A new ionisation network and radiation transport module in PLUTO

Kartick C. Sarkar,1* Amiel Sternberg2,3,4 and Orly Gnat 1
1Racah Institute of Physics, The Hebrew University of Jerusalem, 91904, Israel
2School of Physics and Astronomy, Tel Aviv University, Ramat Aviv, 69978, Israel
3Centre for Computational Astrophysics, Flatiron Institute, 162 5th Avenue, 10010, New York, NY, USA
4Max-Planck-Institut fur Extraterrestrische Physik (MPE), Giessenbachstr., 85748, Garching, FRG

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ABSTRACT
We introduce a new general-purpose time-dependent ionisation network (IN) and a radiation transport (RT) module in the magneto-hydrodynamic (MHD) code PLUTO. Our ionisation network is reliable for temperatures ranging from $5 \times 10^3$ to $3 \times 10^6$ K, and includes all ionisation states of H, He, C, N, O, Ne, Mg, Si, S and Fe making it suitable for studying a variety of astrophysical scenarios. Radiation loss for each ion-electron pair is calculated using CLOUDY -17 data on-the-fly. Photo-ionisation and charge exchange are the chemical heating mechanisms. The IN is fully coupled to the radiation transport module over a very large range of opacities at different frequencies. The RT module employs a method of short characteristics assuming spherical symmetry. The radiation module requires the assumption of spherical symmetry, while the IN is compatible with full 3D. We also include a simple prescription for dust opacity, grain destruction, and the dust contribution to radiation pressure. We present numerical tests to show the reliability and limitations of the new modules. We also present a post-processing tool to calculate projected column densities and emission spectra.

Key words: methods: numerical – radiative transfer – ISM: HII regions

1 INTRODUCTION
Electromagnetic line and continuum radiation from ionised plasma are critical diagnostic probes of the underlying physical mechanisms operating in astrophysical environments. Modelling radiation transport is therefore an important ingredient in astrophysical plasma simulations. Most hydrodynamic plasma models focus on the kinetic and thermal conditions, but with less attention on the actual ionisation states of the heavy element constituents that enable dynamically important energy losses (Cunningham et al. 2005; Stone et al. 2008; Jiang et al. 2012; Rosdahl et al. 2013). The ionisation states are often assumed to be distributed in equilibrium configurations depending only on the local temperature, and/or density of the gas. Examples of such assumptions include temperature dependent collisional ionisation equilibrium (CIE), or density dependent photo-ionisation equilibrium (PIE) in an externally set radiation field. However, equilibrium is valid only when the plasma has enough time to fully respond to changes in the thermal energies or radiation fields. For CIE this requires that the ionisation and recombination timescales, $\tau_{\text{ion}}$ and $\tau_{\text{rec}}$, are much smaller than the time-scale to change the internal energy $\tau_{\text{int}}$. If not, the plasma may be under- or over-ionised, depending on the time-scale-ratio, and the thermal evolution.

For example, for shock heated gas with a temperature $\sim 10^5$ K the radiative cooling time is

$$\tau_{\text{cool}} \sim \frac{1.5 n_0 k_B T}{n_0^2 \Lambda(T, Z)},$$

while the recombination time for a given ion, $i$, is

$$\tau_{\text{rec},i} \sim \frac{1}{n_0 \alpha_i(T)}$$

where, $\alpha_i(T)$ is the total (radiative + dielectronic) recombination rate coefficient. The ratio between the cooling and recombination times is then,

$$\frac{\tau_{\text{cool}}}{\tau_{\text{rec},i}} \sim \frac{1.5 k_B T \alpha_i(T)}{\Lambda(T, Z)},$$

which is independent of density. For C VI$\rightarrow$C V the timescale-ratio is $\sim 0.18$ ($\alpha_{\text{CVI}} = 3.5 \times 10^{-12}$ s$^{-1}$ and $\Lambda(5\times) = 4 \times 10^{-22}$ erg s$^{-1}$ cm$^3$). Therefore, C v will be over-abundant compared to CIE. Clearly, there is a need to consider the time evolution of a non-equilibrium ionisation (NEI) network in addition to the hydrodynamic variables in such cases. Many authors have studied the isochoric/isobaric cooling of a hot gas from $t \sim 10^5$ K to $10^4$ K and shown that the time-dependent ion fractions for ions can differ by orders of magnitude (which in turn affect gas cooling) indicating the importance of the non-equilibrium calculations (Kafatos 1973; Shapiro & Moore 1976; Schmutzler & Tscharnuter 1993; Gnat & Sternberg 2007; Oppenheimer & Schaye 2013; Gnat 2017).

Observationally, the presence of non-equilibrium plasma has

* E-mail: sarkar.kartick@mail.huji.ac.il, kartick.c.sarkar100@gmail.com

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been shown in many environments. Studies including Becker et al. (1980); Claas et al. (1989); Brinkmann (1999); Bamba et al. (2016); Suzuki et al. (2018) found evidence for under-ionised/over-ionised plasma in the X-ray spectrum of young (≤ 2000 yr) SN remnants. Corresponding simulations of the supernovae bubbles also show significant effects of the NEI on observable ions (Hamilton et al. 1983; Shull 1983; Itoh et al. 1988; Slavin & Cox 1992; Slavin et al. 2015; Zhang et al. 2019). Non-equilibrium effects have also been attributed to the non-detection of N v compared to O vi or failure of a CIE fit in the galactic winds (Breitschwerdt & Schmidt 1999; Breitschwerdt et al. 2003; Chisholm et al. 2018; Gray et al. 2019), excess X-ray background (Breitschwerdt & Schmidt 1994), lack of C iv and N v in the local bubble (de Avillez & Breitschwerdt 2012) and the missing baryons in the warm-hot ionised medium (WHIM) in the intergalactic medium (IGM) (Yoshikawa et al. 2003; Cen & Fang 2006; Bertone et al. 2008).

Numerically there have been several considerations of non-equilibrium ionisation effects. Some of the codes (Kafatos 1973; Shapiro & Moore 1976; Schmidt & Tscharnuter 1993; Gnat & Sternberg 2007; Bradshaw 2009; Gnat et al. 2017) only studied the temporal evolution of the ion of a plasma that did not involve spatial dynamics. One approximate method to combine spatial dynamics with the ionisation network is to calculate the cooling and heating rates based on isochoric or isobaric evolution and then use these tables in a full hydro calculation (Sutherland et al. 2003; Vasiliev 2013). More comprehensive 1D steady state codes have been developed to include a self consistent ionisation network that evolves with fluid dynamics. Among them, Shull & McKee (1979); Allen et al. (2008); Gnat & Sternberg (2009) consider a coupling between radiative transfer and the ionisation. However, these models are limited to solving a plane parallel steady state shock for a given shock velocity. Breitschwerdt & Schmidt (1999); Slavin & Cox (1992); Slavin et al. (2015) consider solution in spherical geometry but do not include any radiative transfer.

A popular method of solving the RT problem in a scattering dominated system is to use the Eddington approximation. This is valid when the specific intensity is assumed to be nearly isotropic, or up to a linear dependence on cos(θ) from the direction of propagation (Chandrasekhar 1960; Hummer & Rybicki 1971; Hummer et al. 1973, Rybicki & Lightman 2004). However, this method is inadequate in the optically thin limit as the specific intensity becomes strongly forward peaked. Techniques to overcome this problem is to use a direct flux limiter in the free streaming limit (Levmore & Pomrning 1981) or using M1 closure method (Levermore 1984; Gnedin & Abel 2001; Melon Pakshin & Mignone 2019) in which the second and zeroth moment of specific intensity are connected through an Eddington tensor that works both in optically thick and thin limits. The specific form of the Eddington tensor is, however, chosen in an ad-hoc way. The state-of-the-art method is to use the method of rays to solve for the Eddington tensor at each location and use this tensor for closing the moment equations (Stone et al. 1992; Davis et al. 2012; Jiang et al. 2012).

