Adaptive Mesh Simulations Of Astrophysical Detonations Using the ASCI Flash Code

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Abstract. The *Flash* code was developed at the University of Chicago as part of the Department of Energy's Accelerated Strategic Computing Initiative (ASCI). The code was designed specifically to simulate thermonuclear flashes in compact stars (white dwarfs and neutron stars). This paper will give a brief introduction to the astrophysics problems we wish to address, followed by a description of the current version of the *Flash* code. Finally, we discuss two simulations of astrophysical detonations that we have carried out with the code. The first is of a helium detonation in an X-ray burst. The other simulation models a carbon detonation in a Type Ia supernova explosion.

INTRODUCTION

The Flash Center at the University of Chicago is one of five Level I centers established by the Department of Energy under the ASCI Strategic Alliances Program. The goal of the center is to build a next-generation simulation code for studying Astrophysical Thermonuclear Flashes. These flashes, which result from explosive nuclear burning, are thought to be the cause of a number of observed astrophysical events, including X-ray bursts, novae, and Type Ia supernovae. The complex behavior exhibited by these objects makes them valuable laboratories for the numerical study of a wide range of basic physics phenomena. They are also valuable for what they can teach us about the universe, such as the formation of the elements and the cosmic distance scale.

ASTROPHYSICAL THERMONUCLEAR FLASHES

The three events we wish to model, X-ray bursts, novae, and Type Ia supernovae, all have a great deal in common, although each presents unique computational challenges. Each event begins with a compact star, either a white dwarf (for novae and supernovae), or a neutron star (for X-ray bursts) in orbit around a "normal" star. If the orbital radius is sufficiently small, matter from the normal star will be accreted onto the surface of the compact object over a relatively long period of time compared to the time scale of the flash itself. Due to the orbital angular momentum, the matter cannot fall directly onto the surface of the compact object, but instead accumulates in a disk around it. The angular momentum is slowly diffused outward by poorly understood dissipation processes, allowing the matter to fall onto the surface of the star. This process of accretion may take place at the equator or may be directed to the magnetic poles in the case of highly magnetized stars.

The accreting material that reaches the compact object forms a thin layer on the surface. Once this layer has reached a critical depth, the action begins. For X-ray bursts and novae, a thermonuclear runaway will start at the base of the accreted layer. Due to the extreme temperature sensitivity of the nuclear reactions, any small perturbation will cause the runaway to initiate at a single point rather than simultaneously over the entire surface. A sub-sonic flame front (deflagration) or a supersonic detonation will then propagate outward from this point and consume the entire layer. Little if any material will be ejected from an X-ray burst, due to the enormous gravitational field of the neutron star. However, observations of novae do show an ejected shell of matter that engulfs the companion star, forming a common envelope binary system. These events cause little change to the underlying star, allowing them to recur many times from the same source.

Type Ia supernovae are quite different from the other two events. Here, the accreted material compresses the entire star, causing a runaway to initiate at or near its center. A detonation would result in complete burning to iron group elements, and the intermediate mass elements seen in supernova spectra would not survive. Therefore, burning must propagate as a deflagration front, at least at early times. At late times, the ejected matter becomes supersonic. This has led theorists to suggest that the deflagration undergoes a transition to a detonation at some point during the explosion. In any event, the entire star will be blown apart by the explosion, so that recurrence is impossible.

THE FLASH CODE

Flash [3] is a sophisticated multi-physics simulation code. It was designed to be portable across a wide variety of computers and to run efficiently on massively parallel architectures. An object-oriented framework was added to make maintenance and modification as easy as possible. The code is modular, so that new physics routines and algorithms can be added with a minimum of effort. Parallelization of the code is accomplished using the Message Passing Interface (MPI) library. The Hierarchical Data Format library HDF-5 is used for parallel I/O. The code has been highly optimized and recently achieved a sustained performance of 0.238 TFlops. We were awarded the 2000 Gordon Bell Prize for this accomplishment [1].

At the heart of the *Flash* code is an Adaptive Mesh Refinement (AMR) toolkit, called PARAMESH [4]. AMR concentrates grid points in regions where they are most needed. This capability provides reduced time to solution and decreased memory usage, both of which enable higher resolution simulations.

Simulation of astrophysical thermonuclear flashes requires a wide variety of physics modules. One module solves Euler's equations for compressible gas dynamics using the Piecewise-Parabolic Method [2]. This method was specifically designed for accurate and efficient solution of flows containing discontinuities, such as shock waves, and is therefore ideal for the events we wish to model. The equation of state required for our simulations contains a mixture of partially degenerate and relativistic electrons, an ideal gas component for the ions, and radiation. Modules exist both for analytic computation of the thermodynamic quantities and their derivatives and for a thermodynamically consistent table look up algorithm [6]. Nuclear energy generation is computed by solving a reaction network [5]. The typical networks used by *Flash* contain 10-20 isotopes and more than 100 reactions. The network is represented by a system of linear equations, which are solved using standard linear algebra packages.

