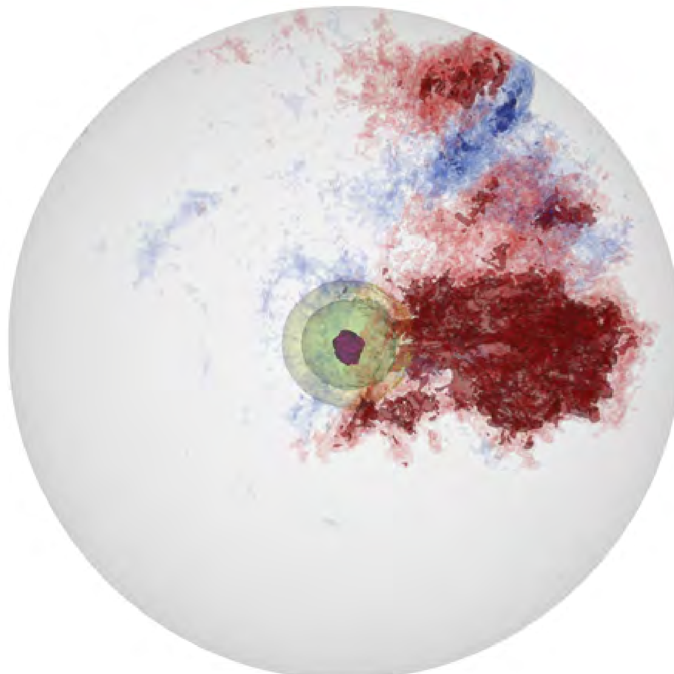

Figure 1: Contours of nuclear energy generation rate (yellow to green to purple) and radial velocity (red is outflow) near the time of runaway for a MAESTRO simulation with an effective resolution of 2.17 km. Only the inner r = 1000 km are shown [142].

own particular computational challenges and our strategy was to use simulation codes specifically optimized for each stage to answer key questions.

2.1.1 Ignition

In that standard model, the dwarf accreted mass at a rate of about 10^{-7} $M_\odot$ y^{-1} and gradually grew to 1.38 $M_\odot$. The matter that accreted could be hydrogen- or helium-rich, but at this accretion rate, both would burn to carbon and oxygen in very thin layers on top of the star. Once the critical mass was reached, carbon would fuse rapidly into heavier elements somewhere near the center of the white dwarf. The central temperature at this "first ignition", when highly screened carbon fusion reactions finally provided more energy than was carried away by neutrino losses from the plasma, was about 3×10^8 K. The star did not explode right away though. For several centuries, the excess energy from carbon fusion was transported outwards by convection with increasing speed that carried increased energy flux. During this time, the central temperature continued to rise at nearly constant density as the white dwarf gradually "thawed out" and attained an adiabatic temperature gradient throughout most of its mass. Eventually, a second critical temperature was reached at the center, $\sim 7.5 \times 10^8$ K, at a density of about 3×10^9 g cm^{-3}, where convection was no longer able to carry away the rapidly escalating energy generation. Because of the extreme degeneracy of the electrons, once convection freezes out, the temperature rapidly escalates to values near 10^{10} K before the pressure rises perceptibly. This rapid rise in temperature sharpens the temperature gradient culminating in the formation of a thin (initially < 1 mm), propagating interface between hot ash and cold fuel called a "flame". During the next few seconds, this flame sweeps through the star causing it to explode, leaving nothing behind.

When we began our SciDAC project, the physics of ignition was one of the major uncertainties in the model. Despite general agreement on the qualitative picture outlined above, it was unclear whether the interaction of convection and burning would frequently lead to ignition at the center of the star or off center. If off-center, by how much, and what was the geometry of the first flame - a point, a sphere, an ellipsoid, or

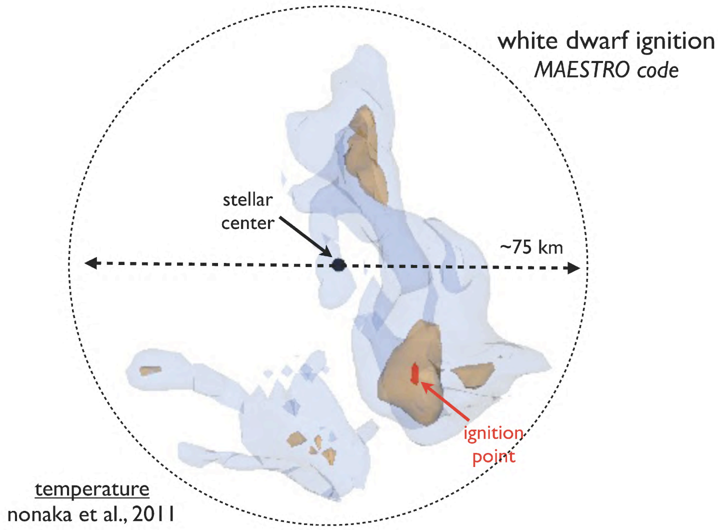

Figure 2: Temperature contours at the innermost 75 km of the white dwarf at the time the runaway ignites. The black dot contains the center of the star and has diameter 4.4 km, corresponding to the cell size from the MAESTRO simulation. The red contour encapsulates the region (one grid cell in this case) where T $> 8 \times 10^8$ K, gold encapsulates T $> 7.8 \times 10^8$, and blue encapsulates T $> 7.5 \times 10^8$. [142].

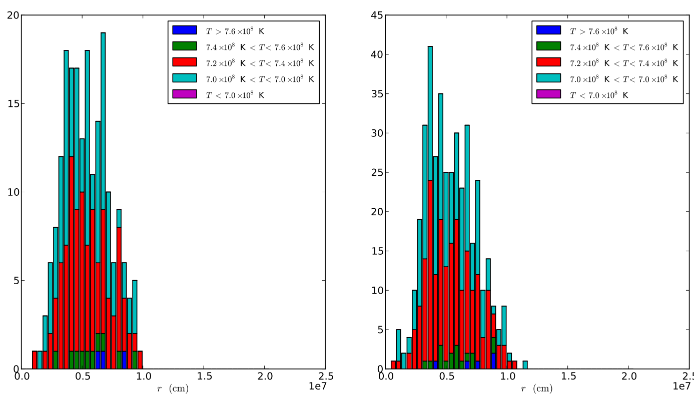

Figure 3: Histograms of the hottest cell, sorted by radius, with the colors representing the average temperature of the hottest cell over the averaging interval for the 4.34 km simulation with (Left) Δt_{hist} = 1.0 s and (Right) Δt_{hist} = 0.5 s [142].

what? Was ignition an ongoing process that happened at many points while the explosion got going or did it only happen once? Did the pre-existing turbulence from the convection affect the propagation of the flame in an appreciable way? Despite some earlier exploratory studies by the Santa Cruz group, the answers to these questions were unknown and major studies by other groups were making contradictory assumptions and getting different answers for the explosion.