Full 3D MHD codes typically include either IN or RT but rarely both of them together. The earliest such attempts was made in YGUAUZ (Raga et al. 1999, 2000) which included a small IN and a radiative transfer. Their technique, unfortunately, is suitable for only a limited number of emitting sources and a constant grid spacing. ASTROBEAR (Cunningham et al. 2005, 2009) contains a network of H and He ions but does not consider any RT or metals. ATHENA++ (Stone et al. 2008; Davis et al. 2012; Jiang et al. 2012) contains a state-of-the-art radiative transfer module (privately distributed) but does not consider the IN dynamics. While FLASH-FERVENT (Fryxell et al. 2000; Baczynski et al. 2015), RAMSES-RT (Rosdahl et al. 2013) contain some form of radiative transfer coupled to chemical network, the network only contains few ions/molecules (mostly, H, He, CO etc.) and the metals are assumed to be in photo-ionisation equilibrium. Most of the 3D radiative transfer modules like SKIRT (Baes et al. 2003), SUNRISE (Jonsson 2006), HYPERION (Robitaille 2011) and RADMC-3D (Dullemond et al. 2012), that have the capability of including a full ionisation network and dust using the Monte-Carlo method, can only be used as post-processing tools due to their massively complex physics and, therefore, slower computation speed. Although TURIS-3D (Harries 2000; Bisbas et al. 2015) solves on-the-fly radiative transfer using the Monte-Carlo technique, it assumes an equilibrium chemistry network.

With our aim of combining both the IN and the RT in a single MHD code, we extend the already existing IN of PLUTO (Mignone et al. 2007; Tesileanu et al. 2008) to include all the ionisation states of H, He, C, N, O, Ne, Mg, Si, S and Fe. The network of ionisation states can be shortened if required. Our radiative transfer module uses a discrete ordinate technique (short characteristics) in spherical symmetry where the RT is solved along different rays fixed in space and angles to transport a spectrum. Spherical symmetry enables methods that speed up the calculation. The method of discrete ordinate has been used in some form or other for various purposes ranging from neutrino transport inside a supernova to the neutron transport problem inside nuclear reactors (see for example Hill 1975; Lewis & Miller 1984; Birnboim 2000). This method does not suffer from the challenges of traversing from an optically thin to an optically thick medium or vice versa. With the inclusion of RT, we also include photo-heating, charge exchange heating/cooling in the IN and radiation pressure on the fluid dynamically calculated at each time step.\(^2\)

In the following sections we describe, one by one, the numerical implementation, equations and standard tests to establish that our module is suitable for studying different astrophysical systems. In a companion paper (Sarkar, Gnat & Sternberg, submitted; paper-II) we make use of this tool to study the time evolution of heavy element column densities in (non steady state) expanding supernova remnant.

2 THE EQUATIONS

2.1 The MHD equations

The MHD equations and numerical implementation of the ionisation network are as described in Tesileanu et al. (2008). We added some more ions and extended this network in terms of new reactions which will be shortly discussed. The ionisation module is suitable for the temperature range of \(5 \times 10^3 \leq T \leq 3 \times 10^8 \) K. The lower boundary of the temperature range is set by our exclusion of molecular chemistry and detailed dust physics. The upper limit is arbitrary but is large enough to include many astrophysical regimes. Our module, therefore, can be applied from early phases of SN to ISM physics to ICM/IGM scales.

The MHD equations for the density (\(\rho\)), velocity (\(\vec{v}\)), and mass...
netic field \( \vec{B} = \vec{B}(\sqrt{\pi}) \) in PLUTO are written in conservative forms as

\[
\frac{\partial}{\partial t} \rho + \nabla \cdot \left( \rho \vec{v} \right) = \rho_s \tag{4}
\]

\[
\frac{\partial}{\partial t} (\rho \vec{v}) + \nabla \cdot \left( \rho \vec{v} \otimes \vec{v} - \vec{B} \otimes \vec{B} + \frac{\vec{T}}{\rho} \right) = -\rho \nabla \Phi + \rho \alpha_d \tag{5}
\]

\[
\frac{\partial}{\partial t} (E + \rho \Phi) + \nabla \cdot \left( (E + p) \vec{v} - \vec{v} \otimes \vec{v} - \frac{\vec{B}}{\gamma} \right) = -\nabla \cdot \mathbf{L} + \rho \vec{v} \cdot \vec{a}_r + \nabla \cdot \vec{F}_c \tag{6}
\]

\[
\frac{\partial}{\partial t} \vec{B} - \nabla \times \left( \vec{v} \times \vec{B} \right) = 0 \tag{7}
\]

Here, \( \rho_t = \rho + B^2/2 \) is the total pressure (thermal + magnetic), \( E = p/(\gamma - 1) + \rho v^2/2 + B^2/2 \) is the total energy and \( \gamma = 5/3 \) is the adiabatic index. The source terms, \( \rho_s, \mathbf{H} \) and \( \mathbf{L} \) are the mass injection rate, thermal heating and thermal cooling rates per unit volume, respectively. The thermal heating term usually includes the photo-heating and charge exchange heating, but can include any external heating term too. The radiation force and the conductive flux in Eqn 6, 7 are given by \( \rho \vec{a}_r \) and \( \vec{F}_c \), respectively. All the source terms except \( \rho_s \) are solved using operator splitting. The mass injection rate in the grid is only added as \( \rho_t dt \) after the end of each time step. This implementation requires that the mass be injected at zero velocity. All the details for solving the above equations can be found in Mignone et al. (2007) and Tesileanu et al. (2008) if not mentioned here.

Our module does not track the radiation energy density and, therefore, does not guarantee the conservation of radiation energy density in a Lagrangian element. This implies that the radiation can do mechanical work on the fluid but the fluid does not do any mechanical work on the radiation. To overcome this problem, ideally, we would need to evolve the radiation energy density with time and treat it like a second fluid in the system. We reserve this issue for a future modification of code. Also notice that in the tests mentioned here, we do not consider a magnetic field and therefore any coupling of the magnetic field with the radiation is neglected.

### 2.2 ionisation network

The ionisation network is solved by treating ions as tracer particles inside the fluid but with a non-zero source function. The ion fraction \( X_{k,i} \) of an ion \( i \) of element \( k \) is given by

\[
\frac{\partial}{\partial t} X_{k,i} + \vec{v} \cdot \nabla X_{k,i} = S_{k,i} \tag{8}
\]

where, \( S_{k,i} \), contains the rate of recomposition and recombination of the ion \((k, i)\) and is given as

\[
S_{k,i} = n_e [X_{k,i+1} \alpha_{k,i+1} - X_{k,i} (\xi_{k,i} + \alpha_{k,i}) + X_{k,i-1} \xi_{k,i-1}] - X_{k,i} \Gamma_{k,i} + A_{k,i} \tag{9}
\]

Here, \( n_e \) is the electron density, \( \alpha_{k,i} \) is the total recombination rate for ion \((k, i)\) to \((k, i - 1)\) and \( \xi_{k,i} \) is the total ionisation rate of ion \((k, i)\) to \((k, i + 1)\). \( \Gamma_{k,i} \) is the photo-ionisation rate and \( A_{k,i} \) is the Auger ionisation rate of lower ions to the current ion.

The ionisation and recombination rates also include charge

### 2.3 Cooling and Heating

The radiative cooling term, \( L \) (erg s\(^{-1}\) cm\(^{-3}\)), includes recombination, free-free, and collisionally excited line radiation terms. The total radiation efficiency, \( A_{k,i} \) (erg s\(^{-1}\) cm\(^{-3}\)), for each ion is taken of computed tables from CLOUDY -17 and similar to the ones given in Gnat & Ferland (2012). The total cooling rate for all the ions is given in terms of the electron density, \( n_e \), and ion density, \( n_{k,i} \), as

\[
L = n_e \sum_{k,i} n_{k,i} A_{k,i}(T) \tag{13}
\]

Also, the cooling rates can be easily updated with a newer version of CLOUDY. We stress that this implementation assumes a coronal level population configuration of electrons for each ion.

\[^3\] the factor of \( 1/\sqrt{4\pi} \) is absorbed in the definition of magnetic field in PLUTO to avoid extra computation.

\[^4\] The statistical CT is assumed only for the highly ionised elements considering that such highly ionised ions have so many energy levels available that a mere collision with a neutral atom can cause charge transfer.
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Heating is taken as

\[
\mathcal{H} = \sum_{k,i,s} n_{k,i} \int_{\nu_{\text{HP},k,i}}^{\infty} \frac{4\pi f_\nu (\nu - \nu_{\text{HP},k,i}) \sigma_{\nu,i}^{\text{PI}}}{h \nu} d\nu + \sum_{k,i} n_{k,i} \left( \sum_{\nu_{\text{HI},k,i}} \Delta_{\nu}^{\text{HI}} \sum_{\nu_{\text{HII},k,i}} \Delta_{\nu}^{\text{HII}} \right)
\]  

(14)

Here, the first term is the usual photo-heating term and the second term is the CT heating/cooling term and only considered if charge is transferred with H ions. The recombination or ionisation energy, \( \Delta_{k,i} \), for each CT case is taken from Kingdon & Ferland (1999) following cloudy -17.