The code also contains modules for diffusive processes, such as radiative transfer and thermal conduction. Self-gravity is computed by solving Poisson's equation. A module for including magnetic field effects is currently being integrated into *Flash*. Future planned additions include a level set front tracking scheme to prevent unphysical diffusion across sharp interfaces and a sub-grid model for treating the effects of turbulent motions that cannot be resolved on the grid.

SIMULATION OF ASTROPHYSICAL DETONATIONS

This section discusses two *Flash* code calculations of astrophysical detonations. The first, a simulation of an X-ray burst on a neutron star, follows the evolution of a 2 km wide section of the stellar surface in an attempt to determine what observational consequences might result from the flash. The second simulation is a study of a very small section of a detonation that might occur in a Type Ia supernova.

X-ray Bursts

As mentioned above, an X-ray burst results from the accretion of material from a binary companion star onto a neutron star. For the parameters we considered, instability occurs after a 110 m thick layer of helium has accumulated onto the stellar surface. At this time the density at the base of the layer is 2×10^8 g cm^{-3} and the temperature is 1×10^8 K. For comparison, the density of the accreting material was only 1×10^{-5} g cm^{-3}. The size of the computational domain was 2,000 m $\times$ 1,500 m with a minimum grid resolution of 1 m.

The runaway initiates at a point at the interface between the accreted material and the underlying neutron star. A detonation front propagates outward from this point, both vertically toward the surface of the accreted layer and laterally around the circumference of the star. The detonation cannot propagate downward toward the center of the star, since there is no fuel there to burn. The detonation approaching the surface of the helium layer dies out due to the lower density and temperature and turns into a stationary deflagration front. The shock wave races ahead into the low density regions of the atmosphere. The detonation propagates laterally through the accreted layer at a constant speed of 1.3×10^9 cm s^{-1}, covering the entire star on a time scale of approximately 3 ms. A series of surface waves are excited by the explosion, which propagate around the star at approximately the same speed as the detonation. The entire atmosphere undergoes violent oscillations with a period of 50 μs. Material is pushed outward at a velocity of 1/3 the speed of light, reaching a height of approximately 10 km above the surface. For a more detailed description of the calculation see [9].

See http://flash.uchicago.edu/research/gallery.html for an assortment of color snapshots and movies of this simulation.

Cellular Detonations

The second set of calculations is relevant to those models of Type Ia Supernovae in which a deflagration to detonation transition is thought to occur. The purpose of this simulation is to determine the detailed structure of the detonation front. Detonations in laboratory experiments exhibit a very complex three-dimensional cellular structure. In order to make a complete model for Type Ia Supernovae, it is necessary to understand what observational consequences this structure might have.

In this case, the compact object is a white dwarf, and the material through which the detonation propagates is assumed to be pure carbon at a density of 1×10^7 g cm^{-1}, the density at which the transition to detonation is thought to occur. The size of the computational grid is $12.8 \times 12.8 \times 256$ cm. The minimum grid resolution is 0.05 cm.

The front propagates for approximately 50 cm before the cellular instability becomes noticeable. At this point the front becomes non-planar, and a series of weak shock waves form perpendicular to the primary shock. Very high pressure spots, called triple points, develop where these shocks collide. These triple points act as tiny explosions, which sustain the propagation of the detonation. The composition distribution behind the front shows both under-reacted and over-reacted regions. Burning continues for a distance of approximately 20 cm behind the front, at which point the solution becomes one-dimensional.

At this density, the cell size is only a few cm, which is much too small to have any observation consequences. However, as the detonation approaches the surface of the white dwarf and the pre-shock density decreases to 1×10^6 g cm^{-1}, the cell size will become comparable to the size of the star. When this happens, it is unlikely that burning will continue to completion and the observed distribution of elements produced by the explosion will be very different from that predicted by one-dimensional theories. The other noticeable effect is in the speed of the detonation front, which is 1-2% slower than predicted by one-dimensional theory. This slight difference is unlikely to have any major impact on supernova models.

See http://flash.uchicago.edu/~fxt/cell3d.html for results of this calculation. A more complete description of the calculation can be found in [7,8].

CONCLUSION

Although it is still under development, the *Flash* code is one of the most sophisticated astrophysics codes currently available. The combination of state-of-the-art numerical algorithms, adaptive mesh refinement, and efficient parallel implementation gives us the capability to attack problems that could only be dreamed of before. The *Flash* code has allowed us to produce the highest resolution, most accurate multi-dimensional simulations of X-ray bursts on neutron stars and detonations in Type Ia supernovae ever performed. Results from other simulations can be viewed at http://flash.uchicago.edu. The code will continue to evolve, as new physics modules are added, making the study of a wider range of astrophysical problems possible.

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