Multidimensional radiative transfer calculations of the light curves and spectra of Type Ia supernovae

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Abstract. The explosion of a white dwarf star in a Type Ia supernova (SN Ia) explosion leads to the burning and ejection of stellar material at a few percent of the speed of light. The spectacle we observe in the months that follow is from the leaking of radiation from this glowing mass of radioactive debris. The modeling of SN Ia light curves and spectra represents a complex problem in time-dependent radiative transfer. Here we discuss numerical methods, in particular Monte Carlo methods, for calculating 3D multi-wavelength radiative transport on massively parallel machines. Our approach involves a newly developed domain decomposition technique in which the memory load is distributed over multiple processors and photon packets are communicated from node to node. We present results for 2-dimensional models that explore white dwarf explosions over a range of explosion paradigms and ignition conditions. These models give insight into how variations in the initial conditions of the explosion affect the light curve we finally observe. We conclude with an outlook (and some initial results) for large scale 3D radiation transport calculations of SNe Ia in an era of petascale computing.

1. Introduction

Among the brightest of stellar explosions are the thermonuclear, or Type Ia, supernovae (SNe Ia). They appear to us as a point source of light, much like a star, but brightening day by day to a peak intrinsic luminosity some billion times greater than that of the sun. We sometimes speak of this transient brilliance as a “supernova explosion,” but in fact the explosion had ended long before, having consumed and disrupted the progenitor star in just a few seconds. What we are actually seeing is the stellar debris, burned and ejected at a few percent the speed of light, and glowing under the heat of its own freshly synthesized radioactivity.

SNe Ia can be seen at great distances, billions of light years, and so can be messengers of the universe at earlier ages. Unlike other kinds of supernovae (SNe), the Type Ia events show an impressive regularity in their luminosity and spectral evolution. Empirically, we find that brighter SNe Ia brighten and fade more slowly than dimmer SNe Ia [1], a relation that can be used to infer the intrinsic luminosities from the light curve shape. In this way, SNe Ia are applied as standard candles to measure cosmological distances, probe dark energy and map out the expansion history of the universe. A persistent concern, though, is that the average properties of SNe Ia could evolve over cosmological time (because of demographic shifts in the
progenitor star population), which would subject the measurements of cosmological parameters to systematic bias.

A theoretical understanding of SNe Ia, based in numerical simulation, would help secure and refine their utility as cosmological probes. The problem is complex and multifaceted and requires a suite of codes to capture the diverse physics at play, which include stellar evolution, hydrodynamics, turbulent combustion, nucleosynthesis, and radiative transfer. Ideally, we want to simulate all aspects of the phenomenon from first principles. In practice, we still face a number of uncertainties concerning, for example, the exact nature of the progenitor star system, the conditions of ignition, and the physics of the flame propagation that unbinds the star.

Validation of supernova explosion simulations comes ultimately from comparing model predictions to observations of real events. Thus we must model the light curves and spectra of the remnant, a difficult problem in time-dependent radiative transport, and one in which several confounding effects must be considered, for example, radioactive energy deposition, differential expansion, line transport, and deviations from local thermodynamic equilibrium. Realistic explosion models also involve some deviation from spherical symmetry, so the transfer calculations must be carried out in three spatial dimensions as well. This problem in its fullest generality is only beginning to be addressed, and should continue to push the limits of high performance computing for years to come.

The focus here is on radiative transfer in SNe Ia. In Section 2, we recount the first ten seconds of the SNe Ia eruption, followed by a description of the light curve and spectrum formation over the following months (Section 3). In Section 4, we discuss numerical methods for radiation transport, in particular Monte Carlo methods, and strategies from parallelization and domain decomposition (Section 5). We then (Section 6) present results for 2D models that explore stellar explosions over a range of ignition conditions. We end (Section 7) with the outlook and some initial results for large-scale 3D radiation transport calculations of SNe Ia in an era of petascale computing.

2. The supernova eruption
We observe Type Ia SNe exploding in galaxies of all types, even those with old (> 1 Gy) stellar populations. Therefore these events cannot signal the death of a massive star (as in the more common case of core-collapse supernovae) because such stars have lifespans of only ~ 10 million years. We believe that SNe Ia are the disruption of compact white dwarf stars supported by electron degeneracy pressure, that have grown to criticality over longer time-scales. In one favored scenario, the progenitor has a binary companion that, after some extended period of stellar evolution, begins transferring mass to the white dwarf. When the white dwarf mass has grown near the limiting Chandrasekhar value of ~ 1.4 $M_\odot$, the increasing central temperature and density initiate carbon burning in the core.

