ENZO+MORAY: radiation hydrodynamics adaptive mesh refinement simulations with adaptive ray tracing

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ABSTRACT
We describe a photon-conserving radiative transfer algorithm, using a spatially-adaptive ray-tracing scheme, and its parallel implementation into the adaptive mesh refinement cosmological hydrodynamics code ENZO. By coupling the solver with the energy equation and non-equilibrium chemistry network, our radiation hydrodynamics framework can be utilized to study a broad range of astrophysical problems, such as stellar and black hole feedback. Inaccuracies can arise from large time-steps and poor sampling; therefore, we devised an adaptive time-stepping scheme and a fast approximation of the optically-thin radiation field with multiple sources. We test the method with several radiative transfer and radiation hydrodynamics tests that are given in Iliev et al. We further test our method with more dynamical situations, for example, the propagation of an ionization front through a Rayleigh–Taylor instability, time-varying luminosities and collimated radiation. The test suite also includes an expanding H$^\text{II}$ region in a magnetized medium, utilizing the newly implemented magnetohydrodynamics module in ENZO. This method linearly scales with the number of point sources and number of grid cells. Our implementation is scalable to 512 processors on distributed memory machines and can include the radiation pressure and secondary ionizations from X-ray radiation. It is included in the newest public release of ENZO.

Key words: hydrodynamics – radiative transfer – methods: numerical.

1 INTRODUCTION

Radiation from stars and black holes strongly affects their surroundings and plays a crucial role in topics such as stellar atmospheres, the interstellar medium (ISM), star formation, galaxy formation, supernovae (SNe) and cosmology. It is a well-studied problem (e.g. Mathews 1965; Rybicki & Lightman 1979; Mihalas & Mihalas 1984; Yorke 1986); however, its treatment in multidimensional calculations is difficult because of the dependence on seven variables – three spatial, two angular, frequency and time. The non-local nature of the thermal and hydrodynamical response to radiation sources further adds to the difficulty. Depending on the problem of interest, some simplifying assumptions may be made.

An important case was considered by Strömgren (1939) for an ultraviolet (UV) radiation source photoionizing a static uniform neutral medium. When recombinations balance photoionizations, the radius of the so-called H$^\text{II}$ region, $R_\text{e} = \left(\frac{3N_\gamma}{4\pi\alpha_B n_H}\right)^{1/3}$, (1)

where $N_\gamma$ is the ionizing photon luminosity, $\alpha_B$ is the recombination rate and $n_H$ is the ambient hydrogen number density. Furthermore, he found that the delineation between the neutral and ionized medium to be approximately the mean free path of the ionizing radiation. His seminal work was expanded upon by Spitzer (1948, 1949, 1954) and Spitzer & Savedoff (1950) who showed that the ionizing radiation heated the medium to $T \sim 10^4$ K. If the density is equal on both sides of the ionization front (I-front), then this overpressurized region would expand and drive a shock outwards (e.g. Oort 1954; Schatzman & Kahn 1955). These early works provided the basis for the modern topic of radiation hydrodynamics of the ISM. A decade later, the first radiation hydrodynamical numerical models of H$^\text{II}$ regions in spherical symmetry and plane-parallel I-fronts were developed (e.g. Mathews 1965; Hjellming 1966; Lasker 1966). They described the expansion of the I-front and the evolution of its associated shock wave that carries most of the gas away from the source. At the same time, theoretical models of I-fronts matured and were classified by Kahn (1954) and Axford (1961) as either R-type (rare) or D-type (dense). In R-type fronts, the ionized gas density is higher than the neutral gas density, and in D-type fronts, the opposite is true. R-type fronts travel supersonically with respect to the neutral gas, whereas D-type fronts are subsonic. Furthermore ‘weak’ and ‘strong’ R-type fronts move supersonically and...
subsonically, respectively, with respect to the ionized gas. The same terminology conversely applies to D-type fronts. ‘Critical’ fronts are defined as moving exactly at the sound speed. These works established the evolutionary track of an expanding H II region illuminated by a massive star in a uniform medium:

(i) Weak R-type. When the star (gradually) starts to shine, the I-front will move supersonically through the ambient medium. The gas is heated and ionized, but otherwise left undisturbed. This stage continues until \( r \sim 0.02 R_s \).

(ii) Critical R-type. As the I-front moves outwards, it begins to slow down because of the geometric dilution of the radiation. It becomes a critical R-type front, which is equivalent to an isothermal shock in the neutral gas.

(iii) Strong and weak D-type. The front continues to slow down, becoming a strong D-type front, and then a critical D-type front. From this point onwards, it moves subsonically with respect to the ionized gas, that is, a weak D-type front. Thus, sound waves can travel across the I-front and form a shock. The I-front detaches from the shock, putting the shock ahead of the I-front.

(iv) Expansion phase. After the shock forms, the H II region starts to expand, lowering the interior density and thus the recombination rates. This increases the number of photons available for ionizing the gas. The sphere expands until it reaches pressure equilibrium with the ambient medium at \( r \sim 5R_s \).