2.4 Conduction

We use pre-existing conduction module in pluto . The conductive flux is given as

\[
\dot{F}_c = \frac{F_{\text{sat}}}{F_{\text{sat}} + F_{\text{class}}} F_{\text{class}},
\]

(15)

where, \( F_{\text{class}} \) is the classical Spitzer conductive flux in the absence of magnetic field and \( F_{\text{sat}} = 5 \phi \rho c_s^3 \) is the saturated flux when the temperature gradient scale is smaller than the electron mean free path. When using thermal conduction (so far isotropic), we set \( F_{\text{class}} = 5.6 \times 10^{-7} \pi^5/3 \pi \nabla T \) erg s\(^{-1}\)cm\(^{-2}\) following Spitzer (1956) and \( \phi = 0.3 \) following Cowie & McKee (1977).

2.5 Radiative transfer

Frequency dependent radiative transfer (RT) is solved at the beginning of each source-splitting loop assuming the light crossing time is much shorter than the typical time-scale for the hydrodynamics to change. The RT equation in a spherically symmetric system is then

\[
\frac{\mu}{r^2} \frac{\partial}{\partial r} \left( r^2 \psi(\mu, r, \nu) \right) + \frac{1}{r} \frac{\partial}{\partial \mu} \left( (1 - \mu^2) \psi(\mu, r, \nu) \right) = j_\nu - \alpha_\nu \psi(\mu, r, \nu),
\]

(16)

where, \( r \) is the radius, \( \mu = \cos \theta \), is the cosine of the angle subtended by a ray with the radial direction, \( \psi \) (erg s\(^{-1}\)cm\(^{-2}\)Hz\(^{-1}\)sr\(^{-1}\)) is the specific intensity of a ray, \( \alpha \) (cm\(^{-1}\)) is the absorption coefficient (we will loosely refer to it as opacity throughout the text) and \( j_\nu \) (erg s\(^{-1}\)cm\(^{-2}\)Hz\(^{-1}\)sr\(^{-1}\)) is the emissivity. Notice that we have retained the derivative with respect to the frequency \( \nu \) in the above equation which assumes that all the velocities are non-relativistic so that no energy is transferred across frequency bands. This assumption is particularly justified if the frequency band width (\( \Delta \nu \)) at any frequency (\( \nu \)) is such that \( \Delta \nu \ll \nu / c \), where \( \nu / c \) is the velocity of a fluid element compared to speed of light. Our RT equation is only applicable in systems where scattering in the given frequency range is negligible and \( \alpha \) is purely dominated by absorption. Our equation demands that the emission and absorption coefficients are spherically symmetric and \( \psi \) is axisymmetric about the radial direction.

The absorption coefficient is calculated at each time step at each frequency band as

\[
\alpha_\nu = \sum_{k,i} n_{k,i} \sum_{s} \sigma_{\nu,i,s}^{\text{PI}}.
\]

(17)

For \( j_\nu \), we assume an isotropic collisional equilibrium emissivity which only depends on the total hydrogen density, \( n_H \) and temperature \( T \). This emissivity is obtained from cloudy -17 for a given metallicity of \( Z_{\odot} \) without the presence of any metagalactic radiation field. Thus, while our IN and RT are consistent with each other, the assumption that \( j_\nu (T) \) is an equilibrium emissivity is not fully consistent with the local non-equilibrium ion-fractions. The computation of the non-equilibrium emissivity could be done via iteration since the ion-fractions also partially depend on the emissivity.

2.6 Dust

Dust plays an important role in the interstellar medium, contributing to extinction, and mediating radiation pressure and thermal heating (Trumpler 1930; Dopita & Sutherland 2000; Draine 2011). Although dust absorption or radiation pressure provided by dust is not very significant in a low density medium, it can play a major role at higher densities. For example, for a Strömgren sphere, we can compare the Strömgren radius \((R_{\text{str}})\) and the mean free path \((\lambda_d = 1/n_H \sigma_{\text{ext},d})\) for a photon in a dusty medium, where \( \sigma_{\text{ext},d} \) is the dust extinction cross section per H nuclei. This produces a lower limit to the density above which the dust becomes important

\[
n_H \sigma_{\text{ext},d} \approx 100 \quad 10^{-4} T_d^{-0.84} \sigma_{\text{ext},d} \ll 21
\]

(18)

where, \( \sigma_{\text{ext},d} \approx 1.0 \times 10^{-21} \) cm\(^2\). This means that in molecular clouds with densities \( \gtrsim 10 \) cm\(^{-3}\), extinction and radiation pressure offered by dust will be very important in the ionisation front dynamics (Spitzer Jr. 1998).

To make our code suitable for studies at higher densities, we include a very simple prescription for dust extinction. We consider extinction tables provided by Weingartner & Draine (2001) for \( R_T = 3.1 \) which is very close to the observed dust properties in the Milky-Way\(^5\). This table provides the extinction cross section per H nuclei \((\sigma_{\text{ext},d})\), the albedo \((\omega)\) and the average angle of scattering \((\langle \cos \theta \rangle)\) as a function of frequency. The total extinction, scattering and absorption opacities are, therefore, given as

\[
\begin{align*}
\alpha_{\text{ext},d} &= n_H \omega \sigma_{\text{ext},d} \\
\alpha_{\text{scat},d} &= \omega \sigma_{\text{ext},d} \\
\alpha_{\text{abs},d} &= \alpha_{\text{ext},d} - \alpha_{\text{scat},d}.
\end{align*}
\]

(19)

Now since the scattering can happen at any direction, the opacity to be used for the radiation pressure is not the same as the total extinction opacity. It is given by

\[
\alpha_{\text{pr},d} = \alpha_{\text{abs},d} + (1 - \langle \cos \theta \rangle) \alpha_{\text{scat},d}.
\]

(20)

The total opacity \((\alpha_{\text{gas}} + \alpha_{\text{dust}})\) to be used while solving the radiative transfer is therefore \( \alpha = \alpha_{\text{gas}} + \alpha_{\text{dust},d} \), and for the radiation acceleration \( \alpha_{\text{gas}} + \alpha_{\text{pr},d} \). We do not model the scattered light from the dust as it is mostly in the infrared which is outside our considered frequency range. We also assume that the photo-electron heating from the dust is negligible compared to photo-ionisation heating from the gas and we do not consider dust heating in our code.

Since dust can be easily destroyed in shocks or in a hot medium, we include a simple prescription for dust sputtering from (Draine 2011, eq 25.13). This rate is given as

\[
\frac{da}{dt} = -10^{-6} n_H \mu \text{m yr}^{-1}.
\]

(21)

Although the extinction curve used in this work consists of a mixture of different dust particle sizes, we assume that the dust sputtering

\[\text{(Available at } https://www.astro.princeton.edu/~draine/dust/dustmix.html \text{)}\]
is well represented by a single population of dust particles with initial size of $a = 0.1 \mu m$ (approximately the wavelength for a $10eV$ photon). The actual dust opacity at any later time is then simply multiplied by $(a(t)/0.1 \mu m)^2$ to account for the dust destruction. We emphasise that this is a ‘proof of principle’ aimed at implementing dust opacity rather than an attempt to model a ‘true’ physical description of dust and its interaction with the ISM. We keep these modifications for a future upgrade of the code.

3 NUMERICAL TECHNIQUE TO SOLVE RADIATIVE TRANSFER

We use the method of short characteristics to solve the RT equation in spherical symmetry. In many applications, radiative transfer is important mainly for its influence on dynamics rather than the exact effects on the ionisation of atoms. Our focus is on the ionisation states themselves. In addition, we want accurate solutions even at the transition layers between optically thick and thin regions since these may host rarer ions and reactions. This is why we employ the method of short characteristics (Lewis & Miller 1984).