To address these issues conclusively, it was necessary to build an entirely new hydrodynamics code, MAESTRO [141] (see also §3). In this "low Mach number code", sound waves were not followed and a background state in tight hydrostatic equilibrium was assumed to exist. The code was thus not restricted by the Courant time, but only by the need to follow the vastly slower convective fluid motion. MAESTRO was built, optimized to run in 3D on up to 100,000 CPU, and equipped with adaptive mesh refinement. Given the right tool - thanks to SciDAC - most of the critical questions about ignition in the Chandrasekhar mass model were answered to our satisfaction.

Our studies [229, 230, 142] showed that the convection has a dipole-like character (Fig. 1). The highest temperatures and ignition occur in outward bound plumes, and the runaway ignites off-center (Fig. 2). Unlike earlier studies by Kuhlen et al., our studies also gave a reliable estimate for the ignition radius (Fig. 3), typically 40 - 75 km off center, but with non-zero probability from 0 to about 110 km. Much of this ignition region would have been inside Kuhlen's inner boundary condition. We then confirmed that this displacement was sufficient that the star burns preferentially on one side, never igniting the far side of the star unless a subsequent detonation occurs (§2.1.2). Initially at least, this sort of supernova will be very asymmetric. Our analysis also shows that ignition will only happen once (Fig. 4). The time between successive recurrences of regions hot enough to run away was considerably longer than one second, the time it takes the star to completely disrupt once it is ignited. Taken together, these are transformational results. SN Ia resulting from the explosion of Chandrasekhar mass white dwarfs will, initially at least, be asymmetric and will not explode unless there is a subsequent detonation (§2.1.2). They only ignite once and the ignition region is irresolvably small, certainly less than 1 km. This means that the initial propagation of the burning, for the first tenth of a second or so, will actually be by a laminar flame.

The existence of a range of ignition radii and not just a single value has significant implications for the light curve. For example, ignition at a larger radius where gravity is stronger leads to more rapid floatation and less burning as the flame moves to the surface of the star. This implies less energy is released and the star expands less prior to detonation. The detonation then moves through matter that is denser and makes more ^{56}Ni and a brighter supernova.

We also analyzed the turbulence created by the pre-explosive convection and found that it has a Kolmogorov character [142]. That turbulence has a smaller intensity on a larger integral length scale than previously thought, 16 km s^{-1} on a length scale of approximately 200 km. Using Kolmogorov scaling, $u \propto L^{1/3}$, this implies turbulent speeds on a 10 km scale of 6 km s^{-1}. This is an order of magnitude smaller than the laminar speed at a density of 3×10^9 g cm^{-3}, suggesting that the initial propagation of the burning (~ 0.1 s) may be governed by the laminar flame speed, not the convective turbulence. Shortly after that the ash with size $\sim$10 km, floats faster than either the background turbulent speed or laminar speed. It seems that the pre-existing turbulence is not a driving factor in how the star explodes, once the first hot spot begins to run away. It may be the source of the initial perturbations though, on an otherwise spherical flow.

The last study employed an effective 4.34 km resolution, and resolved the general flow field properties at an effective 2.17 km resolution. Results obtained with this resolution are consistent with our previous coarser (8.68 km resolution) simulations, suggesting that we have achieved sufficient resolution in order to determine likely ignition radii, at least for the numerical Reynolds number accessible so far.

2.1.2 Explosion

Once the flame is born, a new computational challenge emerges. The ash from the burning has a lower density than its surroundings. It is thus buoyant and floats. Due to the large gravitational potential inside the white dwarf (g times Atwood number $\sim 10^9$ cm s^{-2}), floatation speeds can rapidly approach 10 - 30% of the sound speed. The flame is Rayleigh-Taylor (RT) unstable and experiences the Kelvin-Helmholtz (KH) instability at its boundary due to the high shear. Turbulence is generated and the combination of burning, turbulence, floatation, RT and KH instabilities, and the pressure gradient instability leads to a rapid expansion and advance of the burning, far faster than ordinary conductive, laminar burning alone. This is referred to as the "deflagration stage" of the explosion.

It was widely believed when we started, and we have confirmed (see below), that this deflagration alone will not give rise to SN Ia that closely resemble common events. Some key problems at the time we began our study were:

- What does the initial propagation of the flame look like? How does the flame spread? Is the flame surface always turbulent?

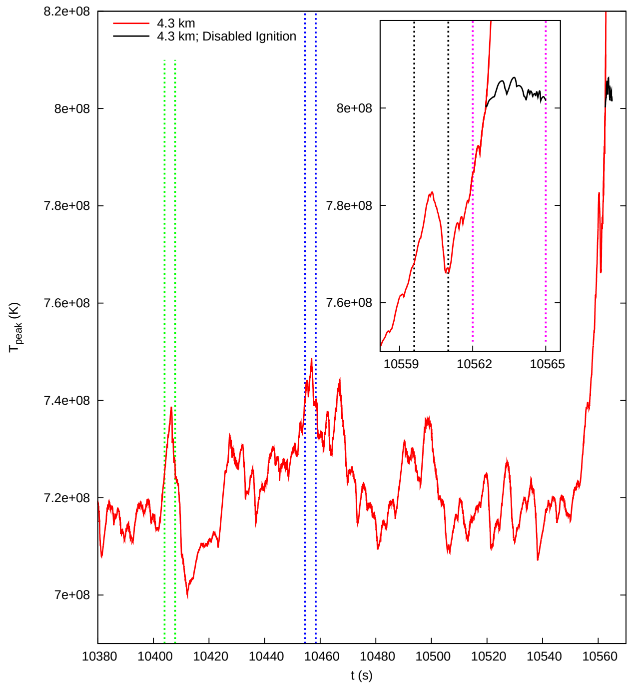

Figure 4: Peak temperature during the ∼200 s preceding ignition for the 4.34 km simulation. The dashed vertical lines indicate time ranges where we will examine whether there are multiple hot spots. The inset plot is a zoom-in of the final ∼5 s preceding ignition. The black curve follows the maximum temperature for a simulation where we disable burning in all cells with $T > 8 \times 10^8$ K. [142]

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- What are the properties of a centrally-ignited deflagration? This problem had been previously considered with the conclusion that deflagration alone gives a supernova with some similarity to SN Ia, but with too little burning to be the common event. We wanted to try our new code and physics on this problem as a test case.
- If the explosion ignites off center, as now appears likely, what happens? How much burning occurs in the deflagration stage and does a delayed detonation occur. Chicago and Munich had both studied the problem and reached different conclusions in their 3D studies.
- What are the key physics, conditions, and site for a potential delayed detonation?
- How does the model outcome vary given various assumptions about the locations of ignition and DDT?
- What are the observables - spectra, light curve, energetics, and nucleosynthesis of the models and how do they compare with observations? What physical variables in the explosion model give rise to the observed diversity of explosions, while maintaining a tight correlation between peak brightness and the width of the light curve?

We were able to make significant advances in answering all these questions, but, unlike the ignition problem, cannot yet claim to have solved them all conclusively.