Carbon burning can continue “simmering” in the white dwarf for several centuries, with the nuclear energy being spirited away by convective flows. Multidimensional models show a complex medium with chaotic fluctuations in entropy that eventually serve as the “sparks” for the explosion [2]. The location of ignition, and whether it happens at one or many points, may profoundly influence the supernova we eventually observe (see Section 6.2). The stochastic nature of this process may be one important reason that not all SNe Ia are exactly alike.

The initial sparks gives rise to a subsonic flame, known as a deflagration, which is modulated by turbulence and fluid instabilities. Because the stellar matter is supported by electron degeneracy pressure, it cannot readily expand in response to the rising temperature, that only promotes further burning. The result is thermonuclear runaway. The details of flame propagation are complex, but within seconds burning has consumed the greater part of the star. The fusion of carbon and oxygen to heavier elements releases sufficient energy ($E \sim 2 \times 10^{51}$ ergs) to unbind the white dwarf and eject the stellar material with velocities of order 10,000 km s$^{-1}$. 

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Nothing is left behind.

About ten seconds later, hydrodynamical and nucleosynthetic processes abate, and the ejecta reach a state-free expansion. The subsequent evolution is peaceful by comparison: the ejected debris expands, with its radius increasing linearly with time and its density dropping as $t^{-3}$ from geometrical dilution. With no further dynamics, the ejecta structure (i.e., the density profile and chemical stratification) retains a self-similar form, and any asymmetry or substructure that was imparted in the explosion is frozen in.

Throughout the entire process described so far, the stellar material remains so opaque that radiative transport is of little importance. By a day or so after the explosion, however, the densities have declined such that diffusion of optical radiation does become significant on the expansion time-scale. It is ultimately the leaking of photons from the hot mass of ejected debris that we observe as the supernova light curve.

3. Light curves and spectra
The material ejected in the thermonuclear explosion is initially quite hot, around $10^9$K, but because of the high velocities it cools rapidly by adiabatic expansion. The thermal energy pool is essentially completely converted to kinetic energy within minutes, well before any appreciable radiation can diffuse to the ejecta surface. If this were the whole story, SNe Ia would lack a luminous display altogether. Remarkably, Nature provides an additional energy reservoir in the form of radioactive isotopes, in particular $^{56}$Ni, which are synthesized in abundance during the explosion.

To first order, the peak brightness of a SN Ia is determined by the quantity of $^{56}$Ni produced.
A typical event makes around 0.6 $M_\odot$, but for some reason (discussed further in §6.2) different explosions have different yields. The decay chain of nickel ($^{56}\text{Ni} \rightarrow ^{56}\text{Co} \rightarrow ^{56}\text{Fe}$) releases $\sim 1\text{MeV}$ gamma rays, which deposit energy in the ejecta primarily through Compton scattering. It is this energy that, through a process of thermalization or excitation/ionization, ultimately re-emerges as the optical/UV radiation we observe.

Figure 1 shows a typical example calculation of a SN Ia light curve. The rate of energy input from radioactive decay follows the half-lives of the isotopes ($\tau_{^{56}\text{Ni}} = 6$ days, $\tau_{^{56}\text{Co}} = 78$ days). At early times, essentially all of the decay products are absorbed locally, but after $\sim 30$ days the Compton opacity has dropped such that gamma rays begin to escape the ejecta straightaway. Any absorbed radioactive energy is re-radiated almost immediately in the optical/UV, but at first it takes some weeks for that radiation to diffuse to the ejecta surface. Thus, the visible light rises to a peak in about 20 days, then declines on a similar time-scale. At late times ($t > 80$ days), when the ejecta are optically thin, the light curve tracks directly the exponential decline of radioactive energy deposition.

The time duration of the SN light curve can be considered a measure of the effective diffusion time of photons and hence depends on the total ejecta mass, the rate of expansion, and the opacity of the supernova ejecta. The opacity is complex, being dominated by literally millions of atomic line transitions, each Doppler broadened by the differential expansion of the ejecta and in aggregate blending together into a pseudo-continuum (see figure 2). Transitions from iron group elements (iron, cobalt, nickel) are the most numerous and have their greatest effect at bluer wavelengths. Because the number of optically thick lines depends on the atomic ionization and excitation state, the opacity is a sensitive function of the ejecta thermal and statistical state.