We solve eq 16 by discretising the $r-\mu$ space in spatial and angular grids represented by $r_i$ and $\mu_j$, respectively. The spatial discretisation is the same as used in solving the hydrodynamics. The angular coordinate is discretised in uniform grids between $\mu = -1$ to $+1$. Use of such an uniform discretisation allows us to avoid the issues encountered in the free streaming limit when the energy preferably flows along $\mu = \pm 1$. While writing the discretised form of eq 16, we use a ‘finite volume’ method which is more accurate in conserving flow of energy between angular/radial bins than the ‘finite element’ method for a given number of bins. To obtain a finite volume-like form we integrate the equation between two grid points. We assume that $J_\sigma$ and $\alpha_\sigma$ are isotropic and remain constant within a radial cell, $\psi$, however, varies linearly in both $r$ and $\mu$ within a single cell. Similar methods have been used previously in different systems from neutron diffusion in nuclear reactors Hill (1975) to neutrino transport inside supernovae Birnboim (2000). These works, however, use a diamond difference scheme (constant $\psi$ between radial/angular cells) which is $O(h^2)$ accurate in estimating $\psi$ at the cell edges, where $h = \alpha_\sigma(r_{i+1} - r_{i-1})/(\Delta[r])$. We assume a linear variation of $\psi$ in both $r$ and $\mu$ directions. This is expected to increase the accuracy of the method to $O(h^3)$ suitable for rays where either optical depth across a cell is high or there is substantial angular variation in intensity (Larsen & Nelson 1982). We also use a better technique for fixing negative intensities as we shall explain.

Integrating the above equation first in the range from $\mu_m$ to $\mu_{m+1}$ and then from $r_i$ to $r_{i+1}$ produces (removing explicit $\nu$ dependence for convenience)$^6$

$$a_{i,m}\psi_{i,m} + b_{i,m}\psi_{i+1,m} + d_{i,m}\psi_{i+1,m+1} + f_{i,m}\psi_{i+1,m+1} = j_i \Delta \mu_m \frac{\Delta V_i}{4\pi}$$

(22)

where, $\Delta V_i = \frac{4\pi}{3}(r_{i+1}^3 - r_i^3)$, $\Delta \mu_m = \mu_{m+1} - \mu_m$ and the time varying coefficients are given as

$$a_{i,m} = -A_m r_i^2 - (1 - \mu_m^2) C_i + \frac{\alpha_i \Delta \mu_m}{2} B_i$$

$$b_{i,m} = A_m r_{i+1}^2 - (1 - \mu_{m+1}^2) C_{i+1} + \frac{\alpha_i \Delta \mu_m}{2} B_{i+1}$$

$$d_{i,m} = \tilde{A}_m r_i^2 + (1 - \mu_m^2) C_i + \frac{\alpha_i \Delta \mu_m}{2} B_i$$

$$f_{i,m} = -\tilde{A}_m r_{i+1}^2 + (1 - \mu_{m+1}^2) C_{i+1} + \frac{\alpha_i \Delta \mu_m}{2} B_{i+1}.$$  

(23)

The constant coefficients are

$$A_m = \frac{\Delta \mu_m}{6} (\mu_{m+1} + 2 \mu_m)$$

$$\tilde{A}_m = -\frac{\Delta \mu_m}{6} (2 \mu_{m+1} + \mu_m)$$

$$B_i = \frac{1}{12 \Delta \mu_i} \left( r_{i+1}^4 - 4 r_i^3 r_{i+1} + 3 r_i^4 \right)$$

$$\tilde{B}_{i+1} = \frac{1}{12 \Delta \mu_{i+1}} \left( 3 r_{i+1}^4 - 4 r_i r_{i+1}^3 + r_i^4 \right)$$

$$C_i = \frac{\Delta \mu_i}{6} (r_{i+1} + 2 r_i)$$

$$\tilde{C}_{i+1} = \frac{\Delta \mu_{i+1}}{6} (2 r_{i+1} + r_i).$$

(24)

For a given emissivity, eq. 22 can be solved by inverting a $(N_r \times N_\mu \times N_r \times N_\mu)$ matrix, but this is time consuming for reasonable numbers of the $r, \mu$ grids. We rather follow a different approach which uses a special analytical solution of equation 16 along $\mu = -1$ and spherical symmetry at the innermost boundary in $r$.

We choose our $\mu$-grids to be symmetric around $\mu = 0$, i.e., $\mu_m = -1, 1, 2, ..., N_\mu/2 - 1, -N_\mu/2, 2, ..., +1$ where the values $\mu_m - N_\mu/2$ have negative values but $\mu_{m+1}$ onward have positive values. We start from the outer boundary, at $i = N_r - 1$ and $m = \mu_0$ to $\mu_{N_\mu}/2$, and specify the background radiation field irradiated on the system as the outer boundary condition. We then solve the RT along $\mu = -1$ where the solution is not dependent on the angular derivative and is given simply as

$$\psi_{i,-1} = \psi_{i+1,-1} \exp(-\alpha_i \Delta r_i) + \frac{j_i}{\alpha_i} \left[ 1 - \exp(-\alpha_i \Delta r_i) \right]$$

(25)

The grid to solve eq 22 is shown in figure 1. The obtained boundary conditions are shown by the green lines and dots. Given this boundary condition and eq 22, we can write down

$$\psi_{i,m+1} = \frac{1}{d_{i,m}} \left( j_i \Delta \mu_m \frac{\Delta V_i}{4\pi} - (a_{i,m} \psi_{i,m} + b_{i,m} \psi_{i+1,m} + f_{i,m} \psi_{i+1,m+1}) \right),$$

(26)

which means that given $\psi_{N_r -2,0} = \psi_{N_r -1,0}$ and $\psi_{N_r -1,1}$ we can determine the value of $\psi_{N_r -2,1}$. This procedure can be applied to obtain $\psi_{i,m}$ for all $i = 0 - (N_r -1)$ and $m = 0 - (N_\mu /2 -1)$. However, it cannot be extended for $m = N_\mu/2$ to $+1$ as we do not have the prior information of the outgoing ray ($\mu > 0$) at the outer boundary. Fortunately, we can apply the spherically symmetric condition at the inner boundary of the sphere, i.e., $\psi_{0,N_r -2} = \psi_{0,N_r -1} = \psi_{0,1}$ and so on. This allows us to write (for the $\mu > 0$ region)

$$\psi_{i+1,m+1} = \frac{1}{f_{i,m}} \left( j_i \Delta \mu \frac{\Delta V_i}{4\pi} - (a_{i,m} \psi_{i,m} + b_{i,m} \psi_{i+1,m} + d_{i,m} \psi_{i+1,m+1}) \right),$$

(27)

which means that given $\psi_{0,N_r/2-1,\mu} = \psi_{1,N_r/2-1,\mu}$ and $\psi_{0,N_r/2} = \psi_{0,1,\mu}$ we can find out the value of $\psi_{1,N_r/2,\mu}$. This method, as before, then can
Figure 1. $r - \mu$ grid to solve radiative transfer equation 22. The green solid line at $i = N_r - 1$ represents the incoming rays (the background), the green line along $\mu = -1$ represents the radially incoming ray for which we have obtained an analytical solution (Eq 25). The green filled circles at $i = 0$ and $m = N_\mu/2$ to $N_\mu - 1$ represent the grids at the inner boundary where the spherically symmetric assumption has been applied to copy the values from $\mu < 0$ rays as indicated by the dashed green lines. The propagation of information in the $\mu < 0$ and $\mu > 0$ region is shown by the blue arrows.

Figure 2. Fixing negative intensity by truestream. The left panel shows the physical geometry whereas, the right panel shows the $r - \mu$ grid structure. An outgoing ray, as an example, has been shown by the solid arrow.

be applied to the rest of the grid. Notice that the propagation of information in this way of solving for the $\psi$ follows the overall direction of photon travel and, therefore, increases the stability of the algorithm (Lewis & Miller 1984). Now, once $\psi$ for all the grids have been calculated, we can find the angular averaged intensity and radiative flux (see section 3.2 and eq 33).