Initial Burning Beginning with single point ignition we studied the early evolution of a burning, floating bubble in a fully resolved calculation using a code similar to MAESTRO [Fig. 5 12]. To avoid reliance on a subgrid model for turbulence, a density, 1.5×10^7 g cm^{-3}, was employed, lower than what is typical in a real explosion. Use of the lower density leads to a thicker laminar flame that is easier to fully resolve. As

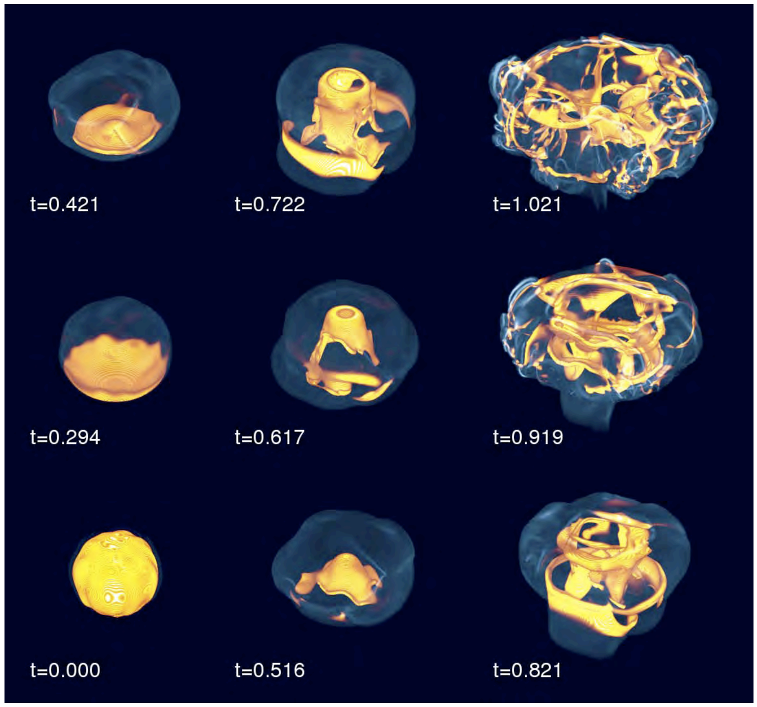

Figure 5: Three-dimensional renderings of the early stages of evolution of a fully resolved burning thermal in a uniform environment (constant gravity, density, initial composition, and pressure). Yellow denotes burning and blue denotes vorticity. All images are at the same scale, where the initial thermal radius was 14 cm. The times corresponding to each image are given in milliseconds (note for context the entire simulated time was 5.6 ms, see Fig. 6 for the evolution after t = 1.021 ms).

discussed by Aspden et al. [12], the results should be qualitatively similar when studied on a larger scale at higher density. This was verified by comparing to thickened flame studies with CASTRO of full star models.

We discovered that there are several stages to the deflagration [124]. Ignition at a single point leads to a "burning floating bubble" that, except for the burning, resembles closely buoyant "thermals" that have been studied in other areas for years. The simulations agree with the predicted power laws and provide constraints for the full-star simulations. The qualitative agreement between the resolved thermals and our full star simulations was gratifying [12]. The flame speed was found to be important during the early-time evolution of the thermal, but played a diminishing role at later times when the evolution became dominated by the large-scale hydrodynamics responsible for entrainment. However, a higher flame speed effectively gave a larger initial ignition kernel, and so resulted in more mass burned. This suggests that future studies should focus on the early-time behavior of these thermals (in particular, the transition to turbulence), and that the choice of turbulent flame speed does not play a significant role in the dynamics, once the thermal has become well established.

Somewhat surprisingly, little turbulence was found in the fuel at the fuel-ash interface, though large turbulence was present in the ash. This leads us to suspect that the critical lateral expansion of the burning may be due more to the baroclinic instability than to turbulence in the fuel. If true, this would greatly reduce the reliance of the results on either a subgrid model for the turbulence or an assumed thick flame speed. This is definitely a topic we want to to explore further.

Centrally Ignited Deflagration Models Using CASTRO and resources at NERSC and ORNL, we have run several 3D models of centrally ignited carbon deflagration in which the burning was represented as a thickened flame with a prescribed speed. Values of 50, 100 and 200 km s^{-1} were employed, which spans the range that is implied by the turbulence and the laminar speed. Results from one of these studies is shown in Fig. 7. For these choices of flame speeds the final synthesis of ^{56}Ni in the three models was 0.56, 0.48,

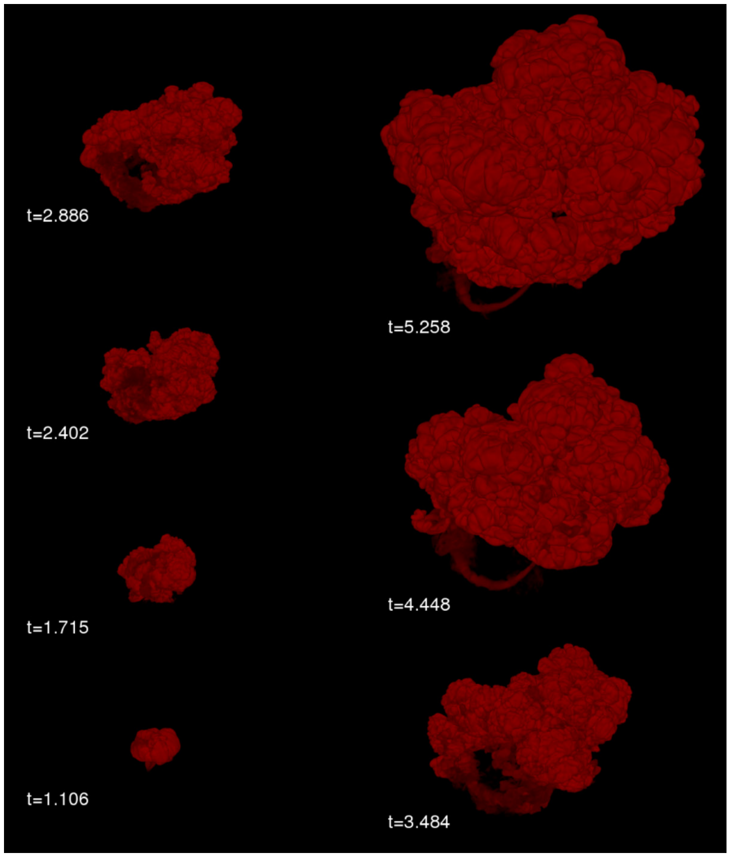

Figure 6: The continued evolution of the burning thermal shown in Fig. 5. Qualitatively similar results were obtained using CASTRO to model the initial burning in a real star using a thickened flame model. At early times shown in Fig. 5, the burning occurs mainly on the underside of the thermal, but at around t $\approx$ 1 ms, a transition occurs and the burning becomes distributed throughout the thermal. Burning thus progresses by entrainment.

and 0.50 $M_\odot$ and the kinetic energies were 1.26, 1.15 and 1.16 $\times 10^{51}$ erg. A mass of 0.16 - 0.17 $M_\odot$ of intermediate mass elements was made in all three models. These results showed a gratifying insensitivity to the uncertain flame speed and are consistent with previous studies, although we found considerably less production of intermediate mass elements than the Munich group. Approximately 0.4 - 0.5 $M_\odot$ of the white dwarf is ejected as unburned carbon and oxygen. As noted by others, this has several deleterious effects. The final explosion speed is too slow and the luminosity too faint to agree with common SN Ia, and the presence of unburned C and O, especially at low velocity, conflicts with the observed spectrum. Centrally ignited deflagrations can only account for a relatively rare class of sub-luminous SN Ia, events that have not been identified in nature. This work formed part of the PhD thesis [122] of Haitao Ma.

