SciDAC Supernova Science Center

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Goals of the Project

The SciDAC Supernova Science Center (SNSC) has as its chief goal a better understanding of supernovae of all types through simulation and model validation. Supernovae are nature's grandest explosions and an astrophysical laboratory in which unique conditions exist that are not achievable on Earth. Understanding these explosions and their signals is therefore important, not only because of their central role in astronomy and nucleosynthesis, but because a full understanding of supernovae may lead us to a better understanding of basic physics. Despite decades of research and modeling, no one understands, in detail, how supernovae work. The problem persists largely because, until recently, computer resources have been inadequate to carry out credible multi-dimensional calculations.

Our core team includes astrophysicists from four institutions: UCSC, the University of Arizona, LANL, and LLNL, i.e., two of the top astrophysics graduate programs in the country and two major DOE Labs. We also have strong collaborations with other groups engaged in supernova simulation at the University of Chicago FLASH Center, the Max Planck Institut für Astrophysik in Garching (MPA), and the Joint Institute for Nuclear Astrophysics at Notre Dame (JINA). Most of the state-of-the-art models for supernovae in the literature have been computed by us and our collaborators.

Our team also includes faculty and grad students in the Arizona Center for Integrative Modeling and Simulation (ACIMS) and High Performance Distributed Computing (HPDC) Laboratory, as well as computer scientists at LANL who will play a key role in optimizing our codes for parallel computers and visualizing the results. We anticipate interactions with other SciDAC Software and Science Centers (see below).

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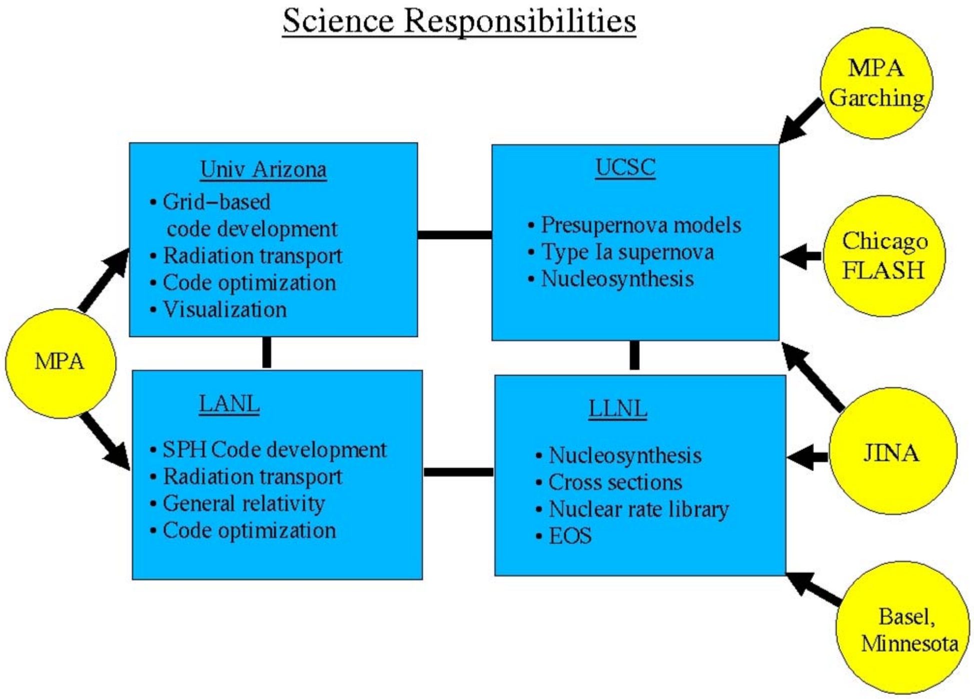

Figure 1: Science responsibilities.

Major Challenges

There are two sorts of supernovae: thermonuclear (*aka* Type Ia) and gravity powered (Type II and Ib). Each offers a unique computational challenge.

The challenge posed by a thermonuclear supernova, stated in the language of fluid mechanics, is the realistic simulation of turbulent (nuclear) combustion at low Prandtl number and extremely high Rayleigh number. A fusion flame is born at the center of a white dwarf which is already turbulent because of prior convection. As the flame proceeds, its ashes lie beneath cold, denser fuel and thus the interface is Rayleigh-Taylor unstable. Non-linear growth of the RT instability leads to shear and increased turbulence. In this environment we want to learn how the flame deforms and, in particular, how fast it moves. Accelerations of roughly 50 times the laminar flame speed are essential to a healthy supernova explosion. The range of length scales (Kolmogorov to stellar) is far too great for full resolution in 3D, so the problem must be attacked in stages in order to develop a realistic sub-grid depiction of the burning.