3.1 Fixing negative intensity

An important issue with the above method is that the assumed linear approximation of $\psi$ in $r - \mu$ grid can break down (since the accuracy is only $O(h^3)$), for example, when a ray peaks very sharply only along a single direction, say, $\delta(\mu)$. In such cases, the linear interpolation predicts excess energy flow from a cell to its neighbouring cell which results in an overall negative intensity from the cell. In such cells we no longer accept values given by eq 22, rather use another method to obtain the solution. We refer this as the truestream method. In this method, if a grid point $(r_i, \mu_m)$ faces a negative intensity, we track individual rays from the previous grid to the current grid. This is done in two steps. First, we find the origin of the given ray at the previous grid ($r_{i-1}$ for $\mu_m > 0$ sweep, for example), say $\mu_p$. This value is given as

$$\mu_p = \sqrt{1 - \left(\frac{r_i}{r_{i+1}}\right)^2 \left(1 - \mu_m^2\right)}$$

for $\mu_m < 0$

$$= \sqrt{1 - \left(\frac{r_i}{r_{i-1}}\right)^2 \left(1 - \mu_m^2\right)}$$

for $\mu_m > 0$ (28)

The intensity at this angle is then found by simple linear interpolation between the two adjacent grids, $r_{i-1}, \mu_i$ and $r_{i-1}, \mu_h$ (see figure 2) as

$$\psi_p = \frac{1}{\mu_p} [ (\mu_p - \mu_i) \psi_{i-1,h} + (\mu_h - \mu_p) \psi_{i-1,l} ]$$

(29)

Note that $\mu_i$ and $\mu_h$ can be anywhere along the ray vector $\mu_m$ and have to be searched for. Now, once we have found $\psi_p$ at $r_{i-1}$, we can find $\psi_{i,n}$ as

$$\psi_{i,m} = \psi_p \exp(-\alpha_{i-1} x) + \frac{\epsilon_{i-1}}{\alpha_{i-1}} \left[1 - \exp(-\alpha_{i-1} x)\right]$$

(30)

where,

$$x = \frac{\sin(\theta - \theta_p)}{\sin\theta_p} r_i$$

for $\mu_m < 0$

$$x = \frac{\sin(\theta_p - \theta)}{\sin\theta_p} r_i$$

for $\mu_m > 0$ (31)

with $\theta = \cos^{-1}(\mu_m)$ and $\theta_p = \cos^{-1}(\mu_p)$. The advantage of this method is that we recalculate the intensity of that grid in an exact way. Unconditionally applying this method throughout the grid can result in slow down of the code.

The above method can, sometimes, ignore the rays that do not pass through other cells but only migrate from $\mu < 0$ half to $\mu > 0$. Such cases may arise at the very inner radii where $\mu_m < \sqrt{1 - (r_{i-1}/r_i)^2}$ for a ray. In such cases $\mu_m = -\mu_m$ and, therefore,

$$\psi(i,m) = \psi(i, N_\mu - m - 1) e^{-2\mu_i \mu_m \alpha_{i-1}} + \frac{\epsilon_{i-1}}{\alpha_{i-1}} \left(1 - e^{-2\mu_i \mu_m \alpha_{i-1}}\right)$$

(32)

where, $2\mu_i \mu_m$ is simply the path length travelled by the ray in that given cell.

3.2 Intensity and Flux

The angular averaged specific intensity (or the mean intensity) and total flux (radially outwards) at any $r_i$ and $\nu$ can be written as

$$J_i = \frac{1}{2} \int_{\phi=0}^{\phi=2\pi} \int_{\mu=-1}^{\mu=1} \psi \ d\mu = \sum_{m=0}^{N\mu} \frac{\Delta\mu_m}{4\pi} (\psi_m + \psi_{m+1})$$

and

$$F_i = \int_{\phi=0}^{\phi=2\pi} \int_{\mu=-1}^{\mu=1} \psi \ d\mu \ d\phi = 2\pi \int_{\mu=-1}^{\mu=1} \psi \ d\mu$$

$$= 2\pi \sum_{m=0}^{N\mu} (A_m \psi_m - \bar{A}_m \psi_{m+1})$$

(33)

following the same assumption of linear interpolation as before. However, notice that these quantities are, by construction, face centred unlike the cell centred hydrodynamic quantities. We, therefore, use the volume averaged values of the $J$ and $F$ at that cell. It is easy to see from Eq 24 that for any quantity that is assumed to vary linearly within a cell $r_i$ to $r_{i+1}$, the volume averaged values are given
Figure 3. Evolution of H, He, C, N and O ions under isochoric cooling for pure photo-equilibrium (dotted lines), G17 results (dashed lines) and new results (solid lines) for isochorically cooling gas. Left column: for $n_H = 1 \, \text{cm}^{-3}$ and Right column: for $n_H = 10^4 \, \text{cm}^{-3}$. Notice how NEq evolution affects the over-ionisation of certain ions. The difference between G17 and the new results are due to the inclusion of statistical charge transfer for higher ions.
by
\[ J = \frac{3}{r_{i+1}^3 - r_i^3} \left( B_i J_i + B_i J_{i+1} \right) \]
\[ F = \frac{3}{r_{i+1}^3 - r_i^3} \left( B_i F_i + B_i F_{i+1} \right). \] (34)

We use these volume averaged values for the calculation of photo-ionisation rates and radiative force on any cell.

4 TESTS

In this section, first, we show that our ionisation network (IN) and radiative transfer (RT) procedure do work separately and then show how they work together. In all the tests, we used a Solar metallicity as given in Asplund et al. (2009).

4.1 Ionisation network

We test the IN by following a zero dimensional simulation where an initial hot plasma \((T = 5 \times 10^6 \text{ K})\) is allowed to cool isochorically to a floor temperature \((T = 5 \times 10^3 \text{ K})\) in the presence of a metagalactic radiation field taken from Haardt & Madau (2012) (hereafter, HM12) at redshift zero \((z = 0)\). This particular kind of test has been performed several times in the literature as mentioned earlier. The results, however, are somewhat dependent on the atomic data used. In this particular test, we compare our results with Gnat (2017) (hereafter, G17).

Figure 3 shows the evolution of the ion fractions for non-equilibrium isochoric cooling using our code (by solid) and from G17 (dashed lines). Equilibrium ion fractions in the presence of the same metagalactic radiation are shown by dotted lines for reference. At high temperatures \((T \gtrsim 10^6 \text{ K})\), the cooling time is much longer than the ionisation/recombination time, therefore the ions remain in equilibrium. The situation changes at lower temperatures \((T \lesssim 3 \times 10^5 \text{ K})\) when \(\tau_{\text{cool}} < \tau_{\text{rec}}\) and the gas departs from equilibrium. Such non-equilibrium effects are much more prominent at intermediate densities (for example, \(n_H = 1 \text{ cm}^{-3}\), shown in the left column) than at lower densities \((n_H = 10^{-4}\text{ cm}^{-3}\), shown in the right column) due to the presence of ionising photons. At lower densities, the temperature of the plasma plays lesser and lesser role in deciding the ionisation state compared to the ionisation parameter. Therefore for a given strong radiation field, the ionisation fraction remains close to the photo-ionisation equilibrium values, and is less dependent on the temperature change. The heating is also elevated for lower density, but is still low with respect to cooling. For example, the cooling to heating ratio at \(T = 10^5 \text{ K}\) for \(n_H = 1\) is \(\sim 10^{-2}\), whereas, the same ratio for \(n_H = 10^{-4}\) is \(\sim 10^{-2}\) (see figure 4 and also noted in Oppenheimer & Schaye (2013)). The main difference between the new results with G17 is due to the inclusion of statistical charge transfer for ions with charge \(\geq 4+\) which mostly affects \(4+, 5+, \ldots\) and, thereafter, propagated to lower ions. Higher ions \((\geq 5+)\) do not make much difference as these ions are not usually present along with \(\text{H}^+ \) or \(\text{He}^+\) in the plasma.

The effect of non-equilibrium cooling and heating is shown in figure 4. The cooling efficiency (green lines) departs from equilibrium only for temperatures \(\lesssim 6 \times 10^3 \text{ K}\). The difference with respect to the photo-ionisation equilibrium case is between a factor of 2 (near \(\sim 10^5 \text{ K}\)) and a factor of 10 (near \(\sim 10^4 \text{ K}\), i.e. isochoric non-equilibrium cooling is slower than the equilibrium cooling. There is no difference in the cooling efficiencies between G17 and our new results despite the additional charge transfer rate. The heating (shown by red lines), however, is lowered by the introduction of the extra charge transfer at \(\sim 10^4 \text{K}\) for \(n_H = 1 \text{ cm}^{-3}\). This difference is, however, not visible at lower densities (see right panel) where photo-ionisation dominates.