These calculations followed only the deflagration stage of the burning and not any ensuing detonation. Later, we implemented detonation in the CASTRO code, and have carried out 2D detonation studies. These are still being written up. Tables have been implemented that speed up the calculation of burning by at least an order of magnitude compared with carrying a (minimal) reaction network.

Models Ignited Off Center According to our studies of ignition (§2.1.1), centrally ignited deflagrations are rare. The common case should be ignition at 30 - 75 km off center. We thus calculated a series of deflagrations ignited at a point (actually a perturbed sphere with radius 20 km) displaced from the center by variable amounts in this range. The results were most sensitive to where the initial off-center deflagration was launched. If the initial ignition was 75 km off center, less mass (0.07 $M_\odot$) burned and the collision of

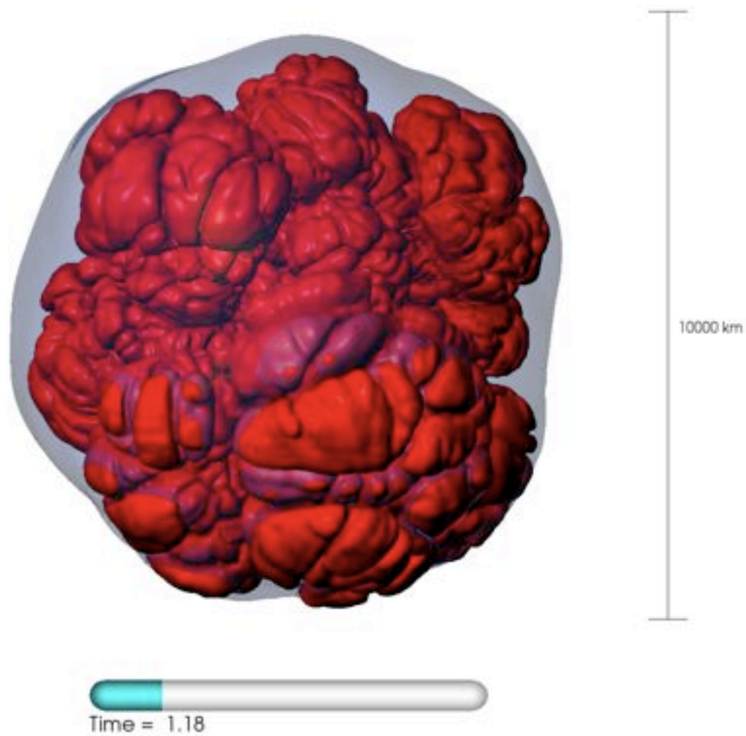

Figure 7: Centrally ignited carbon deflagration calculated with CASTRO at ORNL and NERSC near the end of burning, 1.21 s after ignition. Red shows the interface between ash and fuel and light blue color indicates the star surface where density equals 10^6 g cm^{-3}. The flame speed parameter in this model was 100 km s^{-1}[122]

the ejected ashes on the far side was very energetic, raising the temperature above 2×10^9 K in region with a density greater than 10^7 g cm^{-3}. Such an energetic collision could lead to a detonation. If, on the other hand, the initial ignition was closer in, at 30 km from the center, much more mass (0.11 $M_\odot$) burned and the star expanded more. The collision on the far side was greatly weakened and would not trigger a detonation. Therefore, our results differed not only from those of the Chicago group, who found that the conditions for detonation were robustly achieved for all their off-center calculations; but also from those of the Munich group, who reported that surface detonation would not happen for any of their 3D off-center calculations, especially when the displacements of the initial bubbles were $\leq$ 200 km off center. A key parameter may be not just the outer extent of the ignition, but the *inner* extent.

Our results were also, to a lesser extent, sensitive to the shape of the initial bubble. If the ignition was cylindrically symmetric (like the spherical bubbles considered above), then that symmetry was maintained throughout the rise of the burning bubble and the spread of the ash over the surface. This added symmetry maximized the strength of the collision on the far side. If, however, the initial burning region was not symmetric (for example, an ellipsoid with equatorial radii of 40 km, 20 km and 20 km), the geometry of the entire explosion was changed (Fig. 8) and the collision could be much weaker. Our results showed that when the initial bubbles are far off center (75 km), their shapes are less important: both cases (those with spheroidal and ellipsoidal initial shapes) burned about the same amount of mass (0.07 $M_\odot$) and both resulted in a strong collision on the far side which could lead to detonation. However, when the initial bubbles were close to the center (30 km), the case with the initial ellipsoidal bubble burned far more mass (0.23 $M_\odot$, vs

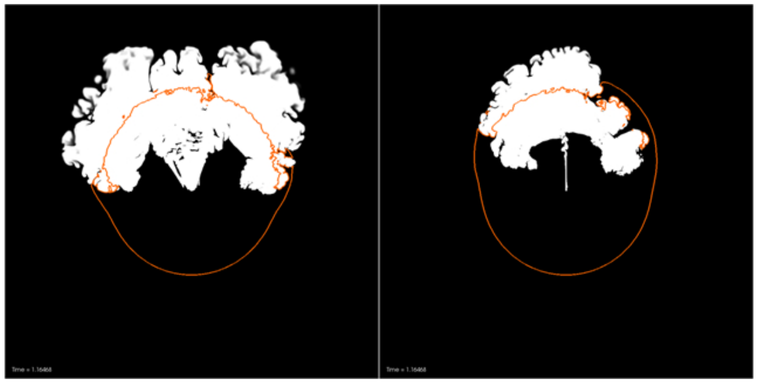

Figure 8: The deflagration of a model ignited in an ellipsoidal region off-center as calculated using CASTRO at ORNL and NERSC. The picture show a slice of the ash right after the burning bubble breaks out of the surface of the white dwarf (orange lines). The left panel is a slice of the x-z plane (with X being the long axis of the initial ellipsoid); the right a slice of the y-z plane. One can see that the geometry of the entire explosion is asymmetric, which will lead to a weaker collision on the far side.

0.11 $M_\odot$ for the spheroidal case), resulting in a much weaker collision. For the 4 models (30 km and 75 km off center, with either spheroidal or ellipsoidal bubble initially) we've done so far, the shapes of initial bubbles don't change the outcome of the collisions. We can, however, reasonably expect that for cases with intermediate displacement of ignition ($\sim$ 50 km off center), the shape of the initial bubble will dictate whether the collision can trigger a detonation.