Modeling gravitational supernovae is even more challenging - and the central theme of our research. The iron core of a massive star collapses to a neutron star radiating a flood of neutrinos for several seconds (roughly 20% of the rest mass of the neutron star converted to pure energy). Inefficient coupling of these neutrinos to the overlaying stellar material launches a shock wave that explodes the star. Convective motions powered by neutrino energy deposition are believed to be key to the success of the model. The computational challenge here is the simulation of fluid flow coupled to the transport of

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radiation (neutrinos) that has a non-thermal spectrum and is making a transition from optically thick to thin. Both the fluid and radiation must be treated in 3D and the added complications of post-Newtonian gravity and a poorly known equation of state for the hot neutron star must be factored in.

Once the hydrodynamic models have been calculated, one must still compute the diagnostics for comparison to observations. Calculating the optical, infrared, and gamma-ray light curves and spectra, nucleosynthesis, neutrino signal, neutron star kicks, and gravitational radiation for the models poses its own special challenges. One must also deal with a fragmented and often uncertain collection of nuclear data.

State-of-the-Art

Two-dimensional models for both types of supernovae have been calculated by several groups. The first 3D models of Type Ia supernovae may be done this year at the MPA. Our own group has just calculated the first 3D model for a gravitational collapse supernova (Fig. 1). However, all these calculations have inadequate spatial resolution and the gravitational collapse model uses a very crude approximation to neutrino transport. None can yet be considered a "solution to the supernova problem".

Our Approach

Our studies of thermonuclear supernovae are, at this time, confined to micro-zoned studies of flame stability and its response to turbulence using the Chicago (PPM-based) FLASH code. We hope, later this year, to begin macroscopic studies of the explosion in 2D and eventually 3D. We are also developing a 3D anelastic code to study the evolution of the white dwarf during the convective stage that precedes explosion in order to understand better the ignition conditions (one point or many).

We are building a library of presupernova stellar models of various masses and compositions. Eighty models, available to the public at our website, have been calculated so far. Nucleosynthesis in these 1D models can be studied (Fig. 2) using a reaction network of up to several thousand nuclei (tens of thousands of reactions). Explosion can be simulated using parameters extracted from the multi-D models. A comprehensive library of nuclear data for astrophysical application is being developed at LLNL.

Using these models of evolved massive stars as a starting point, we will explore the hydrodynamics of core-collapse supernovae with several codes optimized for operation on distributed computers. One uses a Lagrangian grid - Smooth Particle Hydrodynamics (SPH). Others use Eulerian grids - the Arizona PPM-based supernova code, the Chicago FLASH code, and ZEUS-MP are among those currently being explored. One will be

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selected for intensive development. Radiation transport is equally important. In order to have a standard, albeit expensive, calibration calculation, we are developing (at LANL and Arizona) a general purpose 3D Monte Carlo transport code for supernova application. Actually, in a 3D hydrodynamical simulation, 3D Monte Carlo may not be so much more costly than other approaches, but we are also studying the method of ``short characteristics" for solving the radiation transport locally on a grid. An important goal for the next year is to determine just which combination of radiation transport and hydrodynamics will be emphasized. Interaction with the other SciDAC centers may be helpful in this regard.

Optimization of these codes and manipulating and visualizing the large data sets they create will require the involvement of computer scientists at Arizona, LANL, and some of the other SciDAC Centers. In particular, the Arizona Center for Integrative Modeling and Simulation (ACIMS) (http://www.acims.arizona.edu) is developing an "Integrated Astrophysical Runtime and Visualization System" to assist in our efforts.

Recent Developments

The first round of SNSC postdocs has now been hired:

- **UCSC - Mike Zingale** - formerly of the University of Chicago. Co-author of the U-Chicago FLASH code and expert in multi-dimensional hydrodynamics

- **Arizona - Rolf Walder** - formerly of Zurich. Expert in multi-dimensional hydrodynamics and non-LTE radiation transport. Author of the A-MAZE 3D adaptive mesh MHD code.

- **LLNL - Jason Pruet** - formerly of UCSD. Expert in nuclear astrophysics and neutrino physics.

- **LANL - Adrian Gentle** - formerly of Monash. Expert on numerical relativity.

In addition, a total of 13 graduate students are now working on the SNSC team (7 at Arizona including 3 in computer science, 4 at UCSC, and 2 at LANL)

Our first team meeting will be held February 1 and 2 in Tucson, the second will be the first week of June at LANL. Two additional team meetings will happen later this year at LLNL and UCSC.

Milestones and Time Scales

Year 1:

- **First 3D supernova calculations** using smooth particle hydrodynamics - calculations of both the explosion and mixing after the explosion; begin studies of asymmetric explosions (LANL) - **done**.