In the 1970s and 1980s, algorithmic and computational advances allowed numerical models to be expanded to two dimensions, mainly using axisymmetry, to simplify the problem (e.g. Bodenheimer, Tenorio-Tagle & Yorke 1979; Sandford, Whitaker & Klein 1982; Yorke, Tenorio-Tagle & Bodenheimer 1983). One topic that was studied extensively was champagne flows. Here the source is embedded in an overdense region and the H II region escapes from this region in one direction. The interface between the ambient and dense media was usually set up to be a constant pressure boundary. When the I-front passes this boundary, the dense, ionized gas is orders of magnitude out of pressure equilibrium as the temperatures on both sides of the initial boundary are within a factor of a few. In response, the gas is accelerated outwards in this direction, creating a fan-shaped outflow.

Only in the past 15 years, computational resources have become large enough, along with further algorithmic advances, to cope with the requirements of three-dimensional calculations. There are two popular methods to solve the radiative transfer equation in three dimensions:

(i) Moment methods. The angular moments of the radiation field can describe its angular structure, which are related to energy, flux and radiation pressure (Auer & Mihalas 1970; Norman, Paschos & Abel 1998). These have been implemented in conjunction with short characteristics (Stone, Mihalas & Norman 1992, two-dimensional), with long characteristics (Finlator, Özel & Davé 2009), with a variable Eddington tensor in the optically-thin limit (Gnedin & Abel 2001; Petkova & Springel 2009) and with an M1 closure relation (González, Audit & Huynh 2007; Aubert & Teyssier 2008). Moment methods have the advantage of being fast and independent of the number of radiation sources. However, they are diffusive and result in incorrect shadows in some situations.

(ii) Ray tracing. Radiation can be propagated along rays that extend through the computational grid (e.g. Abel, Norman & Madau 1999; Razoumov & Scott 1999; Ciardi et al. 2001; Sokasian, Abel & Hernquist 2001; Alvarez, Bromm & Shapiro 2006a; Mellema et al. 2006; Rijekhorst et al. 2006; Whalen & Norman 2006; Krumholz, Stone & Gardiner 2007b; Trac & Cen 2007; Paardekooper, Kruij & Icke 2010) or particle set (e.g. Susa 2006; Johnson, Greif & Bromm 2007; Altay, Croft & Pelupessy 2008; Pawlik & Schaye 2008, 2011; Hasegawa, Umemura & Susa 2009). In general, these methods are very accurate but computationally expensive because the radiation field must be well sampled by the rays with respect to the spatial resolution of the grid or particles.

Until the mid-2000s, the vast majority of the three-dimensional calculations were performed with static density distributions. One example is calculating cosmological reionization by the post-processing of density fields from N-body simulations (Ciardi et al. 2001; Sokasian et al. 2001; Iliev et al. 2006a, 2007; McQuinn et al. 2007). Any hydrodynamical response to the radiation field was thus ignored. Several radiative transfer codes were compared in four purely radiative transfer tests in Iliev et al. (2006b, hereinafter RT06). Only recently has the radiative transfer equation been coupled to the hydrodynamics in three dimensions (e.g. Krumholz et al. 2007a). In the second comparison paper (Iliev et al. 2009, hereinafter RT09), results from these radiation hydrodynamics codes were compared. Even more rare are ones that couple it with magnetohydrodynamics (MHD) (e.g. Krumholz et al. 2007b). The tests in RT06 and RT09 were kept relatively simple to ease the comparison.

In this paper, we present our implementation, \( \text{ENZO} + \text{MORAY} \), of adaptive ray tracing (Abel & Wandelt 2002) in the cosmological hydrodynamics adaptive mesh refinement (AMR) code \( \text{ENZO} \) (Bryan & Norman 1997; O’Shea et al. 2004). The radiation field is coupled to the hydrodynamics solver at small time-scales, enabling it to study radiation hydrodynamical problems. We have used this code to investigate the growth of an H II region from a 100-M\(_{\odot}\) Population III (Pop III) star (Abel, Wise & Bryant 2007), the early stages of reionization from Pop III stars (Wise & Abel 2008a), the radiative feedback on the formation of high-redshift dwarf galaxies (Wise & Abel 2008b; Wise et al. 2010), UV radiation escape fractions from dwarf galaxies before reionization (Wise & Cen 2009), the negative radiative feedback from accreting Pop III seed black holes (Alvarez, Wise & Abel 2009) and the radiative feedback in accreting supermassive black holes (Kim et al. 2011). We have included \( \text{ENZO} + \text{MORAY} \) in the latest public release of \( \text{ENZO} \) and it is also coupled with the newly added MHD solver in \( \text{ENZO} \) (Wang & Abel 2009).