We show the change in ion ratios \(N_{\text{v}}/O\) and \(C_{\text{v}}/O\) with temperature in figure 5. The non-equilibrium ion ratios are quite different in comparison to equilibrium ratios below \(\lesssim 3 \times 10^5 \text{ K}\). As previously demonstrated, the difference between the G17 and new results only appear at \(n_H = 1 \text{ cm}^{-3}\) and \(T < 3 \times 10^6 \text{ K}\). In the new scenario, the ratios can go to very high values as higher ions like \(\text{O}^v\) can now recombine more efficiently through statistical charge transfer.

4.2 Radiative transfer

4.2.1 slanted beam in a sphere

To show that our radiative transfer can accurately track the movement of rays inside the simulation box, we inject i) a delta ray (\(\psi(\mu') = \delta(\mu - \mu')\)) and ii) a Gaussian beam (\(\psi(\mu') \propto \exp\left[-(\mu - \mu')^2/2\omega^2\right]\)) at the outer boundary \((r_0 = 2 \text{ pc})\) of a sphere. Since the outer boundary condition can only be inwards, we choose \(\mu' = -0.9219\) and set \(\omega\) for the Gaussian beam such that the total energy injected is distributed over only the central 3 rays. The raybeam enters the sphere from outside \((\mu < 0)\) and passes through the tangent point \((r_{\text{tan}} = r_0\sqrt{1 - \mu'^2})\) to finally exit via \(r_0, -\mu'\). The track of the raybeam within the sphere is then given as

\[ \mu(r) = \sqrt{1 - \left(\frac{r_0}{r}\right)^2 (1 - \mu'^2)} \] (35)

This analytic form of \(\mu(r)\) has been compared with the obtained intensity track from the simulations in figure 6 where the opacity and emissivity of the sphere is set to be zero. The sphere is discretised in 1024 and 256 grid points along the \(r\) and \(\mu\) directions, respectively.

Figure 6 shows the \(r - \mu\) track of a delta ray (top panel) and a Gaussian beam (bottom panel). The theoretically expected track (eq 35) is shown as the white dotted line in each panel. In both cases, the track of the ray is well reproduced by the simulations except a small discrepancy in the delta ray case. This is because tracking a single ray suffers from limitations due to the linear interpolation method used between the cells. The mismatch of the theoretically predicted line (Eq 35) vs computed smeared intensity curve (red/yellow region in fig 6) for the delta ray also disappears once we increase the angular resolution. The discrepancy also disappears as the energy is distributed among a few rays, as can be seen for the Gaussian beam.

Another issue that is immediately apparent in the top left panel of fig 6 are the negative intensities and corresponding fringes. As explained earlier (sec 3.1), negative intensities arise due to the linear interpolation between the cells and only if the intensity is strongly peaked to only one ray. Since the technique to solve RT (sec 2.5) guarantees energy conservation, a negative intensity in some cells results in excess intensity in nearby rays which creates the fringes. Notice that these artefacts only appear on the outer side (larger radii) of the predicted raybeam. This is understandable as the information only propagates from the bottom-right corner to top left corner for \(\mu < 0\) and from bottom-left to top-right corner for \(\mu > 0\) (see fig 1 and section 2.5).

Fortunately, both the negative intensities and the fringes tend to disappear in the Gaussian beam case as soon as the energy is distributed among several rays. We, in any case, employ our negative
Figure 4. Heating and cooling functions for isochoric cooling in the presence of HM12 \((z = 0)\) radiative. Left panel: for \(n_H = 1\) cm\(^{-3}\) and right panel is for \(n_H = 10^{-4}\) cm\(^{-3}\). The dotted lines show the cooling/heating functions in case of a photo-collisional equilibrium (PE) case, the dashed lines represent a time dependent isochoric cooling (TDP) case from G17 and the solid lines show the new results. The orange line in the right panel shows the heating, \(\mathcal{H}/n_e n_H\) (erg s\(^{-1}\) cm\(^3\)), for our new results to compare with the cooling.

Figure 5. N \(\nu\)O vi vs C \(\nu\)O vi as a function of temperature of the plasma (shown in colour palette). The dotted lines show a photo-collisional equilibrium case, the thick dashed line shows the results from G17 and the thin solid line shows the new results. Left panel is for \(n_H = 1\) cm\(^{-3}\) and Right panel is for \(n_H = 10^{-4}\) cm\(^{-3}\). The ratio evolves as the plasma cools to lower temperatures as indicated by the colour palette.

intensity fixing technique (sec 3.1) and the result is shown in the right column of figure 6. For both the \textit{delta ray} and \textit{Gaussian beam} cases, the negative intensity and fringes almost vanish from the map. The corresponding energy conservation is shown in figure 7 for both the \textit{delta ray} and \textit{Gaussian beam} cases. The figure compares the angular averaged specific intensity for the incoming raybeam \((\mu < 0)\) and the outgoing raybeam \((\mu > 0)\). In an ideal case where the energy of the raybeam is conserved, the averaged intensity for both incoming and outgoing rays should be equal in the absence of any absorbing/emitting medium. This is exactly what we see in Fig 7. Without negative intensity fixing, the angular averaged intensity conserves energy very accurately despite the fringes. With fixing, the energy is conserved very accurately for a \textit{Gaussian beam} but not for the \textit{delta ray}. For the \textit{delta ray}, the energy conservation is not very good at the outer radii when the energy is supposed to be only along a single ray. The conservation is much better once the ray travels slightly inwards.

4.2.2 spherical attenuation

In this test, we exclude radiation from outside the simulation box and assume that the inner boundary \((r = r_c)\) of the spherical grid behaves like a black body surface with brightness \(\psi'\). The outward flux from the central surface is then simply \(\pi r_c \psi'\). We set the rest of the simulation box to have no emissivity and a constant absorption coefficient \(a_0 = 3.7133 \times 10^{-18}\) cm\(^2\) (representing hydrogen at \(T = 10^4\) K, right after Lyman limit). We also perform tests with varying absorption. The results are shown in Fig. 8 and compared with the theoretical curves\(^7\)

\[
F(r) = 2 \pi \psi' \int_{\cos(\theta_c)}^{1} e^{-a(r \xi - \sqrt{r_c^2 - r^2 + \xi^2})} \xi d\xi
\]

where, \(\theta_c = \sin^{-1}(r_c/r)\) is the maximum angle at \(r\) that contains the central source (see Rybicki & Lightman (2004), their Fig

\(^7\) See Appendix B for the derivation.
Figure 6. Expected versus the obtained track of a delta ray (top panel) and a Gaussian beam. The colour shows the sp. intensity. The theoretically expected track is over plotted as the white dots.

Figure 7. Conservation of angular averaged sp. intensity ($J$) along the ray/beam track without neg intensity fixing (left panel) and with negative intensity fixing (right panel). Red represents inwards rays ($\mu < 0$) and blue represents outgoing rays ($\mu > 0$). In most part of the plot red is hidden behind the blue lines implying a very good energy conservation along the ray/beam.
represents a popularly used flux formula, \( \varepsilon_j \) represents the opacity. The open circles represent the simulation results, and the solid lines represent the predicted behaviour of the flux (Eq 36). All the cases have emissivity \( j_0 = 0 \), except the cyan points (see text). The dashed gray curve represents a popularly used flux formula, \( F(r) \approx r^{-2} \exp \left[-\alpha (r - r_c)\right] \), for a radiating surface.

The exponential term appears due to the fact that \( \alpha > 0 \). For \( \alpha = 0 \), the above integration would produce the standard result, \( F(r) = \pi \psi'(r_c/r)^2 \). However, for a non-zero \( \alpha \), one needs to integrate the above equation. The figure shows a good match with the expected curves both at high and low opacities over several orders of magnitude. It is clear that the heated interior of the shell is over-pressurised with respect to the temperature inside the IF due to photo-heating. The heating is not only restricted to the inner region of the IF but also extends beyond the IF. This heating increases the temperature of the background medium from \( 6 \times 10^3 \) K to \( 10^4 \) K before the passage of the IF through it.