The emergent spectra of SNe Ia are characterized by broad absorption/emission line features superposed on a pseudo-blackbody continuum (figure 3). The line features allow us to diagnose the chemical composition and (by measuring Doppler shifts) the expansion velocity of the ejecta. At early times (about 20 days after the explosion) SN Ia spectra are dominated by features of intermediate mass elements (IME) such as silicon, calcium, and sulfur. A few weeks later the opacity has dropped and one peers deeper into the ejecta; the spectrum then evolves to one dominated by iron group features. This leads to a picture in which the iron group elements are concentrated in the ejecta core, which is surrounded by a shell of IME and, perhaps, an outermost clumpy layer of unburned carbon and oxygen.

4. Multidimensional radiative transfer

SN light curves are modeled by post-processing the output of explosion simulations that have been run to the free-expansion phase. At that point, the ejecta structure (i.e., the density, velocity, and chemical composition defined on a spatial mesh) fully determines the emergent light curves, spectra, and spectropolarization. Several codes, using various numerical techniques, have been developed to model aspects of the radiation transport phase in SNe, for example, [3, 4, 5, 6, 7]. We focus here on SEDONA [8], which solves the time-dependent multi-wavelength transfer problem in one, two, or three spatial dimensions.

The full light curve calculation is actually built of several subproblems, with the work flow as follows: (1) calculate the radioactive decay rate and the transport and absorption of emitted gamma rays; (2) determine the material state (i.e., temperature, degree of ionization/excitation) at each spatial point; (3) compute the wavelength-dependent opacity at each spatial point, given the local state; and (4) solve the transport of visible radiation through the rapidly expanding, optically thick ejecta. In fact, the radiation field affects the material state through heating and radiative ionization/excitation, so steps (2) and (4) are coupled together in a nonlinear way.

The radiation field is, in general, a function of 3 spatial dimensions $(x, y, z)$, as well as time $t$ wavelength $\lambda$ and (because isotropy does not typically hold) of direction as defined by the two propagation angles $\theta$ and $\phi$. The radiation transfer equation is thus formally a differential
Figure 2. The opacity of SNe Ia is dominated by numerous Doppler-broadened lines that blend together into a pseudo-continuum opacity, here shown for a parcel of cobalt/iron rich gas. The thin red line is calculated by using a restricted atomic linelist of $\sim 500,000$ lines, while the thick black line is the result by using the full list of $\sim 42$ million lines. The horizontal dashed line marks the level of electron scattering opacity.

equation involving seven independent variables. Methods for direct numerical solution of the equation using accelerated lambda iteration techniques have recently been implemented in the context of 3D supernovae [9]. More often, approximate schemes are adopted to reduce the dimensionality of the problem by neglecting, for example, the angular dependence (e.g., flux-limited diffusion), the wavelength dependence (grey transport), or time (stationarity approach). Our goal is to address the problem in its full generality.

Given the complexity and high-dimensionality of the problem, Monte Carlo (MC) methods are appealing and the approach adopted in SEDONA. In the MC scenario, packets of radiant energy (“photons”) are emitted throughout the ejecta and tracked through randomized scatterings and absorptions until they escape the envelope. Each packet possesses a unique wavelength and polarization Stokes vector, which are updated at each scattering event. Packets passing through a grid cell are tallied to construct estimators of the local radiation field, and the corresponding rates of radiative heating, ionization, and excitation. Packets escaping the grid can be used to construct the emergent spectrum and light curve. All calculated quantities possess statistical noise, which is reduced as the number of propagated packets is increased.

Photon packets diffuse through all dimensions of the problem: stochastically through space, forward in time and – due to absorption and remission processes – back and forth in wavelength space. Because the ejecta is in differential expansion, the packet wavelength is also constantly Doppler shifting with respect to the local co-moving frame, causing packets to sweep through lines one by one. In this case, line scattering and absorption processes can be simplified by adopting the narrow-line limit, or Sobolev approximation, which is appropriate for media in high differential expansion [10]. Here, the ejecta properties are assumed constant over the small spatial region in which the photon Doppler shifts into resonance with a line. A more exact treatment of line transport, which we have also begun implementing, requires very high
wavelength resolution ($\sim 10^5$ points) in order to resolve individual line profiles. The memory requirements in 3D are therefore extreme but should be accessible using current high performance platforms and new parallelization strategies (see Section 5).