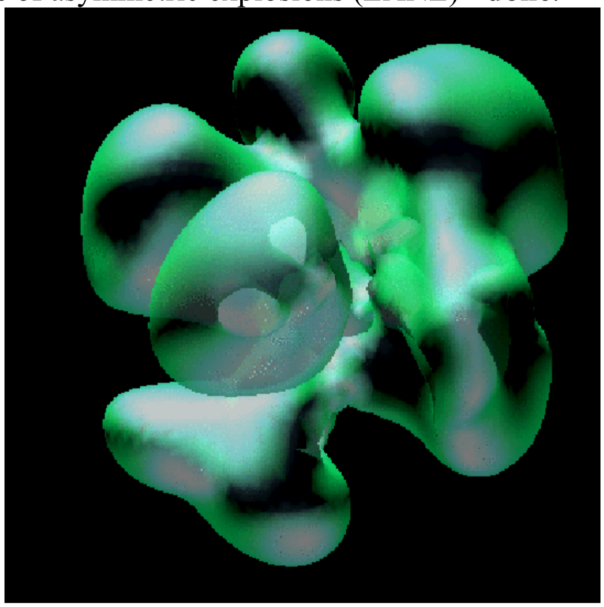

Figure 2: Velocity iso-surfaces (1000 km s^{-1}) 60 ms after core collapse and bounce in a 15 solar mass supernova. Calculated by Fryer and Warren at LANL using the SPH code (with 300,000 particles). Neutrinos are treated as either trapped or untrapped, i.e., the “grey” region is not well represented. The figure shows a region about 1000 km in size.

- **Library of presupernova models** of massive stars - 11 to 60 solar masses, various metallicities (UCSC) - **done**.

- **Integrated Astrophysical Runtime and Visualization** System parallel programming design methodology, benchmarking and evaluation of ZEUS-MP on NERSC seaborg (IBM-SP), visualization infrastructure (Arizona) - **done**.

- **The all-purpose Monte Carlo code** to calibrate the 1D, 2D, and 3D neutrino and photon Boltzmann solvers. Complete coding and initial testing. (LANL, Arizona)

- **1D implicit and explicit neutrino radiation-hydro codes**, employing the Feautrier tangent-ray method and the method of short characteristics to solve the Boltzmann transport equation, coupled to a variety of grid-based hydro codes. Code development (Arizona).

- **Studies of turbulent flame propagation (in 2D)** relevant to the Type Ia supernova problem. First cut 2D Type Ia supernova models using FLASH code (UCSC).

- **Library of standard nuclear data** for astrophysics on web. Version 1 (LLNL).

Year 2:

- **Further 3D supernova models using SPH.** Incorporate implicit flux-limited neutrino diffusion. Co-process with Monte Carlo. First studies of rotation and kicks. Nuclear yields from asymmetric explosions (LANL).

- **Time-dependent Monte Carlo transport and parallel short-characteristics Boltzmann solvers for 2D and 3D** for both neutrinos and photons, coupled to an ALE or other hydrodynamics code. Coding finished end of year 2 (Arizona).

- **Integrated Astrophysical Runtime and Visualization System -** development of component-based adaptive runtime system, collaborate with High-Performance Data Grid Toolkit, Scalable Systems Software and other SCIDAC projects to make our codes interoperate and utilize the high performance software tools developed by these projects (Arizona).

- **Nucleosynthesis library** from simulated 1D explosions. See Fig. 2 (UCSC).

- **First 3D SN Ia models** using the FLASH code. (UCSC, MPA, Chicago).

- **Studies of 3D stellar convection** coupled to nuclear burning in massive stars, with and without rotation, using anelastic hydrodynamics (UCSC).

- **Complete nuclear astrophysical data archive.** Begin computation of improved theoretical rates (LLNL).

Year 3:

- **Grid-based 3D Calculations of core-collapse supernovae** (Arizona).

- **2D light curves and spectra** (Arizona).

- **3D-GR models using SPH** Complete model from collapse to one year after explosion. Gravitational wave predictions for all models. (LANL).

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- **3D Monte-Carlo studies of radiation transport in all models** (LANL, Arizona).

- **Integrated Astrophysical Runtime and Visualization System** - continue the development of adaptive runtime, problem solving environment, and assist efforts at other SNSC sites (Arizona).

- **First 3D MHD calculations of rotating stellar evolution** using anelastic hydro. Studies of onset of thermonuclear runaway in Type Ia supernovae. Build up to do protoneutron star formation (UCSC).

- **Nucleosynthesis studies in all models** (all teams).

- **Improved theoretical nuclear reaction rates** (LLNL).