With AMR we were also able to follow the spread of the ash over the surface of the star and found that a region of high shear developed between the hot ash and the unburned fuel. Given that the shear speeds were a substantial fraction of the sound speed, this makes such regions a possible site for developing a detonation [216].

2.1.3 Delayed Detonation

Perhaps the greatest uncertainty in the standard model was the physics of the deflagration-detonation transition (DDT). Everyone agreed that such a transition was necessary if the model was to give good agreement with observations, but how and where it happened was and remains a difficult problem in turbulent combustion. We adopted two approaches to the problem. One was to study the physics that might lead to a spontaneous DDT in calculations on a small physical size that resolved the relevant physics. The other was to search in models of the full star where these conditions might be achieved.

Using a combination of 3D simulation [9, 10, 11], coupled with more highly resolved calculations using the Linear Eddy Model [216], we were able to reach some useful conclusions. First, the transition to detonation can only occur for a limited range of densities, $\rho = 0.8 - 1.6 \times 10^7$ g cm^{-3}. It is here that turbulence with the expected intensity can begin to disrupt the flame mixing hot ash and cold fuel together to produce a warm, potentially explosive mixture. In terms of combustion physics, the Karlovitz number must be substantially greater than 1, in fact we found $Ka > 10$. However, simply reaching low density is not sufficient to make a detonation happen. Otherwise it would be very easy. The turbulent intensity must also be very large on a macroscopic length scale. That is the Damkohler number, Da, must be $\lesssim$1. The scale over which the turbulence mixes must be larger than the critical mass required to initiate a detonation, around 1 - 10 km in the preferred density range, and the turbulence must mix the region sufficiently that it runs away simultaneously within a sound crossing time. This requires turbulence that is itself already nearly sonic. Because of random excursions in turbulent intensity, which we studied, and because the burning could sit and burn inductively for a time before running away, the necessary condition was relaxed a little. Turbulence with a characteristic speed of 20% sonic on a scale of 10 km might rarely initiate a detonation. At 30 - 50% the result was more robust. We also found that a DDT could possibly happen at a somewhat higher density,

$2-3\times10^7$ g cm^{-3} in the thick turbulent oxygen flame that trails the carbon burning flame [220, 11], but the results there were less conclusive.

In the full star models, we located three sites where these sorts of conditions might be realized. One is the region where the burning first breaks out in models that are ignited off-center. Another is in the collision on the far side of the burning ashes, a confirmation of the Chicago GCD model. The third, which we presently find most appealing is in the interface between the hot ash as it spreads over the surface and the cold white dwarf beneath (Fig. 8). Each of these three choices will give a different sort of supernova and each will need to be explored. Detonation at break out will happen when the white dwarf has expanded only a little and will make a lot of ^{56}Ni, hence a high energy, very bright SN Ia. Detonation in the sliding layer will give a variety of results, but also rather bright supernovae. The GCD model postpones detonation to the latest time, and will be fainter.

2.2 Merging White Dwarfs

During the course of the grant it became clear that other kinds on models than the then standard Chandrasekhar mass model might be needed to explain the empty progenitor boxes observers found for some nearby SN Ia [147, 18]. We thus explored both 1D and multi-dimensional models for merging white dwarfs.

Ramirez-Ruiz and collaborators at UCSC carried out 3D simulations of merging white dwarf binaries [178, 70]. They have focused on the high-accretion rate phase that precedes merger in a dynamically unstable system where the secondary is either a pure helium white dwarf or a helium-carbon-oxygen hybrid.

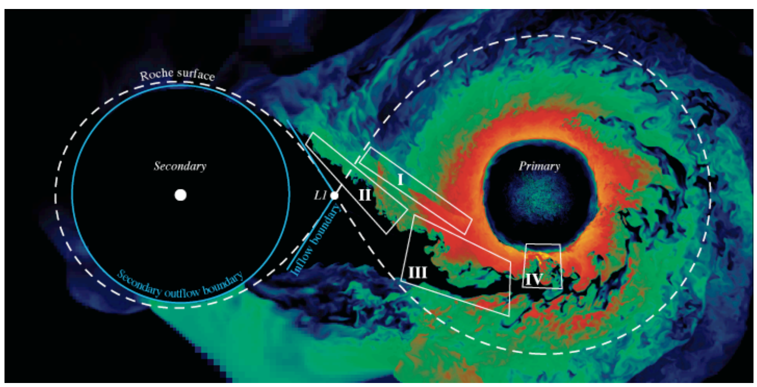

Figure 9: Hydrodynamical simulation of two merging white dwarfs during their last few orbits [70]. The color scheme shows log T through a slice of the orbital plane. The cyan circle shows the spherical outflow boundary condition centered about the secondary, while the cyan wedge shows a cross section of the cone used as the mass inflow boundary. The dashed contour shows the systems Roche surface. The white boxes with labels show the development of a standing shock (I); a region where shear leads to RT instability (II); and the place where gravity changes sign and all wave modes become unstable (III).

They found that for dynamically unstable systems where the accretion stream directly impacts the surface of the primary, the final tens of orbits preceding the merger can have mass accretion rates that range from 10^{-5} to 10^{-3} M$_\odot$ s^{-1}, leading to the rapid accumulation of helium on the surface of the primary. After $\sim10^{-2}$ M$_\odot$ of helium has been accreted, the ram pressure of the hot helium torus can deflect the accretion stream such that the stream no longer directly impacts the surface. The velocity difference between the stream and the torus produces shearing which seeds large-scale Kelvin-Helmholtz instabilities along the interface between the two regions. These instabilities eventually grow into dense knots of material that periodically strike the surface of the primary, adiabatically compressing the underlying helium torus. If the temperature of the compressed material is raised above a critical temperature, the timescale for triple-α

reactions becomes comparable to the dynamical timescale, leading to the detonation of the primary's helium envelope. This detonation drives shock waves into the primary which tend to concentrate at one or more focal points within the primary's carbon-oxygen core. If a relatively small amount of mass is raised above a critical temperature and density at these focal points, the carbon-oxygen core may itself detonate.

Later at the end of the grant, the mergers of two carbon-oxygen white dwarfs were studied by Raskin, Moll, Woosley and Kasen [128, 167]. Most of this work was supported by a subsequent grant from DOE-HEP and is not discussed here.

2.3 Sub-Chandrasekhar Mass Models for SN Ia

"Sub-Chandrasekhar" models were studied in 1D [221] and in 3D [127]. The 1D models were particularly useful in delineating just what will and won't work for common SN Ia's. The primary carbon-oxygen white dwarf for this model class must have a mass of 1.0 ± 0.1 $M_\odot$and it must be capped by 0.05 ± 0.02 $M_\odot$ of helium. This range of CO dwarf masses gives the right amount of ^{56}Ni for the light curve. More than 0.07 $M_\odot$ of helium gives a bad spectrum and less than 0.04 $M_\odot$ will not detonate.