The line opacities and emissivities depend on the ionization and excitation state of the ejecta gas. Under the condition of local thermodynamic equilibrium (LTE) the calculation of these is relatively simple, as they are well-defined functions of the local temperature, density, and composition. Unfortunately, in the tenuous atmospheres of SNe, thermalizing processes (collisions) are rare, and radiative transitions and radioactive excitation can drive the material out of equilibrium. In this case, one must address the full non-LTE problem by solving a set of nonlinear coupled equations describing the rates into and out of each atomic level. Typically, several 100’s levels per ion are considered, coupled by 10,000’s of line transitions. The matrix must be solved at all spatial points and at all times, making fast algorithms essential.

We have implemented a non-LTE solver into SEDONA that uses tallies of Monte Carlo packets to estimate the rates of radiative transitions (treated in the Sobolev formalism). Figure 3 compares a LTE synthetic spectrum to a non-LTE spectrum for a 1D SN Ia model at maximum light (20 days after explosion). Clearly LTE provides a good qualitative approximation, which justifies its use in our initial multidimensional calculations. In detail, however, the color of the spectrum and the strength of individual line features are sensitive to non-LTE effects. At yet later times (> 70 days after explosion) LTE breaks down altogether.

Realistic opacity calculations require extensive atomic data – we use an atomic linelist from

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**Figure 3.** The spectrum of the observed Type Ia SN 1981B compared to the synthetic spectra of a 1-D SN Ia model (black line) computed assuming LTE (top) and non-LTE (bottom). While LTE is a generally good approximation, it overpredicts the emission component of strong line features and gives too red a color for the pseudo-continuum.
Figure 4. Weak scaling (left) and strong scaling (right) results for the domain-decomposed Monte Carlo test problem. The blue dashed line represents “perfect” scaling. The points are actual code performance on the Franklin supercomputer at NERSC.

[11], which provides data for over 40 million bound-bound transitions. Even this list is likely incomplete or inaccurate to some degree, especially at longer wavelengths (figure 2). Input from experiments and advancing theoretical calculations will, we hope, improve the atomic data set for astrophysics in the future.

5. Parallelization and domain decomposition strategies
For simple 1D problems, Monte Carlo methods can be computationally inefficient because a very large number of photon packets must be propagated to achieve reasonable noise levels. The MC approach, however, becomes of increasing benefit when facing problems of higher complexity and dimensionality. For 3D multi-wavelength radiation transfer, MC methods could rival or surpass deterministic methods, especially when made to run efficiently and scalably on massively parallel machines.

In problems involving one or two spatial dimensions, where memory requirements are fairly modest, Monte Carlo is “embarrassingly parallel.” Each processor holds a copy of the entire grid and propagates packets independently, with the emergent packet statistics being combined at the end of the calculation. This approach, known as “full replication,” scales perfectly and without limit, since communication is isolated to a few well-defined, deterministic parts of the program. Unfortunately, it also restricts the grid resolution to the memory available on an individual node, typically only several gigabytes. The requirements for a well-resolved 3D radiative transfer problem far exceed this. A typical calculation would use order 100^3 spatial points and 10^3 to 10^5 wavelengths points, requiring storage of ~ 10^{11} values of opacity, emissivity, and radiation field tallies. At double precision, this necessitates several hundreds of gigabytes to 1 TB of memory.

The situation is complicated by industry trends, which drive new high-performance computing architectures away from massively parallel, shared-memory systems toward systems with fewer CPUs and less memory per node, but faster internode communication. To most effectively use such machines for 3D radiative transfer, we have recently developed and implemented an algorithm for domain-decomposed Monte Carlo (DDMC), in which the model grid is distributed over a large number of CPUs. As packets propagate they “diffuse” from node to node, not unlike the diffusion of photons in the real supernova debris. With DDMC, grid sizes of a few terabytes are accessible, at the expense of a significant increase in communication.

