Modeling Emission from the First Explosions: Pitfalls and Problems

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Abstract.
Observations of the explosions of Population III (Pop III) stars have the potential to teach us much about the formation and evolution of these zero-metallicity objects. To realize this potential, we must tie observed emission to an explosion model, which requires accurate light curve and spectra calculations. Here, we discuss many of the pitfalls and problems involved in such models, presenting some preliminary results from radiation-hydrodynamics simulations.

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INTRODUCTION

JWST will advance our current picture of first-generation stars, which is now based on theory and indirect constraints from nucleosynthetic yields, by directly observing the explosions of these stars. Such observations will vastly improve our understanding of the structures and masses of Pop III stars. How much information these observations provide depends upon the accuracy of our simulations of the emission from primordial supernovae. In this paper, we discuss the problems and pitfalls that can befall such models.

Recent supernova light curve calculations have focused on thermonuclear explosions of white dwarfs: so-called Type Ia supernovae. The usual approach in these models is to first simulate the explosion in a purely hydrodynamic calculation. The trajectories from this explosion are then used in a radiation transport calculation. The transport calculation assumes that an equilibrium between radiation and matter exists and allows this equilibrium to set the matter temperature based on the radiation flow due to the decay of radioactive nickel.

This approach, separating the hydrodynamic and radiation transport calculations, will not work for the first stars. Indeed, we know that radiation-only calculations of light curves for all massive star supernovae are incorrect. This is because the light curve is not just powered by radioactive decay. A second heat source exists - that of shock heating. Depending upon the initial radius of the star and the immediate surroundings of the explosion, shock heating can dominate the light curve out to late times [3, 4]. Including the effects of shock heating in a supernova emission model requires a coupled radiation-hydrodynamics calculation.

As we shall show here, accurate estimates of supernova emission require modeling the
FIGURE 1.  *Left:* Maximum shock velocity versus time in two models of a Wolf-Rayet star supernova: a purely hydrodynamic calculation with no radiative losses and a simulation with radiative losses in a single-group, flux-limited diffusion model. In the hydrodynamic-only calculation, the shock accelerates dramatically as it crosses the sharp density gradient at the edge of the star, reaching speeds above the speed of light in this non-relativistic model (meaning that the flow is relativistic with high Lorentz factors - shock breakout was once argued as a way to produce gamma-ray bursts [1]). It is clear from the transport calculation that radiative losses diminish this acceleration dramatically. Even at late times, well after shock breakout, the maximum velocities in these two models are very different. *Right:* Effective radiation temperature defined by \((E_{\text{rad}}/\sigma)^{1/4}\) (top) and velocity (bottom) versus radius for 4 snapshots in time during shock breakout in a pair-instability supernova explosion. In the initial two snapshots, the radiation is trapped in the flow of the shock. By the third snapshot, the radiation has begun to lead the shock but is still coupled strongly with the material ahead of the shock and preaccelerates it. In this manner, the radiation flow, not the hydrodynamic flow, determines the position and velocity of the shock. The position of the shock changes faster than the shock velocity/Sedov solution would predict. In the last snapshot, the radiation is becoming decoupled completely from the matter and the radiation front is no longer able to accelerate the matter. This is the true escape of the radiation. Note that radiation decoupling effects span a range of time with a variety of effects, and that one can not simply mimic these effects with a cooling term.

departure of radiation and matter from equilibrium. This departure is most pronounced when the radiation in the shock first becomes untrapped: at shock emergence or shock breakout. The shock breakout signal dominates the observable transient in first stars, making accurate models of this nonequilibrium process crucial for understanding detections of these outbursts. In this paper, we discuss the physics of shock breakout and light curve calculations, concluding with the current LANL approach for a new generation of light curve models.
**PITFALLS IN MODELING SHOCK BREAKOUT**

The engine for both core-collapse and pair-instability supernovae is launched in the stellar core. While it is deep within the photosphere, the radiation is trapped in the flow, carried outward with the shock. But as the shock breaks out of the star, the radiation begins to lead the shock and ultimately decouples from it.

**Energy Loss:** In a purely hydrodynamic simulation, the explosion is well described by the Sedov similarity solution \([2]\): 
\[
\nu_{\text{shock}} \propto t^{(\omega - 3)/(5 - \omega)}
\]
where \(\omega\) defines the density structure of the medium: \(\rho \propto r^{-\omega}\). As the shock reaches the edge of the star, the density drops rapidly (\(\omega\) becomes large) and the shock can accelerate dramatically (as seen in the purely hydrodynamic calculation in the left panel of Fig. 1). But this calculation assumes that all of the internal energy in the shock is able to accelerate the material in front of it. If some internal energy, and hence shock pressure, is released, the acceleration will be much lower. This is exactly what happens when the radiation decouples from the matter. In our sample Wolf-Rayet simulation (Fig. 1, left), radiative losses sap the energy in the shock, and acceleration by pressure in the sharp density gradient is heavily reduced. The maximum material velocity is much lower than what would be expected from the Sedov solution (or a purely hydrodynamic calculation). Clearly, a pure hydrodynamic calculation does not produce the accurate flows needed for these light curve calculations.

**Radiative Acceleration:** If the only effect of radiation on the hydrodynamical evolution were energy loss, it could be modeled with a cooling term in the explosion calculation. But radiative effects in shock breakout are much more complex than just energy loss. As the radiation begins to decouple from the shock, it interacts with the matter in front of the shock strongly enough to accelerate it (right panel of Fig. 1). The position of the shock will thus be further out than predicted by a purely hydrodynamic model with a cooling term. Radiation, not matter pressure gradients, governs the position and velocity of the outmoving shock. The maximum velocity of this radiation-driven shock can also be faster than the Sedov solution would predict (counteracting the effect of radiative losses). This is visible in the early rise in the shock velocity in the sample Wolf-Rayet simulation (Fig. 1, left panel).

