Emission from cooling supernova shocks in MHD simulations

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Abstract. Each supernova (SN) injects \(10^{51}\) erg into the interstellar medium (ISM). The blast wave shocks the gas and heats it up to \(10^7\) K; the gas subsequently cools by emitting radiation across the electromagnetic spectrum. Typically, about 70% of the initially injected SN energy is lost by radiative cooling. Thus an understanding of the radiative losses is needed to understand the evolution of supernova remnants, and to allow for comparisons between simulations and observations.

We present a post-processing module for the FLASH code which calculates the cooling radiation from shock-heated gas in different energy bands. Using modern collision excitation data from MAPPINGS V, we produce maps of the SN emission at different wavelengths, allowing for a comparison to real observations of supernova remnants (SNRs) and for testing observational diagnostic tools. Here, we focus on optical line emission arising from the interaction between the shock wave and dense gas of a nearby molecular cloud and on the use of optical line ratios for determining the shock parameters.

1. Introduction
Massive stars live short lives and sometimes end their lives still surrounded by their natal molecular environment. As such, a number of supernova remnants have been found to interact with dense, molecular gas. The density of the gas hit by the expanding supernova shock greatly affects the evolution of the shock such as the shock velocity and temperature (e.g. [5], [22], [13], [11]). In turn, the SNR shock also affects the molecular gas, heating and ionizing it and driving turbulence.

Supernova remnants can be studied across different energy bands due to the cooling radiation covering the entire wavelength range. Most SNRs are observed at radio wavelengths due to their non-thermal synchrotron emission. In an early evolutionary stage they may be observed in the X-ray as the hot, shocked plasma cools. In the later stages of evolution when the dense, shocked gas has cooled, one may observe SNRs in the Optical. However, these observations are rarer, both because of extinction in the Optical and because significant optical emission only occurs when high density gas is shocked. In the Green catalog ([10]) only about 20 percent of the SNRs have optical observations. When they can be observed, optical line emission can allow one to learn a great deal about the parameters of the environment in which the SN exploded and about the evolution of the SNR. Moreover, the morphology of the line emission is typically filamentary and/or clumpy, revealing the distribution of the dense gas.

In this work, we use our new pipeline to produce optical line emission maps of a simulated SNR, which is interacting with a dense molecular cloud. We present the evolution of the line...
emission and test the accuracy of using line ratios in determining the parameters of the supernova shock.

2. Simulations
We use high-resolution, hydrodynamical simulations from [21] carried out with the adaptive mesh refinement (AMR) code FLASH 4.3 [9]. This simulation is part of the SILCC project [26] and SILCC-Zoom project [20]. As such, it includes self-gravity, supernova-driven turbulence, and the galactic external potential and follows the formation of molecular clouds from the multi-phase interstellar medium in solar neighborhood conditions. We use the estimate of [6] for the strength of the interstellar radiation field (ISRF) and take $G_0 = 1.7$. The radiative transfer of the diffuse ISRF is modeled self-consistently (see [27] for a detailed description of the method). Moreover, a non-equilibrium chemistry network following the formation of H$_2$ and CO coupled to the gas heating and cooling processes is included. Because molecular hydrogen forms on dust, we include a simple dust model: the dust-to-gas ratio is fixed and the dust temperature is calculated separately from the gas temperature assuming thermal equilibrium. For example, it takes into account the photo-electric effect associated with the absorption of the ISRF photons.

The simulation reaches a maximum resolution of $\sim 0.1$ pc. After the forming molecular cloud is fully refined ($t_0 = 11.9$ Myr), we explode a single supernova ($t_{SN} = t_0 + 1.53$ Myr) at distance of $d = 25$ pc from the center-of-mass of the cloud along the $x-$direction. At the moment, the cooling radiation from the SN is not taken into account, but this is subject to future work in this project.

Figure 1. Time evolution of the density (top row) and temperature (bottom row) for times 0.06 Myr, 0.12 Myr and 0.18 Myr after the SN explosion (from left to right). The slices are taken at $z = 0$. 
Figure 2. The derived emission in the Optical, UV and X-ray bands for times 0.06 Myr, 0.12 Myr and 0.18 Myr (top to bottom) as in Fig. 1.

3. Post-processing

To calculate the cooling function in different energy bands, we use the MAPPINGS V code [24] in a post-processing step. This code assumes collisional ionisation equilibrium and by considering emission from hydrogen, helium and metal atoms and ions, as well as non-atomic emission such as free-free emission, one may produce a detailed cooling curve at any given temperature and density.