Our specific DDMC algorithm alternates between propagation and communication cycles. The model atmosphere is divided into a number of contiguous spatial “chunks,” each assigned
to a single CPU. Each chunk is further subdivided into 3D Cartesian mesh of “cells” within which the values of physical variables are defined. Each CPU is responsible for propagating energy packets through its chunk of the model domain. When a packet reaches a chunk boundary, it is buffered, awaiting communication to a neighboring CPU.

When all CPUs have propagated their load of packets to chunk boundaries, the propagation phase ends and communication begins. Our implementation uses the Message Passing Interface (MPI): and to avoid the overheads in passing numerous small messages (packets are less than 100 bytes each), packets are sent in large batches. Distinct MPI calls (both a send and a receive) must be performed at each of the six faces of the chunk cube, accomplished by looping over dimension \((x, y, z)\) and oscillating a send/receive between the even/odd chunk pairs. An alternative approach of “global array” (GA) parallelism is attractive because it is designed to reduce overheads transparently and obviate the two-phase approach, but GA seems to be less universally available than MPI for the present.

If the required memory for the entire grid is less than the aggregate memory available, the grid can be duplicated on further sets of CPUs to recover some of the favorable scaling properties of the “full replication” approach. Another option is to use spare CPUs for load balancing. Chunks representing the dense inner regions of the supernova ejecta typically have a heavier scattering load than do those located near the outer boundaries. Replicating the heavily loaded chunks on additional CPUs can mitigate the latency induced in the propagation phase, but incurs a further communication cost. Hence the load-balancing option may require intelligent tuning.

We have performed both weak and strong scaling tests of our DDMC code with a simple grey opacity test problem (figure 4). To probe weak scaling, we kept the average number of scatterings per CPU constant and enlarged the problem grid (adding chunks in proportion to the number of CPUs). In the strong scaling tests, the same physical volume was progressively gridded at higher resolution, reducing the per-CPU workload. The results (which depend also on the opacity, and hence propagation load, of the particular model) show a weak scaling increase of only 38% out to 1,000 processors. Both the weak and strong scaling results are promising, especially considering the range of grid sizes tested. Moreover, the block of 1000 processors can now be replicated 10 or 100 times over on additional processors with no further losses in inefficiency. Thus DDMC will permit large-scale radiative transfer calculations to be performed effectively on petascale machines.

6. Results for 1D and 2D Type Ia models
Although several aspects of SN Ia explosion process remain uncertain, progress can be made by parameterizing areas of ignorance and comparing model observables to real data. In previous work [13, 14], we studied the diversity of SN Ia light curves using simplified 1-D explosions that bypassed the details of turbulent nuclear combustion. These studies gave insight into how SN Ia light curves depend on ejecta properties and helped clarify the underpinning of the important width-luminosity relation.

In particular, our radiation transfer calculations emphasized the importance of the opacity’s dependence on the ionization state. In SNe Ia, gradual cooling of the ejecta promotes the recombination of Fe III to Fe II soon after the light curve peak. Because optical/infrared lines are more numerous for Fe II than for Fe III, this cooling increases the line opacity and enhances the fluorescence of blue photons to longer wavelengths. The effect of wavelength redistribution in Fe II lines explains why the infrared light curves of SNe Ia rise to a “secondary” peak several weeks after the first (Figure 5). In dimmer SN Ia models, which are generally cooler, we find that recombination sets in earlier and the secondary maximum is hastened, a trend also noted in observations [15]. For the same reason, the flux in the blue bands disappears more quickly in the cooler SNe, resulting in a faster declining B-band light curves for dimmer SNe Ia. Such effects are at the heart of the Type Ia width luminosity relation.
Figure 5. Left: Light curves (in the blue wavelength band) of parameterized 1D SN Ia models with $^{56}$Ni mass varied between 0.35 and 0.70 $M_\odot$. The brighter models decline more slowly than their dimmer ones. Right: Near Infrared light curves of the same models. The secondary maximum is due to the redistribution of flux from bluer to redder wavelength, which is enhanced as the ejecta cool and the ionization state lessens.

6.1. 2D deflagration models

While parameterized 1D models are useful for understanding how SN Ia light curves vary with the ejecta properties, they do not constrain the physical origin of such variations. To this end, we have pursued a survey of 2D models based on a more realistic treatment of the explosion physics as captured by the SN Ia code developed by SciDAC collaborators at the Max Planck Institute for Astrophysics. To explore the sensitivity to initial conditions, we parameterized the white dwarf ignition process by inserting randomly distributed “hot spots” around the stellar center. The subsequent propagation of the deflagration flame was tracked under a level-set approach and employed a subgrid-scale model to describe turbulent energy on unresolved scales.

