The Light Curves and Spectra of Supernova Explosions: Multi-Dimensional Time-Dependent Monte Carlo Radiative Transfer Calculations

Daniel Kasen\textsuperscript{1,2}, Stan Woosley\textsuperscript{2}, Peter Nugent\textsuperscript{3}, Friedrich Röpke\textsuperscript{4}

\textsuperscript{1} Johns Hopkins University/Space Telescope Science Institute, Baltimore, MD
\textsuperscript{2} Department of Physics and Astronomy, University of California, Santa Cruz, CA
\textsuperscript{3} Lawrence Berkeley National Laboratory, Berkeley, CA
\textsuperscript{4} Max Plank Institute for Astrophysics, Garching, Germany

E-mail: kasen@pha.jhu.edu

Abstract. While the disruption of a star in a supernova explosion lasts only seconds, the ejected stellar material, much of it newly radioactive, continues to shine brightly for several months. Multi-physics simulations of supernova are now illuminating the physics of the stellar explosion itself, but further post-processing of models with a radiative transfer code is needed to predict the visible emission and compare directly to astronomical observations. Here we discuss Monte Carlo techniques for addressing multi-group time-dependent radiative transfer in 3-dimensional, rapidly expanding atmospheres. We have developed the SEDONA code, which calculates detailed angle dependent light curves, spectra, and polarization, and have applied it to study the nature and cosmological utility of supernovae. The code is scalable and is typically run on high-performance computers using 1024 processors.

1. Introduction
Some stars will live for a few billion years, then die in a few violent seconds of a supernova explosion. So brief is their final disruption that we almost never catch a glimpse of it. Only rarely do we find historical images of the progenitor star before it had been ripped apart. What we do typically observe in the months and years that follow is emission from the processed stellar material ejected in the explosion (the supernova ejecta). Powered by the decay of freshly synthesized radioactive isotopes (or lingering thermal energy from the shock itself) the ejecta can glow as bright as a billion suns; bright enough to be seen billions of light years away.

One class of supernova explosions – the thermonuclear, or Type Ia supernovae (SNe Ia) – show an impressive regularity in their luminosity evolution, or light curve. At peak, normal SNe Ia have similar brightness to within a factor of \( \sim 2 \). An empirical correlation can be used to further calibrate the luminosity – brighter SNe Ia rise and decline more slowly than dimmer SNe Ia [8]. Using this width-luminosity relation, SNe Ia are applied as standard candles to measure cosmological distances and map out the expansion history of the universe.

Normal SNe Ia are widely believed to be the explosion of compact white dwarf stars, composed chiefly of carbon and oxygen and near the limiting Chandrasekhar mass of \( \sim 1.4 \, M_\odot \). The accretion of material from a companion star is thought to trigger an ignition under degenerate conditions, leading to thermonuclear runaway (see Woosley et al., Lamb et al., this volume). The
energy released unbinds the star, ejecting the stellar material (much of synthesized to radioactive isotopes) with velocities of order 7,000 km s\(^{-1}\), a few percent of the speed of light.

A theoretical understanding, based on numerical simulation, of how SNe Ia explode is important for securing and refining their use as cosmological probes (as well as interesting in its own right). Our SciDAC collaboration is modeling the numerous and complex physical processes at play using a suite of codes (see Woosley et al., this volume). The models still face a number of uncertainties concerning, for example, the nature of the progenitor star system, the location of ignition, and the physics of the turbulent nuclear combustion. There are several promising research directions, but as yet no agreed upon standard model of SNe Ia.

Explosion models of SNe Ia predict the density, velocity, and compositional structure of the ejecta. In order to make a direct comparison to astronomical observations, post-processing is needed. Here we discuss Monte Carlo radiative transfer calculations of the detailed emission — light curves, spectra, and polarization — of SN models. Our ultimate goal is to develop an end-to-end simulation of the event — from the moments leading up to ignition, to the months and years following explosion — that captures the essential features of the observations without resorting to any ad-hoc tuning of model parameters.