2.4 Light Curves and Spectra

Our radiation transport calculations with SEDONA have shown that multi-dimensional effects in the ignition and explosion of white dwarfs are a critical source of diversity of SNe Ia. We carried out a survey of over eighty 2D delayed detonation models, which covered a wide range of ignition conditions and criteria for initiating a DDT in the Chandrasekhar mass model [103]. We found that the luminosity of the models varied by a factor of more than 3 depending upon the geometry of the ignition. The synthetic light curves showed a correlation between peak brightness and light curve duration similar to the observed WLR. In addition, the asymmetry of the ejecta led to variations of $\sim 20 - 30\%$ in brightness depending on the angle at which the supernova was viewed (see Fig. 10). This orientation dependence caused scatter in the WLR, suggesting that the dispersion in calibrated SNe Ia luminosity can be largely traced to asymmetries developing in the explosion.

In addition, we used delayed-detonation models to explore potential systematic errors arising from variations in SN Ia progenitors. In particular, we varied the metal content (metallicity) of the white dwarf, a quantity that is expect to evolve over cosmic time. A significant change in luminosity lead to variations of $\sim 15\%$ in the optical band luminosity. Interestingly, the application of the standard WLR partially, but not totally corrected for this systematic effect, with the residual error being around 2%.

We made our database of synthetic SN Ia spectra available to the observational community, and our models are now being used by most of the leading supernova cosmology surveys, including the PTF, SN Factory, SNLS, SDSS II, the CfA, and others. In one comparative analysis [16] we used cross-correlation techniques to determine the goodness of fit of 48,000 of our model spectra relative to the CfA database of over 500 observed spectra. This provided an important and comprehensive validation of our simulations. The quality of fit was found to be high for most of our synthetic spectra, but certain models did not match the spectra of any known observed SNe Ia, allowing use to rule out regions of model parameter space. Interestingly, the spectroscopically peculiar models also tended to be the outliers in the Phillips relation (see Figure 10) illustrating the value of simulations in calibrating SNe Ia for cosmology.

2.5 Enabling Better Studies of Dark Energy

Our group and others have used our simulated light curves to improve the standardization of SNe Ia for cosmology. In one analysis [60] we showed that the intrinsic color of SNe Ia correlated with the ejecta velocity (as measured from the Doppler shift of the Si II line) in both observed SNe Ia and in our models. Because the intrinsic color of SNe Ia must be known to properly correct for dust extinction, such color variations have implications for standardization. We found that dispersion in SNe Ia luminosity could be reduced by including velocity information in the calibration. We gave a physical basis for these effects, showing that the color-velocity relation arose naturally in certain asymmetric models due to a viewing angle

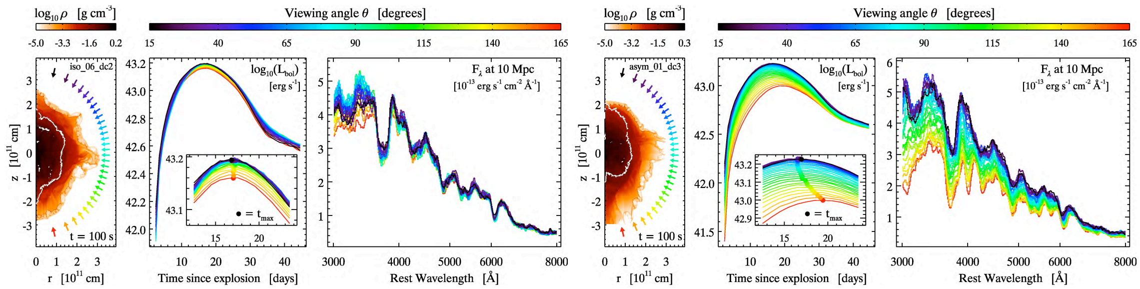

Figure 10: Top left: Total mass density distribution in a central ignited 2-D delayed detonation model. The arrows denote the 30 different viewing angles considered in our radiative transfer calculations. Top center: Bolometric light curves as a function of viewing angle. Top right: Optical spectra as a function of viewing angle. Bottom row: Same as above but for a model ignited off-center showing a significant variation in peak brightness and spectral properties. From [16].

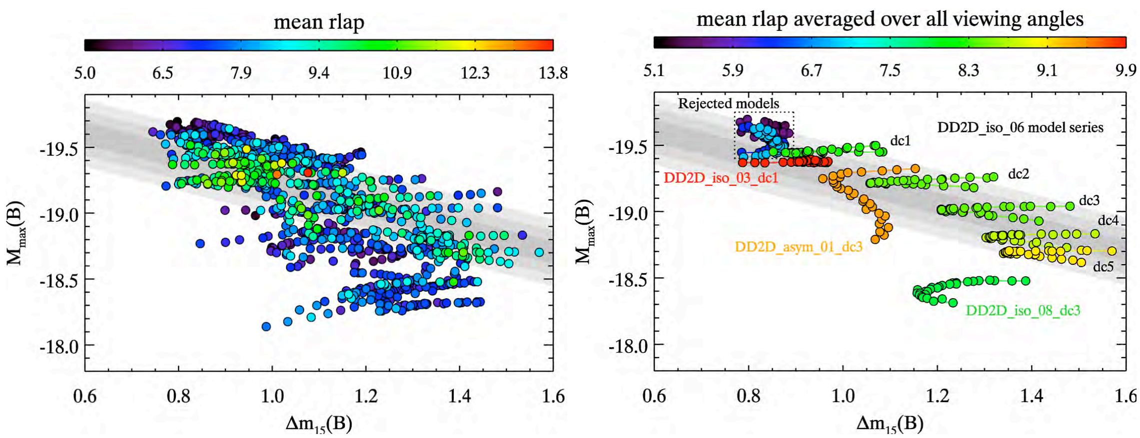

Figure 11: Left panel: Width luminosity relation for the our full set of 2-D delayed detonation model. Each model has 30 associated data points, each corresponding to a specific viewing angle. Each point is color-coded according to the mean value of the goodness of fit compared to observations (SNID rlap parameter). The grey contours show the observed width-luminosity relation. Models with spectra that do not well match those of observed SN Ia also tend to be outliers in the WLR. Right: Same as left panel but for a subset of models. From [16].

effect. This further supports the notion that much of the dispersion in observed SN Ia luminosities is the result of asymmetries which develop in the ignition/explosion phase. Our models and their analysis have thus brought us closer to specifying physically motivated secondary parameters needed for calibrating SNe Ia.

Our models have also impacted our understanding of potential systematic errors in SN Ia cosmology. In an important paper, Sullivan et al., reported that the luminosity of SNe Ia in elliptical galaxies differs systematically from SNe Ia in star forming galaxies, *even after the WLR and other calibrations had been applied*. Sullivan et al, used comparisons with our models to show that the effect was consistent with what we found for metallicity variations in galaxies. The nature of the error was decidedly non-trivial – SNe Ia in low-metallicity elliptical galaxies tended to be intrinsically dimmer, but application of the WLR tended to over-correct them, causing the calibrated luminosity to be too bright. Understanding such complex, non-linear effects will be critical for future dark energy experiments, and will require comparison to realistic simulations.