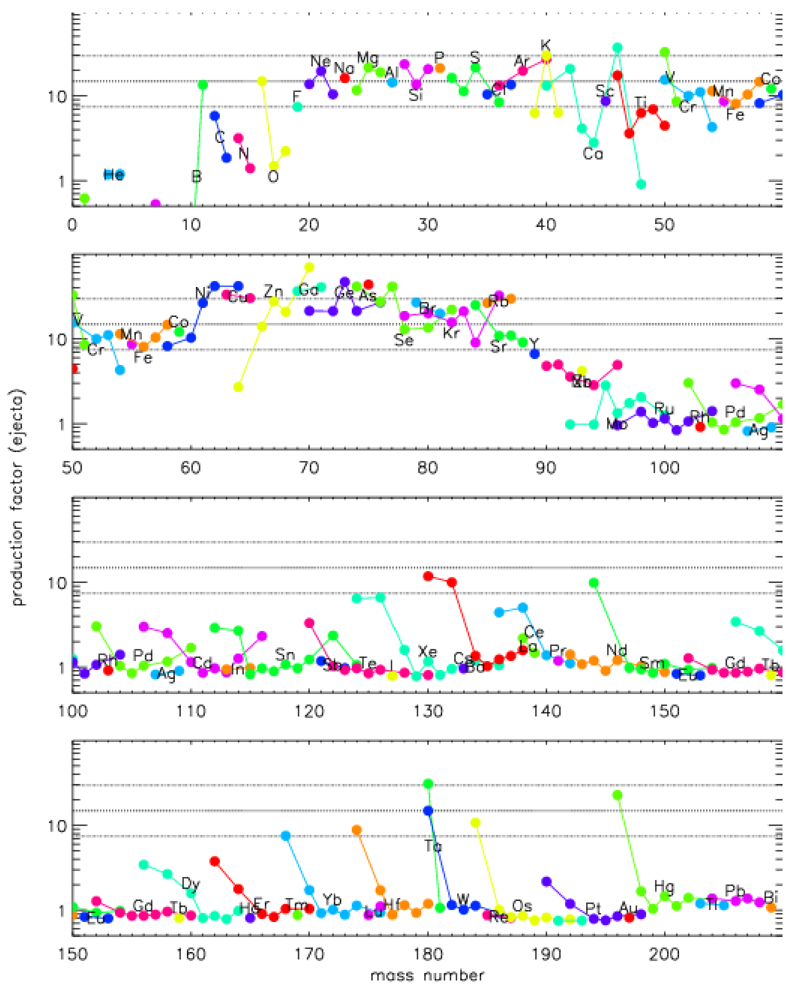

Figure 3: Nucleosynthesis in a 25 solar mass supernova model compared with solar abundances. Abundances for over 2000 isotopes from hydrogen to polonium were followed in each of approximately 1000 stellar zones throughout the life of the star and its explosion as a supernova. Our library will eventually include 300 such models.

Interaction with Other Projects

- **Terascale Supernova Initiative** - Ours is but one of two SciDAC Centers dedicated to the study of supernovae. We will provide pre-supernova models and reaction rate information to the TSI and plan joint meetings to discuss our mutual findings.

- **High-Performance Data Grid Toolkit** and **DOE Science Grid** - these two National Co laboratories and Networking Centers, working together with the computer scientists on our team at Arizona, can help us migrate our codes to large scale distributed high performance computing environments (Grid computing). The PIs of these projects have on-going interactions with our team members at the HPDC laboratory.

- **Algorithmic and Software Framework for Applied Partial Differential Equations Center** - Phil Collela is a co-author of one of our main codes (PPM). We are also interested in learning new numerical techniques from him and and John Bell, especially for studying low Mach number fluid flow.

- **Terascale High-Fidelity Simulations of Turbulent Combustion with Detailed Chemistry** - perhaps surprising is the considerable overlap in scientific goals between the SNSC and the chemical combustion community. Type Ia supernovae are prime examples of turbulent combustion. We have already worked with experts at the Sandia Combustion Facility at Livermore for four years.

- **Scalable Systems Software Center** and **Center for Component Technology for Terascale Simulation Software** - We will collaborate with the researchers of these two Integrated Software Infrastructure Centers to make our codes scalable, component-based, and run efficiently in Grid computing environments.

- **Terascale Optimal PDE Simulations** - We will work with these experts on optimal strategies for dealing with the large matrices generated by our non-LTE radiation transport programs and nuclear reaction networks.

- **Terascale Simulation Tools and Technologies Center** - We are working with Jim Glimm and students applying their adaptive grid capabilities to the study of mixing in supernova explosions.

- **Common Component Architecture** - Though our codes are still in a developmental stage, we intend to develop them according to CCA principles. Our team members at the ACIMS will work with Armstrong and colleagues.

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