In the deflagration phase, burned ash is buoyant with respect to surrounding cold fuel, resulting in hot rising bubbles subject to shearing and other fluid instabilities. The resulting ejecta structure exhibits irregular plumes of processed material ($^{56}$Ni and IME) embedded in a substrate of unburned carbon/oxygen (figure 6). The deflagration itself fails to consume all available fuel but burns enough to explode the star. The result is a subenergetic event, with relatively low $^{56}$Ni yield (in this particular model only 0.2 $M_\odot$).

Postprocessing with our radiative transfer code gives a synthetic spectrum that bears little resemblance to that of observed SNe Ia at maximum light (figure 6). This model failed to synthesize an abundance of high-velocity IME and so does not reproduce the observed blueshifted absorption features from silicon, sulfur, and calcium. The strength of the deflagration phase can be enhanced by increasing the number ignition points (and will be greater yet in full 3D calculations) but even the most vigorous 3-D deflagrations seemingly do not burn enough material to match the properties of the more typical SNe Ia [16].
6.2. Delayed-detonation models

The speculation is that in real supernova the deflagration flame transitions at some point to a supersonic detonation wave, which sweeps through the star, burning away any remaining fuel, so producing a healthy explosion. The physics of the transition is still not completely understood, although progress is being made in this direction. One possibility is that deflagrating bubbles may break out from the white dwarf surface, initiating large-scale flows that collide and compress the fuel [17]. Another possibility, reconsidered recently in [18], is that a detonation occurs spontaneously as a result of vigorous turbulent mixing of fuel and ash on small scales.

We have introduced a spontaneous detonation transition into our 2D models by simply inserting the detonation by hand once the deflagration flame has reached a density of $10^7$ g cm$^{-3}$, (roughly the conditions when mixing is intensified as a result of burning in the “distributed regime”). The left side of figure 7 shows the final ejecta structure of one such “delayed-detonation” model, which resulted in a stratified compositional structure and 0.64 $M_\odot$ of $^{56}$Ni. On the right side of the figure is a time-series of synthetic spectra calculations compared to observations of a typical SNe Ia. The week-by-week evolution follows spectrum formation in progressively deeper layers of the ejecta – at early times ($t < 30$ days) in the outer layers of IME and later in the $^{56}$Ni core. The overall good agreement of the model with observations is impressive, especially considering that, apart from the ignition conditions and detonation criterion, the model was not tuned in any way.

The results of figure 7 strongly support some sort of delayed detonation model of SNe Ia.
Even more interesting, in our specific adopted paradigm we find that the peak brightness of the supernova depends sensitively on the ignition conditions. Increasing the number of ignition “hot-spots” gives (perhaps surprisingly) a less luminous event (see figure 8). The reason is that the amount of $^{56}$Ni produced by the detonation wave is determined primarily by the density of the material it passes through. Stronger ignition conditions give a stronger deflagration phase, which leads to greater pre-expansion of the white dwarf (hence lower overall densities) at the moment of detonation. A variation of the number of ignition points from $N = 20$, to $N = 150$ leads to a variation in peak brightness of a factor of 2, which is a large part of the luminosity range observed in normal SNe Ia. Inspection of the detailed maximum-light spectra show features that correlate with peak brightness as well. For example, the more luminous models have bluer colors and a weaker ratio of Si II features near 6000 Å.

6.3. Off-center detonation models
The centrally ignited delayed-detonation models discussed so far retain approximate spherical symmetry (see figure 7). Slight asymmetry in the ignition conditions, however, can lead to pronounced global asphericities in the final ejecta structure. Actually, models of the simmering phase of non-rotating white dwarfs find that convection has a dominant dipolar mode, in which case ignition may be expected to occur off-center. We have explored the possibility by distributing the initial hot spots within a cone of opening angle $\pi/4$. The resulting deflagration flame (and subsequent detonation) burned to completion more thoroughly on one side of the
star, leading to a predominance of $^{56}$Ni on the ignition side ($y > 0$) and of silicon group elements on the other (figure 9). As the deflagration phase in this model was weak (being confined to one side of the star), the $^{56}$Ni production was large, $\sim 1.0 \, M_\odot$. The light curve shape and peak brightness also depend sensitively on the orientation, varying by nearly 25% depending on the viewing angle. When viewed from the ignition side ($\theta = 0^\circ$), the model is as luminous as the brightest SN Ia ever found [19].