3 CODES DEVELOPED

3.1 CASTRO

CASTRO uses a compressible flow formulation in Eulerian coordinates and includes self-gravity, multi-group flux-limited diffusion and reaction networks. CASTRO incorporates hierarchical block-structured adaptive mesh refinement and supports 3D Cartesian, 2D Cartesian and cylindrical, and 1D Cartesian and spherical coordinates. See [5] for a detailed description of the hydrodynamics and gravity solver in CASTRO.

The hydrodynamics in CASTRO is based on the unsplit methodology introduced by Colella. The code has options for the piecewise linear method and the unsplit piecewise parabolic method (PPM). The hydrodynamics options are designed to work with a general convex equation of state.

CASTRO supports two different methods for including Newtonian self-gravitational forces. One approach uses a monopole approximation to compute a radial gravity consistent with the mass distribution. The second approach is based on solving the Poisson equation,

$$-\Delta\phi = 4\pi G\rho,$$

for the gravitational field, ϕ. The Poisson equation is discretized using standard finite difference approximations and the resulting linear system is solved using geometric multigrid techniques. A third approach in which gravity is externally specified is also available.

Radiation transport in CASTRO is based on flux-limited diffusion and includes both gray [226, 227] and multigroup approximations. The code also includes the capability to model multigroup neutrino diffusion with multiple neutrino flavors, which incorporates an implicit coupling of Y_e into the system. The flux limiters are based on the formulation of Levermore. CASTRO is based on a nonrelativistic formulation; however, the code uses a mixed frame approach that distinguishes the laboratory and comoving frames for the radiation. In this approach the radiation quantities are computed in the laboratory frame while the opacities are measured in the comoving frame. The formulation includes order $O(v/c)$ terms arising from the mixed frame formulation that can cause significant differences in the dynamic diffusion limit where radiation transport is dominated by motion of the fluid. The approach used in CASTRO splits the system into two parts, one part that couples the radiation and fluid in a hyperbolic subsystem, and another part that is a system of coupled parabolic equations that evolves radiation diffusion over all the groups (along with Y_e in the neutrino case) and source-sink terms. The hyperbolic subsystem is solved explicitly with a high-order Godunov scheme as part of the hydrodynamic component of the algorithm, whereas the parabolic part is solved implicitly with a first-order backward Euler method. The primary computational expense of the radiation is in the solution of linear systems as part of the iteration over energy groups. We rely on the *hypre* library for solving these systems on large parallel machines.

Our approach to adaptive refinement 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. During the regridding step, increasingly finer grids are recursively embedded in coarse grids until the solution is sufficiently resolved. An error estimation procedure based on user-specified criteria evaluates where additional refinement is needed and grid generation procedures dynamically create or remove rectangular fine grid patches as resolution requirements change.

For pure hydrodynamic problems, synchronization between levels requires only a "reflux" operation in which coarse cells adjacent to the fine grid are modified to reflect the difference between the original coarse-grid flux and the integrated flux from the fine grid. For processes that involve implicit discretization, the synchronization process is more complex. The synchronization for self-gravity is similar to the algorithm introduced by Miniati and Colella. The AMR treatment of radiation is similar to the approach of Howell and

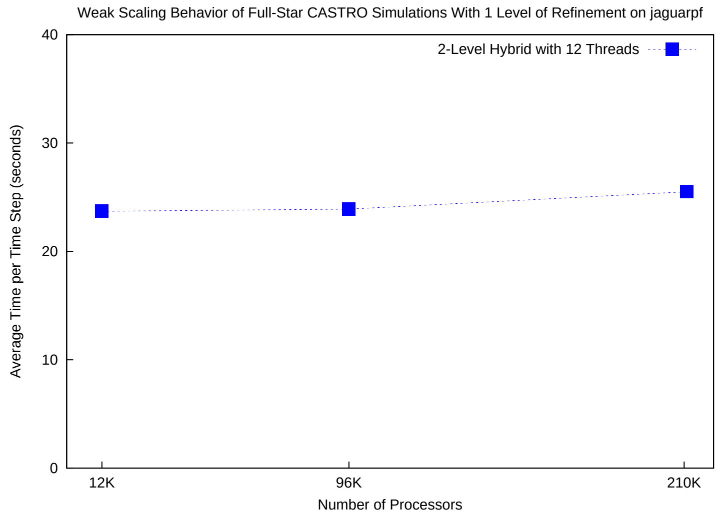

Figure 12: Weak scaling of CASTRO hydrodynamics with AMR

Greenough; however, CASTRO uses an alternative specialized procedure for synchronization of the radiation solution between different levels of the adaptive mesh hierarchy. In this approach, the synchronization corrections are deferred and become part of the next coarse level advance. This adds complexity to the regridding operation but eliminates the need for the multilevel linear system solutions, resulting in dramatic improvements in both computational time and scalability.

CASTRO uses a hybrid parallelization strategy based on MPI + OpenMP using the BoxLib framework. The basic strategy is to distribute grids within the AMR hierarhcy to computational nodes. This provides a natural coarse-grained approach to distributing the computational work. A dynamic load balancing technique is needed to adjust the load. Although the code supports both a heuristic knapsack algorithm and a space-filling curve algorithm for load balancing, the data-locality properties make the space-filling curve the method of choice for problems with radiation or when a Poisson equation is used to compute the gravitational field. For multicore architectures we then use OpenMP directives to distribute the computations on grids over the available cores on the node. Using this model we have been able to obtain nearly ideal weak scaling of the CASTRO hydrodynamics to more than 200,000 cores [4] as shown in Figure 12. We have also demonstrated near ideal scaling of the gray radiation solver to more than 32,000 cores [226] as shown in Figure 13.

3.2 MAESTRO

MAESTRO is a low Mach number hydrodynamics code for simulating highly stratified flows under astrophysical conditions using block-structured adaptive mesh refinement (AMR) [228, 4, 141]. In the low Mach number formulation, the pressure is decomposed into a dynamic and thermodynamic component, the ratio of which is of order Mach number (M) squared. The star is assumed to be in hydrostatic equilibrium, such that the one-dimensional base state density (the average density at a given radius) is in hydrostatic equilibrium with the one-dimensional base state (thermodynamic) pressure. The total pressure is replaced by the thermodynamic pressure everywhere except the momentum equation. In order to constrain the density, composition, and enthalpy so that they remain in thermodynamic equilibrium with the base state pressure, a divergence constraint on the velocity field is enforced, derived from integrating the equation of state along particle paths. The divergence constraint is similar to that used for incompressible hydrodynamics, modified to account for background stratification and local compressibility effects due to compositional changes, heating, and thermal diffusion. The result is that sound waves are filtered out of the system, allowing for