The density distribution in the Strömgren sphere is shown in the top panel of figure 9. Despite the photo-heating and the expansion of the IF, the density does not change throughout the sphere except at the very centre and near the IF. The over-pressure central material expands outwards and creates a significant dip in density within central \( \leq 10 \) pc over a sound crossing time-scale of \( \approx 400 \) Kyr. A significant density shell-like feature also appears near the IF containing the swept up material from lower radii. Although this sweeping up does not change the interior density by more that few \%, the shell can contribute to a \( \approx 10\% \) change in the density. It is clear that the heated interior of the shell is over-pressure and will expand to larger radii over sound crossing time-scale much like the \( \text{H} \alpha \) regions considered in literature (Spitzer 1968; Dyson & Williams 1980; Raga et al. 2012). This can cause a significant reduction of the density inside the \( \text{H} \alpha \) region. In the cases where the central source is a stellar cluster, the expansion of the ionised region can even cause the disruption of the parent cloud itself.

We show a more quantitative picture in Fig 10 for the evolution of the IF (taken as the radius where \( X_{\text{HF}} = 0.5 \)) for two cases. In the first case, we switch off the local emission at every cell (but include radiation losses) which means that any photon that is emitted by a recombining plasma is not re-absorbed. This is similar to case A.

Note that the use of the HM12 spectrum at the inner boundary is completely arbitrary. This is just to test the effectiveness of the code and does not imply any realistic physical scenario.
Figure 9. Structural evolution of a Strömgren sphere with time (represented by different colours). Quantities shown are, Hydrogen number density $n_H$ (top panel), temperature (second panel), Hydrogen ionisation fraction, $X_{HI}$ (third panel) and the radial flux (erg s$^{-1}$cm$^{-2}$ Hz$^{-1}$) in a 13.61 – 14 eV band (lowest panel).

Figure 10. Evolution of the ionisation front for an ionising luminosity of $Q = 2.16 \times 10^9$ s$^{-1}$, $n_H = 1.0$. The horizontal lines show the expected radius of the Strömgren sphere and the circles show the IF from the simulation. Blue represents the simulation with zero emissivity, whereas, red shows the case with emissivity turned on.

recombination in an optically thin medium with coefficient $\alpha_A$. In the second case, we turn on the local emission from the plasma, this means that the emitted photons from a recombination can be re-absorbed in the same medium after the recombination. This allows the gas to approach "case B" recombination. The expected sizes of the Strömgren spheres for cases A and B are

$$R_{d,A} = \left(\frac{3 Q}{4 \pi n_H^2 \alpha_A}\right)^{1/3} \approx 83 \text{ pc}$$

$$R_{d,B} = \left(\frac{3 Q}{4 \pi n_H^2 \alpha_B}\right)^{1/3} \approx 98 \text{ pc}$$

(37)

Where we have assumed the temperature of the recombining plasma to be $1.5 \times 10^4$ K following figure 9 for both the cases and $\alpha_A = 4.13 \times 10^{-13} T^{-0.7131}$ cm$^3$ s$^{-1}$ and $\alpha_B = 2.56 \times 10^{-13} T^{-0.8163}$ cm$^3$ s$^{-1}$ (Draine 2011).

Figure 10 shows a good match between the "no-emissivity" model and "case A" (blue). When emissivity is included, the size of the ionised region is smaller than expected for "case B" (red). We speculate that this underestimation of $R_{IF}$ in the $\alpha_B$ case may be for several reasons. Most importantly, the assumption of the case B recombination rate. This recombination rate is important only if the optical depth is $\gg 1$ ('on-the-spot' absorption) unlike the Strömgren sphere where the optical depth is $\sim 1$. The actual recombination rate for a Strömgren sphere, therefore, should be between $\alpha_A$ and $\alpha_B$. Other reasons include the use of band averaged opacities which are weighted by the UV background. This may underestimate or overestimate the actual instantaneous opacity depending on the hardness of the local spectrum compared to the UV background. It is also possible that the average temperature inside the ionised bubble for the case when we turn on emission from gas is slightly lower than compared to the zero emissivity case. Additionally, the analytical estimation for the Strömgren sphere depends on the assumption of a constant density, temperature and a sharp boundary for the ionised
sphere. In reality, none of these assumptions are true as can be seen in Fig. 9. In addition, we also estimated Strömgren’s radius by equating the total recombination rates in these two cases with the Q from the central star. These radii are about 106 pc and 118 pc for the case of zero emissivity and full emissivity, respectively. These radii, once used in Strömgren’s radii calculation (Eq 37) also indicate smaller average temperature inside the ionised sphere of the full emissivity case. Hence, we do not consider the underestimation of $R_{\text{st}, B}$ as a drawback to the simulation, rather a success of the test.

5 RESULTS

5.1 Emission spectra

We also present a tool to calculate the emergent spectra from the sphere. Our tool contains a separate script to solve the frequency dependent radiative transport at a given time. The RT method is the same as presented in section 2.5 but with a much higher frequency resolution suitable to include the impact of line emission. The emissivities and opacities required to perform the RT are obtained from CLOUDY -17 by using the local density, temperature and non-equilibrium ion-fractions. The spectra, therefore, may contain signatures of non-equilibrium ionisation for comparison to observations and predictions. The emergent spectra, at $r = 92.5$ pc, where $x_{HI} = 0.95$ at $t = 200$ Kyr, is shown in Fig 11 as a function of impact parameter from the centre of the ionised sphere. The impact parameters ($b$) plotted in this figure are simply converted from the $\mu$ values at that radius since $b = r \sin \theta = r \sqrt{1 - \mu^2}$. The deep black line shows the surface averaged spectra which is same as the angle averaged spectra, $\langle \psi \rangle = \int_0^1 \psi(\mu) \, d\mu = \sum_{m=N_{e}}^{m=N_{\mu}} \frac{3}{2} \left( \psi_{m} + \psi_{m+1} \right)$, in case the remnant is not resolved. The sudden rise in emission and drop thereafter at $\lambda = 1216$ Å is due to the Ly-$\alpha$ emission and scattering (since the scattering is treated as absorption in the first step but is considered as emission in the next time step). The final drop of emissivity happens at $\lambda \leq 912$ Å ($E \geq 13.59$ eV) due to the neutral H absorption.

Figure 11. Synthetic spectra from a Strömgren sphere at $t = 200$ Kyr emerging from a radius of $r = 92.5$ pc for $n_H = 1$, including emission but without including any dust. The colour of the lines represent the impact parameter from the centre of the SN remnants. The deep black spectra is the surface averaged value of all the spectra.

5.2 Effect of dust

To examine the effect of dust absorption we run the simulations in section 4.3 with and without dust at two different densities, $n_H = 1$ and $30$ cm$^{-3}$. The results are shown in figure 12. The figure shows the evolution of the ionisation fronts normalised by their corresponding theoretical Ströngek radius, $R_{\text{st}, B}$ and its establishment time, $t_{\text{est}} = 1/n_H a g(T)$ at $T = 1.5 \times 10^4$ K. The figure clearly demonstrates the effect of dust in denser medium. We find $\approx 30\%$ decrease in the final radius for $n_H = 30$ cm$^{-3}$ compared to only $\approx 13\%$ decrease for $n_H = 1$ cm$^{-3}$. This verifies our discussion regarding the effect of dust in denser medium (Eq 18) and shows that our code is well suited for the studies where dust plays a major role.

6 CONCLUSIONS

We have presented a new module to PLUTO -4.0 that contains an upgraded ionisation network for almost all the important metals, their ionisation states and contribution to cooling. This network is also coupled to a frequency dependent radiative transfer module that calculates the local intensities and flux on-the-fly, assuming spherical symmetry. We also employ some dust physics to account for dust attenuation of the ionising radiation field.

We present several tests to demonstrate the accuracy of the ionisation network and radiative transfer, both individually and when coupled together. This is a major upgrade from the previously existing but smaller ionisation network. Although the radiation transfer module works only in spherical symmetry compared to recent development of 3D radiative transfer module in PLUTO, our RT module is frequency dependent and employs a discrete ordinate technique (short-characteristic) that does not use an ad-hoc Eddington tensor to close the moment equations. Moreover, the employment of the short characteristic method enables us to accurately compute the densities of ions that occur near the boundary between optically thin a thick medium. In addition, the multi-frequency approach enables calculation of very accurate ionisation rates of different elements and their ions without assuming a single opacity/emissivity for all of them.