2. Light Curve and Spectrum Calculations

In its fullest sense, the SN light curve problem includes all of the following computational challenges: (1) Treatment of the transfer and absorption of decay products (primarily gamma-rays from the decay of radioactive \(^{56}\)Ni) which power the visible light curve. (2) Calculation of the ionization/excitation state of the SN ejecta gas over the grid. While the approximation of local thermodynamic equilibrium (LTE) is a useful expedient, a full solution of the non-LTE rate equations is desirable. (3) Calculation of the ejecta opacities/emissivities given the gas state and using an extensive atomic database of over 10 million bound-bound line transitions. (4) A solution of the transfer of visible radiation through the rapidly expanding, optically thick ejecta. (5) Calculation of the ejecta temperature structure through the balancing of radiative heating and cooling. Because the temperature is needed in step 2 but cannot be determined until after step 4, iterations are usually needed to arrive at a self-consistent model.

Monte Carlo (MC) methods offer an appealing solution to the radiative transfer problem encountered in steps 1 and 4 above. In the MC approach, packets of radiant energy (“photons”) are emitted throughout the ejecta and tracked through randomized scatterings and absorptions until they escape. The photon diffusion timescale is comparable to the expansion timescale, such that packets must be tracked through a temporally evolving space-time grid. Packets passing through a grid cell are tallied to construct estimators of the local rates of heating, ionization, and excitation. Packets escaping the grid are used to construct the emergent spectrum as observed from earth. All calculated quantities possess statistical noise, which is reduced as the number of propagated packets is increased.

MC methods are flexible, general, and intuitive, but for simple 1-dimensional (1D) calculations they are also computationally inefficient compared to direct numerical solution of the transfer equation. The real advantages of MC are only realized for highly complex systems like SNe Ia, which require multi-wavelength transfer in 3 spatial dimensions while including the effects of time-dependence, differential expansion, and polarization. MC algorithms typically scale very well (in many applications perfectly) and large calculations can be profitably run on massively parallel computers.

Our MC radiative transfer code SEDONA [4] solves the SN light curve problem described above in 1,2 or 3 spatial dimensions. It implements several of the stabilization and variance reduction techniques described in the literature [6, 7, 1]. The code is written in C++ and parallelized using a hybrid of MPI and openMP. It has shown scaling up to 1024 processors on machines such as the Linux cluster ATLAS at LLNL and the IBM SP Seaborg at NERSC.
3. Validation and Results

Although a first-principles understanding of how SNe Ia explode is still lacking, many aspects of the phenomenon can be captured using simplified models. In [9] we developed parameterized hydrodynamical models of Chandrasekhar mass white dwarf explosions. In these 1D “toy” models we bypassed the difficult issues of nuclear combustion and simply took as free parameters the end products of burning (i.e., the amount and distribution of nickel, iron, and silicon group elements produced). The implied energy release was then used to calculate the final ejecta velocities and densities. Figure 1 shows SEDONA radiative transfer calculations for one such model. The impressive agreement of the synthetic light curves and spectra with observations of normal SNe Ia provides important validation of our calculations.

We have used sets of these parameterized 1D models to study the diversity of SN Ia light curves. The abundance of radioactive $^{56}$Ni turns out to be the primary determinate of the peak brightness of the event. Figure 2 shows six models in which we have varied the total mass of $^{56}$Ni in the ejecta by a factor of 2 (from 0.35 to 0.70 $M_\odot$) while holding the energy of the explosion fixed. The range in model peak brightness resembles the variation observed among normal SNe Ia. Moreover, the observed width-luminosity relation (WLR) is reproduced, with brighter models having broader light curves in the blue wavelength band. In [5] we discussed in detail the transfer physics underlying this relation, noting that the model WLR reflected the strong dependence of the ejecta opacity on the ionization state.

In [9] we expanded our parameter study to a grid of 130 SN Ia models which spanned the range of conceivable explosions of a Chandrasekhar mass white dwarf. As expected, $^{56}$Ni remained the dominant parameter controlling peak brightness, however the light curve width was sensitive to additional parameters, in particular the explosion energy and the radial distribution.
Figure 2. Left: Light curves (in the blue wavelength band) of SN Ia models with $^{56}\text{Ni}$ mass between 0.35 and 0.70 $M_\odot$. Right: Relationship between the models’ peak brightness and light curve width (the latter measured as the drop in magnitude from peak to 15 days after). The shaded band shows the observed width-luminosity relation of [8].