The SNR evolution can be divided into different stages. The most important ones for this work are: (i) the Sedov-Taylor (ST) phase (about 72% of the initial SN energy is converted into thermal energy; during the energy conserving ST phase the shock evolves adiabatically); (ii) the transition (TR) phase (an intermediate period, in which radiative cooling becomes important); and (iii) the pressure-driven snowplough phase in which the evolution is dominated by radiative losses (almost all thermal energy is radiated away). Usually, a SNR is observed during the radiative phase (TR phase). In this work, we will consider emission before, during and after the TR stage for comparison. Following the calculation from [11] for the environmental density of
the studied SNR \( (n = 1 \text{ cm}^{-3}) \), our transition time is \( t_{TR} \approx 0.12 \text{ Myr} \). In Fig. 1, we show the density and temperature distributions for three different snapshots at times 0.06 Myr, 0.12 Myr and 0.18 Myr, i.e. before, at, and after \( t_{TR} \). From the gas temperature which is given by the FLASH simulation, we calculate the emitting luminosity for every cell in the 3-dimensional computational domain from the MAPPINGS V cooling tables. In addition to the total emitting luminosity \( (\Lambda \text{ [erg/s/cm}^3]) \), we calculate the radiative cooling in three different energy bands using MAPPINGS V: the non-ionizing ultraviolet (UV) and Optical \((E < 13.6 \text{ eV})\), the ionizing UV \((13.6 \text{ eV} < E < 100 \text{ eV})\) and for the X-ray regime \((E > 100 \text{ eV})\). Projecting this onto a 2D plane, we produce emission maps for each band (see Fig. 2). The figure clearly shows that even though the SN explosion is initially symmetric, the remnant morphology strongly depends on the molecular cloud distribution. The density of the molecular cloud gas is several orders of magnitude higher than in the typical interstellar medium \((n_H > 10^3 \text{ cm}^{-3})\). Therefore, the velocity of the shock wave towards the center of the cloud is much smaller, and in places almost stops. Moreover, hitting such a dense medium leads to rapid ionization of the gas and launches strong reverse shocks that travel into the ejecta. Figure 1 shows that the explosion cannot spread to the center of the molecular cloud (the area of highest density), but continues to expand into the more diffuse area in the lower right corner on the emission maps, forming dense filaments which are also commonly found in real observations.

Figure 3 shows a mass-weighted phase diagram for the computational domain containing the SNR and the molecular cloud. Generally, the ISM is split into three different phases which are in approximate pressure equilibrium: a cold and dense phase, \( T < 300 \text{ K} \), a warm and diffuse phase, \( T \sim 10^4 \text{ K} \), and a hot and diffuse phase, \( T > 10^6 \text{ K} \) [8, 26]. One can clearly see over-pressured, hot gas at densities of \( \rho \sim 10^{-24} \text{ to } 10^{-25} \text{ g cm}^{-3} \) which lies above the equilibrium curve; this is the shocked gas due to the expanding SNR.

Figure 3. Mass-weighted temperature-density phase diagram at \( t = 0.12 \text{ Myr} \) after the SN explosion.
4. Optical diagnostic

BPT diagrams (Baldwin-Phillips-Terlevich diagrams, see [2]) are a standard excitation diagnostic tool to separate different ionizing sources. Typically they are used to distinguish between H\textsc{ii} regions and active galactic nuclei (AGNs) due to differences in the hardness of their exciting radiation fields. Here we use them to investigate the distribution of shocked gas by the SNR. The diagrams are based on the ratios of strong optical emission lines: [OIII] (\(\lambda 5007\))/H\textbeta{} and [NII] (\(\lambda 6583\))/H\textalpha{}. Figure 4 shows a BPT diagram which contains two observational lines separating galaxies dominated by AGN emission, and those dominated by H\textsc{ii} regions. We also plot a theoretical line derived from our MAPPINGS V data, i.e. the expected line ratios from a parcel of gas at a given temperature in collisional ionization equilibrium (CIE). On top of this we plot the mean line ratios of our emission maps, i.e. from the SNR, over the course of the simulation (\(\Delta t = 0.56\) Myr). The SNR line ratio lies close to the boundary between H\textsc{ii} regions and AGN-dominated emission, as well as close to gas in CIE at a temperature of a few \(10^4\) K. Moreover, there is very little movement in the line ratios with time. Due to this overlap it is therefore difficult to fully distinguish between SNR-dominated, H\textsc{ii} region-dominated and AGN-dominated emission from unresolved galaxies using a BPT diagram.

In addition to the typical BPT line ratios we make use of the [SII] (\(\lambda 6731\))/H\textalpha{} ratio, which has been shown to be elevated in SNRs compared to H\textsc{ii} regions (see Fig. 5). This is due to the fact that the UV photons in an H\textsc{ii} region are sufficiently high energy to doubly ionize sulphur; however, there typically exist a large recombination region behind the SNR shock front, which contains singly ionized sulphur. Previous observations and models show that typical values for the [SII] (\(\lambda 6731\))/H\textalpha{} ratio are 0.1 - 0.5 for H\textsc{ii} regions and 0.5 - 1.0 for SNRs (see more in [15]). We also include the [OIII] (\(\lambda 5007\))/H\textbeta{} and [NII] (\(\lambda 6583\))/H\textalpha{} ratios which, including the previous line ratios, comprises a Veilleux-Osterbrock diagram [25] (an extension of the BPT diagram).

We summarize these ratios from our simulations in table 1. They are all consistent with the observed ratios for a SNR.