This module is suitable for studying systems with no radiation
as well as ones which have highly varying radiation field in both time and space. One such example is shown in section 4.3 as a standard test. In a companion paper (Sarkar, Gnat & Sternberg, submitted; paper-II) we use our new tool to study the time evolution of heavy element column densities in (non steady state) expanding supernova bubbles and shells. We hope that this tool will help us understand many unanswered questions in astrophysics and will prove to be a powerful tool to the community to better predict the resulting metal column densities and emission spectra of a numerical simulation.

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**APPENDIX A: RADIATIVE TRANSFER METHOD**

Starting from eq 16, we can remove the differentials by integrating it first in \( \mu \)-direction and then in \( r \) direction within a \( r - \mu \) cell. Integrating it from \( \mu \) to \( \mu_{m+1} \) we obtain

\[
\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \int_{\mu_\text{m}}^{\mu_{m+1}} \mu \, d\mu \right) = \frac{1}{r} \int_{\mu_\text{m}}^{\mu_{m+1}} \mu \, d\mu \quad \text{(A1)}
\]

At this stage we assume that \( \psi \) is linear between any \( \mu_m \) and \( \mu_{m+1} \), i.e.

\[
\psi(\mu) = \frac{\psi_{m+1} - \psi_m}{\mu_{m+1} - \mu_m} (\mu - \mu_m) + \psi_m
\]

\[
= \frac{\psi_{m+1} - \psi_m}{\mu_{m+1} - \mu_m} + \frac{\psi_m}{\mu_{m+1} - \mu_m} (\mu_m - \mu) \quad \text{(A2)}
\]

Now we can write down different moments of \( \psi \) as

\[
\int_{\mu_\text{m}}^{\mu_{m+1}} \psi \, d\mu = A_m \psi_m - \bar{A}_m \psi_m + 1
\]

\[
\int_{\mu_\text{m}}^{\mu_{m+1}} \mu \, d\mu = A_m \mu_m + \bar{A}_m \psi_m + 1
\]

where,

\[
\Delta \mu_m = \mu_{m+1} - \mu_m
\]

\[
A_m = \frac{\Delta \mu}{6} (\mu_m + 2\mu_m)
\]

\[
\bar{A}_m = -\frac{\Delta \mu}{6} (2\mu_{m+1} + \mu_m)
\]

The RTE then becomes

\[
\frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 (A_m \psi_m - \bar{A}_m \psi_m+1) \right] + \frac{1}{r} \int_{\mu_\text{m}}^{\mu_{m+1}} \left( (1 - \mu_{m+1}) \psi_{m+1} - (1 - \mu_m) \psi_m \right) d\mu = -\alpha \frac{\Delta \mu}{2} (\psi_{m+1} + \psi_m) + j \Delta \mu
\]

\[
\Rightarrow \frac{\partial}{\partial r} \left[ r^2 (A_m \psi_m - \bar{A}_m \psi_m+1) \right] + \left( (1 - \mu_{m+1}) \psi_{m+1} - (1 - \mu_m) \psi_m \right) = -\alpha \frac{\Delta \mu}{2} \psi_m + j \Delta \mu r^2
\]

We can now continue to use this method and integrate the above equation between two radial grids \( r_i \) and \( r_{i+1} \) assuming that \( \psi \) can be linearly interpolated between the radial grids too. The moments are

\[
\int_{r_i}^{r_{i+1}} r^2 \psi \, dr = B_i \psi_i + B_{i+1} \psi_{i+1}
\]

\[
\int_{r_i}^{r_{i+1}} r \psi \, dr = C_i \psi_i + C_{i+1} \psi_{i+1}
\]

**APPENDIX B: FLUX FROM A BLACK BODY**

Let us consider a spherical backbody of radius \( r_c \) and surface brightness \( \psi' \) is located at \( r = 0 \). The sphere thus subtends and angle \( \theta_c = \sin^{-1}(r_c/r) \) at any distance \( r \) from the centre. Now the intensity received at \( r \) from an angle \( \theta \) and \( \theta + d\theta \) travels a distance

\[
r' = r \cos \theta - \sqrt{r^2 - r^2 \sin^2 \theta}
\]

(see figure B1). The specific intensity
received from this angle, therefore, is $\psi' \exp(-ar')$, where $a$ is the absorption coefficient of the medium. Hence, the total flux at $r$ is

$$F(r) = \int_0^{2\pi} d\phi \int_0^{\theta_c} \psi' \exp[-ar'] \cos \theta \sin \theta d\theta$$

$$= 2\pi \psi' \int_0^{\theta_c} \exp \left[-a \left( r \cos \theta - \sqrt{r^2 - r^2 \sin^2 \theta} \right) \right] \cos \theta \, d(\cos \theta)$$

$$= 2\pi \psi' \int_{\cos(\theta_c)}^{1} \exp \left[-a \left( r \xi - \sqrt{r^2 - r^2 + r^2 \xi^2} \right) \right] \xi \, d\xi \quad \text{(B1)}$$

This equation reproduces the standard results $F(r) = \pi \psi'(r_c/r)^2$ for $a = 0$ but has to be integrated numerically for any $a > 0$. This is also the reason why a direct method to compute the radiative transfer using this technique is computationally expensive.

**APPENDIX C: TABLES USED**

The frequency bands considered in our computation is identified by its left edge and right edge. We choose our frequency bands carefully so that the bands recognise the ionisation edges. For example, near the H ionisation edge, we choose our band to extend only from 13.58 eV to 13.61 eV to make sure that the edge is recognised and so that the emissivities and opacities near the edge is treated properly.

### Table C1. Frequency bands (left column) and their central values (right column) considered in this paper. The middle column shows the averaged UV background (such that the total energy in a band remains constant) from HM12 ($z = 0$) for reference.

| $h_P \nu$ (eV) | $J_{\nu,uvb}$ (erg s$^{-1}$ cm$^{-2}$ Hz$^{-1}$ sr$^{-1}$) | $h_P \nu \xi$ (eV) |
|----------------|-------------------------------------------------|-----------------|
| 1.000          | 9.6478e-21                                     | 3.000           |
| 5.000          | 1.3389e-21                                     | 6.570           |
| 8.139          | 5.6456e-22                                     | 8.154           |
| 8.169          | 3.8152e-22                                     | 9.259           |
| 10.349         | 1.6254e-22                                     | 10.364          |
| 10.379         | 1.3201e-22                                     | 10.814          |
| 11.249         | 9.5417e-23                                     | 11.264          |
| 11.279         | 3.6504e-23                                     | 12.429          |
| 13.579         | 8.2525e-24                                     | 13.594          |
| 13.609         | 7.7788e-24                                     | 13.804          |
| 13.998         | 7.3787e-24                                     | 14.498          |
| 14.998         | 6.3202e-24                                     | 15.998          |
| 16.998         | 5.0948e-24                                     | 18.498          |
| 19.998         | 3.8055e-24                                     | 22.288          |
| 24.577         | 2.5129e-24                                     | 24.593          |
| 24.608         | 3.1698e-24                                     | 24.802          |
| 24.998         | 2.8943e-24                                     | 25.997          |
| 26.997         | 2.1110e-24                                     | 31.047          |
| 35.097         | 1.3758e-24                                     | 35.116          |
| 35.137         | 1.1388e-24                                     | 41.464          |
| 54.363         | 6.8136e-25                                     | 54.413          |
| 54.463         | 6.1679e-25                                     | 57.229          |
| 59.992         | 5.3038e-25                                     | 69.992          |
| 79.992         | 4.5026e-25                                     | 89.992          |
| 99.988         | 3.5575e-25                                     | 124.988         |
| 149.984        | 2.5598e-25                                     | 174.984         |
| 199.980        | 1.6667e-25                                     | 249.976         |
| 299.968        | 1.1469e-25                                     | 324.968         |
| 349.964        | 9.8931e-26                                     | 374.964         |
| 399.960        | 8.7015e-26                                     | 449.961         |
| 499.961        | 7.9968e-26                                     | 524.940         |
| 549.961        | 7.7044e-26                                     | 574.940         |
| 599.920        | 7.2500e-26                                     | 649.920         |
| 699.920        | 6.4461e-26                                     | 849.921         |
| 999.880        | 5.3771e-26                                     | 1249.881        |
| 1499.841       | 4.5649e-26                                     | 1749.842        |
| 1999.802       | 4.0462e-26                                     | 2249.762        |
| 2499.763       | -                                               | -               |