More realistic models of SNe Ia must capture the details of nuclear burning and radiative transfer in multiple dimensions. We are pursuing such models in 3D, and have begun a survey of 2D models which explore white dwarfs under a range of ignition conditions. All 2D models show some deviation from sphericity due to the chaotic nature of ignition and instabilities in the burning front. Asymmetrical ignition can sometimes lead to pronounced global asphericities. Figure 3 shows the final chemical structure of a model in which the star was ignited off-center near the symmetry axis. The deflagration flame (which later transitioned to a supersonic detonation wave) burned to completion more thoroughly on one side of the star, leading to a predominance of $^{56}\text{Ni}$ on the ignition side ($y > 0$) and of silicon group elements on the other. Not surprisingly, the emission from this asymmetric model shows strong orientation effects. In the 2D SEDONA calculations of Figure 3 (center), both the light curve shape and peak brightness of the off-center model vary by nearly 25% depending upon viewing angle. In the day 20 spectrum (Figure 3, right), the depth and Doppler shift of line absorption features due to silicon and calcium also vary by a large amount. Such an asymmetry could be an important source of dispersion in the WLR. It may also explain some of the spectroscopic diversity and line polarization features detected among SNe Ia [3].

4. Further Code Developments
Recent code developments have improved both the applicability and physical accuracy of our radiative transfer calculations. While previous SEDONA calculation have adopted the LTE
Figure 3. Left: The final ejecta structure of a 2D (axially symmetric) SN Ia model which was ignited off-center. The color scale indicates the average atomic mass, with red corresponding to $^{56}$Ni and light blue to silicon group elements. Center: B-Band light curve of the 2D model as seen from different viewing angles ($\theta = 0$ corresponds to the view looking down along the y-axis). Right: Spectrum of the 2D model at 20 days after explosion from various viewing angles.

assumption, we have now implemented a non-LTE solver to calculate the occupation number of atomic levels in statistical equilibrium. We solve the non-linear set of coupled rate equations of atomic models that include over 2,000 levels coupled by over 10,000 line transitions. To expand to even larger atoms, efficient parallelized solvers of sparse matrices are needed.

Our MC calculations scale perfectly and without limit as long as the memory requirements are modest. For 1D and 2D calculations, for instance, the grid is replicated on each processor and packets propagated independently, with the results communicated only at calculation end. For well-resolved 3D calculations, on the other hand, the gas opacities must be stored on a 5-dimensional grid (3 spatial, 1 time, 1 wavelength dimension) requiring several hundreds of GBs. This grid must be distributed among processors and packets communicated between processors as they propagate stochastically. Proper load balancing is a challenge. Algorithms for domain decomposed MC have been developed and some have been shown to scale well (on simple problems) up to 244 processors [2]. Blocks of processors with requisite memory can themselves be replicated to extend the scaling without limit. Improving and implementing such scalable algorithms are a major focus of our current code development.

Acknowledgements: Support for this work was provided by the DOE SciDAC Program under grant DE FC02-0641438. We are grateful for computer time provided by LLNL on the ATLAS machine, by ORNL through an INCITE award, and by NERSC.

References
[1] Brooks, E. & Fleck, J. 1986, J. Comp. Phys. 67, 59
[2] Brunner, T., Urbatsch, T., Evans, T., & Gentile, N. 2005, American Nuclear Society, UCRL-CONF-208
[3] Kasen, D., & Plewa, T. 2007, ApJ, 662, 459
[4] Kasen, D., Thomas, R. C., & Nugent, P. 2006, ApJ, 651, 366
[5] Kasen, D., & Woosley, S. E. 2007, ApJ, 656, 661
[6] Lucy, L. B. 1999a, A&A, 344, 282
[7] —. 1999b, A&A, 345, 211
[8] Phillips, M. M., Lira, P., Suntzeff, N. B., Schommer, R. A., Hamuy, M., & Maza, J. 1999, AJ, 118, 1766
[9] Woosley, S. E., Kasen, D., Blinnikov, S., & Sorokina, E. 2007, ApJ, 662, 487