Table 1. All line ratios calculated from our synthetic emission maps covering the entire evolution of the SNR (\(\Delta t = 0.56\) Myr).

| Name                      | Obtained values |
|---------------------------|-----------------|
| [OIII] (\(\lambda 5007\))/H\textalpha{} | [0.99, 1.14]    |
| [SII] (\(\lambda 6717\))/([\(\lambda 6731\)] | [1.00, 1.03]    |
| [SII] (\(\lambda 6731\))/H\textalpha{}       | [0.44, 0.98]    |
| [NII] (\(\lambda 6583\))/H\textalpha{}       | [0.57, 0.99]    |
| [OIII] (\(\lambda 5007\))/H\textbeta{}        | [1.1, 1.29]     |

The [SII] emission lines are extremely useful in determining SNR shock properties. One may estimate the electron temperature and the electron density from the combination of the [SII] \(\lambda 6731/\lambda 6717\) ratio and the [SII] ((\(\lambda 4069 + \lambda 4076\))/([\(\lambda 6716 + \lambda 6731\)])) ratio. We use the PyNeb tool [16] - a PYTHON package which computes emission lines using an n-level atom approach. It should be noted that this technique will only be sensitive to emitting gas which is of the order of \(10^4\) K due to the abundance of S\textsuperscript{+}; at higher temperatures the sulphur is more highly ionized and at lower temperatures it is atomic. We obtain \(n_e \approx 320 - 400\) [cm\(^{-3}\)] and \(T_e \approx 8000 - 10000\) [K]; indicating a dense, cooling post-shock recombination layer, as expected.
Figure 4. A BPT-diagram. The red dot shows the volume-weighted mean line ratio from our simulation, it moves from right to left as a function of time. Two reference lines are plotted which distinguish between H\textsc{ii} region-dominated and AGN-dominated emission from galaxies; dotted from [15] and dashed from [14]. The coloured line shows the expected line ratios from a parcel of gas at a given temperature in collisional ionization equilibrium. The colour bar shows the temperature.

Combining these results with the fact that the SNR has a diameter of approximately 40 pc (see Fig. 1), one may calculate the energy of the explosion from the following equation:

\[ E = 5.5 \times 10^{43} n_e D^3 \text{ ergs}, \]  

where \( n_e \) is the electron density in cm\(^{-3} \) and D is the SNR diameter in parsec [17]. This results in \( E \approx 1.1 \times 10^{51} - 1.4 \times 10^{51} \text{ erg} \). This is comparable to energies estimated in observations and is consistent with the energy which is injected into the simulation, \( 10^{51} \text{ erg} \). In this particular case we have an error of about 40\%, but the diameter can also be a factor that adds inaccuracy in this calculation (after all, our SNR is clearly not spherically symmetric, see Fig. 1), so some more statistical data is needed to draw a conclusion and accuracy of the method.

In addition to determining these quantities, one may also estimate the shock velocity and magnetic field strength using 1D radiative shock models. We compare our mean line ratios from figure 4 with a grid of models from [1]. We find that the best fit is with models with a shock velocity of 400–475 [km s\(^{-1} \)] and an extremely weak magnetic field. This is a reasonable estimate of the true shock velocity, and the magnetic field value is consistent with our simulations.

5. Conclusions
We have developed a post-processing module for the FLASH code, which uses the updated collision data from MAPPINGS V to reproduce realistic emission maps of simulated supernova remnants. We investigate the following line ratios: [O\textsc{iii}] (\( \lambda 5007 \))/H\textsc{\( \alpha \)}, [S\textsc{ii}] (\( \lambda 6717 \))/(\( \lambda 6731 \)),
Figure 5. Example of emission map (projection) at time 0.26 Myr after the SN event. Left: S[II] (λ6731); right: Hα.

[SII] (λ6731)/Hα, [NII] (λ6583)/Hα, [OIII] (λ5007)/Hβ, and find them to be consistent with observations. We show that our SNR does not appear distinct in a BPT plot, but lies in the boundary region between AGN and HII region-dominated emission. Furthermore, using [SII] lines we calculate a mean electron density of $350 \pm 50$ cm$^{-3}$ and an electron density of $T_e = 8000 - 10000$K. This is consistent with observations and shows the presence of a dense, cooling post-shock recombination layer in the SNR. Using the calculated electron density we estimate the initial supernova energy and find values of $E \approx 1.1 \times 10^{51} - 1.4 \times 10^{51}$ erg, consistent with the energy deposited in the simulation, $10^{51}$ erg. In addition, we use shock models to estimate the shock velocity and find a value of $400 - 475$ km s$^{-1}$. So far, we only make a weak judgment whether the obtained parameters correlate with the assumed ones. In order to draw a conclusion about the accuracy of each method we need to investigate more statistical data.

The pipeline we produced allows for a comparison with real optical observations (e.g. [23], [4], [19]); here we presented a line ratio analysis while in future we will present a detailed morphological study focusing on the formation and evolution of the bright optical filaments seen in figure 4. We also want to study the effect of projecting the 3D data on the appearance of the filaments (for example, as in work [12]). While this work has focused on the optical emission, we will extend this comparison to higher energies such as the X-rays in the future. Combining X-ray data with other energy bands helps to better understand the physics of SNR shocks and constrain the physical parameters. We wish to test these diagnostics and propose new ones.

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