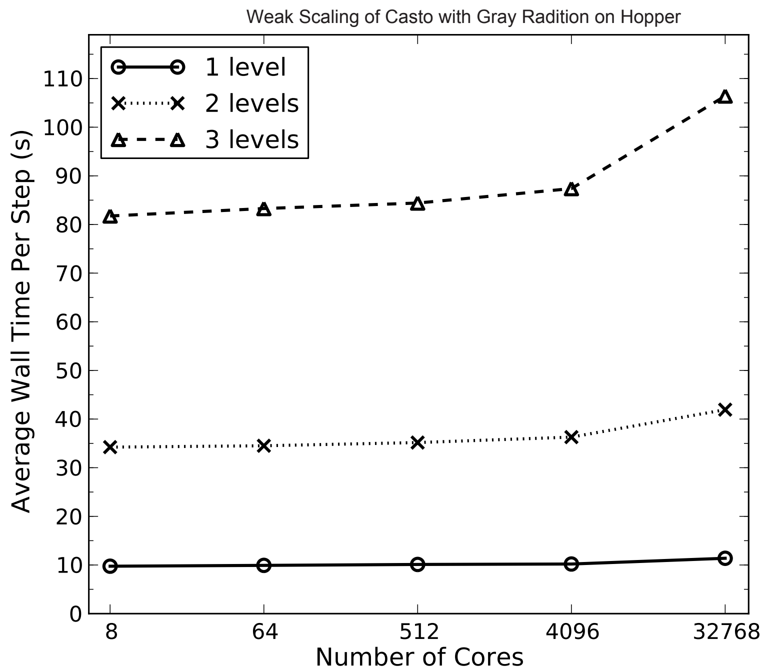

Figure 13: Weak scaling of gray radiation solver in CASTRO

much larger (by a factor of $1/M$) time steps than those used in corresponding compressible codes.

The algorithm in MAESTRO is based on a second-order accurate approximate projection method originally developed for incompressible flows. First, the density, composition, velocity, and enthalpy are advanced to the new time level using an unsplit Godunov method. As part of this process, reactions and thermal diffusion are incorporated through an operator splitting approach that retains second-order accuracy of the overall algorithm. The updated thermodynamic variables are then used to evaluate the generalized divergence constraint, accounting for stratification and local compressibility effects. The velocities are then projected onto the space that satisfies this divergence constraint. The projection step involves the solution of an elliptic equation, computed iteratively using multigrid. The base state density and pressure also evolve over time, capturing the expansion of the star due to large-scale heating and convection. MAESTRO uses the same hybrid parallelization strategy as CASTRO and has demonstrated nearly ideal scaling to more than 96,000 cores [5] as illustrated in Figure 14.

3.3 SEDONA

SEDONA is a multi-dimensional time-dependent multi-wavelength radiation transport code built on an implicit Monte Carlo (IMC) approach, and including modern acceleration and variation reduction techniques [108]. In the IMC approach, the radiation field is represented by discrete particles (e.g., "photons") which are tracked through randomized scatterings and absorptions until they escape the computational domain. Particles passing through each zone are tallied to construct estimators of the local radiation field and its influence on the matter, e.g., the rates of radiative heating, ionization, and excitation. Particles are also used to construct the emergent spectrum and light curve. All calculated quantities possess statistical noise, which is reduced as the number of propagated particles is increased. SEDONA includes the option of employing discrete diffusion techniques to ameliorate the well-known inefficiency of standard Monte Carlo methods is regimes of high opacity. In this approach, particle motion in opaque regions is sampled from the diffusion approximation, rather than the full Boltzmann equation.

SEDONA was designed to calculate synthetic light curves, spectral time series, and spectropolarimetry

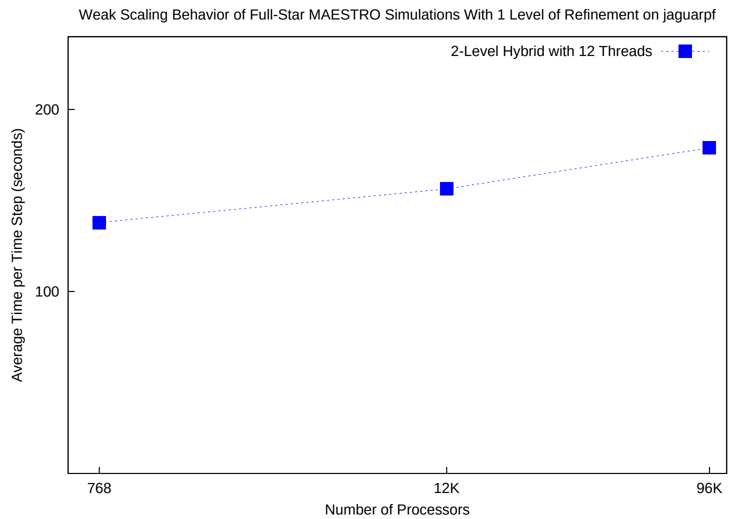

Figure 14: Weak scaling of MAESTRO with refinement

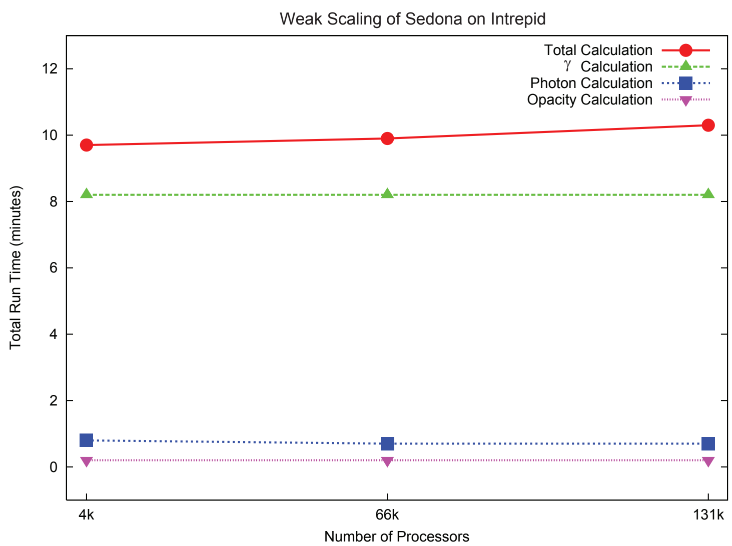

Figure 15: Weak scaling of the SEDONA IMC transport code in full-replication mode for a 2-D spectrum calculation.

of multi-dimensional explosion models. This is done by post-processing hydrodynamical simulations once the ejecta had reached the phase of free, homologous expansion. The code includes a detailed treatment of the transport and absorption of radioactive decay products – primarily gamma-rays which heat the ejecta through Compton scattering and photo-ionization. We compute the optical opacity for arbitrary compositions including the aggregate effects of Doppler broadened lines using an extensive atomic database that includes several tens of millions of transitions. For multi-dimensional problems, the atomic level populations are typically approximated to be in local thermodynamic equilibrium (LTE), however, a non-LTE solver has been implemented as well and has been used so far in 1-dimensional calculations.

SEDONA is written in C++ and is parallelized using a hybrid MPI + OpenMP. For problems with modest memory requirements (2-D or low resolution 3-D calculations) the entire computational domain can be replicated on a single node, which independently propagates a fraction of the particles. We have demonstrated that in full-replication, the code shows weak scaling beyond 100,000 cores (Figure 15).

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