Astronomical imaging of the geometry of SNe Ia would clearly give deep insight into the nature of the explosion physics. Unfortunately, virtually all observed SNe are too distant to be directly resolved in the initial phases. In this case, our only direct probe of asphericity is through observations of the polarization of SN light. Electron scattering in the ionized SN envelope will polarize the light, but the net effect will cancel unless there is a preferred direction (i.e., departure from spherical symmetry) in the scattering medium. Spectropolarimetric observations are typically very challenging, as the light from SNe is dim and quickly fading, and the observed polarization levels are typically small, $P \sim 1\%$. Nevertheless, intrinsic polarization has now been clearly detected in several SNe Ia, both in the lines and the continuum [20, 21, 22], demonstrating that in general SNe Ia aspherical to some extent.

Deriving the detailed ejecta geometry of SNe Ia from polarization observations is a difficult inverse problem which can only really be attempted by comparison with multi-dimensional radiation transfer calculations. Figure 10 shows the polarization spectrum at maximum light of an off-center detonation model. From some orientations, the model resembles observations of particular SNe Ia (e.g., SN 2004dt [23]) with a low continuum polarization but large line polarization peaks at the location of prominent absorption features. Although the agreement with observations is suggestive, the solution may not be unique, and other geometries could make
similar polarization predictions. The path forward is to obtain spectropolarization observations for a statistical sample of SNe Ia, which probe many different viewing orientations, and compare to the predictions of individual models.

7. Initial results and outlook in 3D
When compared to fully 3D simulations, the 2D explosion models only approximate the ejecta morphology and do not reproduce the correct energetics, $^{56}\text{Ni}$ yields, or detailed sub-structure. Ultimately, the SN Ia problem must be addressed, at all stages, in 3D. The computational expense is then naturally much greater, and a much smaller grid of parameter space can be explored.

While a few full-star 3D SN Ia explosion calculations have been carried out [24, 25, 26, 27], the modeling of synthetic spectra and light curves in 3D is largely unexplored territory. Figure 11 shows one of our milestone calculations – the first high-resolution 3D model of a SN spectrum at maximum light. In this example, an asymmetric geometry was artificially constructed by distorting a spherically symmetric SN Ia model. The transfer calculation, which relied on our newly developed domain-decomposition algorithms, was performed on a grid of $200^3$ spatial points and $10^4$ wavelength points, amounting to over 1 TB of memory.

Our 3D spectrum run took approximately 10,000 CPU-hours on 1,000 processors on the Cray XT4 machine Jaguar at Oak Ridge National Laboratory. We anticipate that full light
Figure 10. Flux spectrum (bottom) and polarization spectrum (top) of an off-center delayed detonation model at maximum light, as seen from one particular viewing angle. The aspherical distribution of IME in the SN ejecta leads to large polarization peaks over line absorption features.

Figure 11. Synthetic spectrum calculation of a model SN Ia calculated in full 3D using the domain decomposition parallelization approach. The underlying model ejecta was constructed artificially by distorting a 1D model.
curve calculations, now under development, will require upwards of 500,000 CPU-hours per model. The introduction of certain Monte Carlo variance reduction techniques may be able to reduce the execution time significantly, but already 3D time-dependent multi-wavelength transfer calculations for supernovae are within our reach.

The ultimate goal is to develop an end-to-end simulation of SNe Ia, from the moments of ignition to the months following explosion, which help us to infer how variations in the SN Ia progenitor system affect the luminosity of the event. This theoretical understanding would be of great help in limiting and controlling the potential evolution of SN Ia properties with redshift, a possible source of systematic error in cosmological studies of dark energy. First-principle calculations of SNe Ia will require our increased understanding at every stage of the event, in particular the precise conditions of ignition, the physics of the deflagration to detonation transition, and the effects of non-LTE on the spectra and light curves. Our SciDAC group has parallel efforts on all these fronts. The advancing numerical methods should continue to make good use of massively parallel machines in the coming era of petascale computing.

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