As the radiation further decouples, it begins to sap the shock strength (see our Energy Loss discussion), leading to lower velocities. These two radiative effects compete: radiative acceleration causes the shock to move faster than expected from a purely hydrodynamic calculation and radiative losses cause the shock to move more slowly. Radiation hydrodynamics is needed to capture both effects.

**LIGHT CURVE MODELS AND OPACITIES**

A simple way to compute supernova light curves during shock breakout is to calculate the location of the photosphere, determine the temperature at the photosphere, and estimate the bolometric luminosity by assuming blackbody radiation: 
\[
L_{\text{SN}} = 4\pi r_{\text{ph}}^2 T_{\text{ph}}^4.
\]
Depending upon the mass loss in the wind, the photosphere can be at the edge of the star or deep within the star’s wind profile. Many theoretical estimates of the bolometric luminosity use such a simple approximation. Comparing this analytic estimate to an actual simulation in which a full spectrum is calculated and then summed to get a
bolometric luminosity reveals that the analytic approach can overestimate the bolometric luminosity by over an order of magnitude (Fig. 2, left). The crude estimate of the opacity in the analytic approach accounts for a large fraction of this discrepancy. The photosphere is not at a single location, but depends on wavelength and the wavelength dependent opacity. Because the luminosity is proportional to $T^4$ and the temperature gradient is so steep at breakout, small errors in the shock position can produce large changes in the total predicted luminosity. Detailed opacities as a function of wavelength are crucial for accurate breakout luminosity predictions. Another assumption typically used in computing opacities is that the atomic level states are in equilibrium with the matter temperature. In shock breakout, this is not necessarily true and non-LTE effects may alter the opacities, and hence luminosities.

**LANL APPROACH**

LANL has begun to leverage off of its expertise in radiation hydrodynamics techniques as part of the Advanced Simulation and Computing (ASC) program. Under this program, LANL has developed the multi-dimensional radiation-hydrodynamics code RAGE (Radiation Adaptive Grid Eulerian), which was designed to model multi-material flows [5]. RAGE is an adaptive mesh refinement (AMR) code with a second-order, direct-Eulerian
Godunov hydrodynamics solver and multi-group flux-limited diffusion radiation transport with operator-split coupling. A discrete-ordinate scheme has been added to model non-thermal photon transport [4] along with implicit Monte Carlo (IMC) transport with full angular information for thermal photons.

There is some confusion in the astrophysical literature between the “diffusion” schemes used in most stellar evolution codes and the flux-limited diffusion (FLD) used in transport. Diffusion schemes in stellar models tend to be akin to conduction schemes, allowing energy flow from hotter to colder zones that is determined by the temperature gradient and the radiative diffusion coefficient. Such equilibrium diffusion/conduction schemes are appropriate in optically thick media where the radiation is fully coupled to the matter. FLD schemes model the radiation flow separately from the matter (the radiation energy is not set by the matter temperature). The simplifying assumption in these schemes is that the angular distribution of the radiation has a specific form. Full, or higher-order, transport schemes make no assumptions about the angular distribution but instead calculate it. The FLD transport in RAGE can model the decoupling of the radiation field from the shock in our breakout calculations.

Some astrophysical implementations of higher-order transport have made assumptions that the radiation and matter are fully coupled. Although these schemes include the angular distribution of the radiation field, they are little better than conduction codes in modeling shock breakout. These are sometimes referred to as 1-temperature algorithms, while codes that evolve radiation flux and matter temperature separately are known as, somewhat confusingly, 2-temperature codes. It is important to know what scheme is used when analyzing results from theory calculations. At LANL, all our transport algorithms (including our discrete ordinate and Monte Carlo methods) are full 2-temperature schemes.

At present, we assume that the level populations of the atoms in our shocks are in equilibrium with the matter. If the radiation field is exciting these atoms, this thermodynamic equilibrium is certainly not valid, but the database of nonequilibrium opacities are not yet sufficiently complete for our calculations (LANL’s atomic physicists are currently working on such a database). In addition, the modeling of radiation flow during shock breakout is very sensitive to the operator-split coupling term and it is likely that our current scheme is introducing errors.

With these caveats, we conclude with a brief discussion of our initial results. Figure 2 (right) shows the wealth of spectral data in the shock breakout light curves for a 250 M⊙ pair-instability explosion. Both emission lines and absorption lines (especially in the ultra-violet) are present. Many of these lines will appear in the visible spectrum at high redshift. We show the light curves of this supernova in a variety of bands in Fig. 3. At low energies, the peak in the light curve can occur a year after the explosion. Redshifted to first stars, this peak would occur 10 - 20 years after the explosion. Such a supernova would not be detected as a transient. The shock breakout itself will exhibit a broad peak lasting up to 200 days.

The prolonged pair-instability light curves, coupled with high-redshift time dilation effects, limit the potential of high-redshift transient surveys. JWST may only detect the shock breakout emission. Modeling this emission not only requires true 2-temperature radiation-hydrodynamic calculations, but probably nonequilibrium opacities as well. Until all of this is done accurately, any theoretical prediction must be taken with some
FIGURE 3. Light curves (luminosity versus time) for a number of spectral bands for a 250 M⊙ pair-instability supernova out to 1 year. We have included two bands consistent with the JWST bands assuming that the source is at a redshift of 10. Here, we have included both the wavelength shift of the source emission and time dilation. Note that the shock breakout emission lasts a week in the JWST frame. The differences between the plots on the left and on the right is the inclusion of the Lyman break, which cuts off any emission shortward of 1216 Å. Most high-redshift supernova searches for these pair-instability supernovae will detect the shock breakout.

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