We have structured this paper as follows. In Section 2, we describe the mathematical connections between adaptive ray tracing and the radiative transfer equation. Furthermore, we detail how physics other than photoionization and photoheating are included. We then derive a geometric correction factor to any ray-tracing method to improve accuracy. We end the section by describing a new computational technique to approximate an optically-thin radiation field with ray tracing and multiple sources. In Section 3, we cover the details of our radiation hydrodynamics implementation in \( \text{ENZO} \), specifically (1) the ray-tracing algorithms; (2) coupling with the hydrodynamics solver; (3) several methods to calculate the radiative transfer time-step; and (4) our parallelization strategy. We present our results from the RT06 radiative transfer tests in Section 4. Afterwards in Section 5, we show the results from the RT09 radiation hydrodynamics tests. In Section 6, we expand on these tests to include more dynamical and complex setups to demonstrate the flexibility and high fidelity of \( \text{ENZO} + \text{MORAY} \). Section 7 gives the results from spatial, angular, frequency and temporal resolution measurements.

1 http://enzo.googlecode.com
2 TREATMENT OF RADIATIVE TRANSFER

Radiation transport is a well-studied topic and we begin by describing our approach in solving the radiative transfer equation, which in comoving coordinates (Gnedin & Ostriker 1997) is

$$\frac{1}{c} \frac{\partial I_\nu}{\partial t} + \frac{\hat{n} \cdot \nabla I_\nu}{\bar{a}} - \frac{H}{c} \left( \frac{\partial I_\nu}{\partial \nu} - 3I_\nu \right) = -\kappa I_\nu + j_\nu. \quad (2)$$

Here $I_\nu \equiv I(\nu, x, \Omega, t)$ is the radiation specific intensity in units of energy per time $t$ per solid angle per unit area per frequency $\nu$. $H = a/a$ is the Hubble constant, where $a$ is the scalefactor. $\bar{a} = a/a_{em}$ is the ratio of scalefactors at the current time and time of emission. Table 1 lists the symbols used in our treatment of radiative transfer and its implementation into ENZO. The second term represents the propagation of radiation, where the factor $1/\bar{a}$ accounts for cosmic expansion. The third term describes both the cosmological redshift and the dilution of radiation. On the right-hand side, the first term considers the absorption coefficient $\kappa_\nu \equiv \kappa_\nu(x, \nu, t)$ and the second term $j_\nu \equiv j_\nu(x, \nu, t)$ is the emission coefficient that includes any point sources of radiation or diffuse radiation. We neglect any $(\nu/c)$ terms in equation (2) that become important in the dynamic diffusion limit [$k\nu(\nu/c) \gg 1$], where $\nu$ is the characteristic size of the system. This occurs in relativistic flows or very optically thick systems, such as stellar interiors or radiation-dominated shocks (see Krusholz et al. 2007a) for a rigorous derivation that includes $(\nu/c)$ terms to second order.

Solving this equation is difficult because of its high dimensionality; however, we can make some appropriate approximations to reduce its complexity in order to include radiation transport in numerical calculations. Typically time-steps in dynamic calculations are small enough so that $\Delta a / a \ll 1$; therefore, $\bar{a} = 1$ in any given time-step, reducing the second term to $\hat{n} \partial I_\nu / \partial x$. To determine the importance of the third term, we evaluate the ratio of the third term to the second term. This is $H L/c$, where $L$ is the simulation box length. If this ratio is $\ll 1$, we can ignore the third term. For example, at $z = 5$, this ratio is 0.1 when $L = cH(z = 5) = 53$ proper Mpc. In large boxes where the light-time crossing is comparable to the Hubble time, it becomes important to consider the cosmological redshifting and dilution of the radiation. Thus, equation (2) reduces to the non-cosmological form in this local approximation:

$$\frac{1}{c} \frac{\partial I_\nu}{\partial t} + \frac{\hat{n} \cdot \nabla I_\nu}{\bar{a}} = -\kappa I_\nu + j_\nu. \quad (3)$$

We choose to represent the source term $j_\nu$ as point sources of radiation (e.g. stars, quasars) that emit radial rays that are propagated along the direction $\hat{n}$. Next we describe this discretization and its contribution to the radiation field.

2.1 Adaptive ray tracing

Ray tracing is an accurate method to propagate radiation from point sources on a computational grid, given that there are a sufficient number of rays passing through each cell. Along a ray, the radiative transfer equation reads

$$\frac{1}{c} \frac{\partial P}{\partial t} + \frac{\partial P}{\partial r} = -\kappa P, \quad (4)$$

where $P$ is the photon number flux along the ray. To sample the radiation field at large radii, ray tracing requires at least $N_{ray} = 4\pi R^2/\Delta x^2$ rays to sample each cell with one ray, where $R$ is the radius from the source to the cell and $\Delta x$ is the cell width. If one were to trace $N_{ray}$ rays out to $R$, the cells at a smaller radius $r$ would be sampled by, on average, $(r/R)^2$ rays, which is computationally wasteful because only a few rays per cell, as we will show later, provide an accurate calculation of the radiation field.

Table 1. Variable definitions used in Sections 2 and 3.

| Variable | Description |
|----------|-------------|
| $A_{cell}$ | Cell face area |
| $a$ | Scalefactor |
| $C_H$ | Collisional ionization rate of hydrogen |
| $C_{inf}$ | Courant–Friedrichs–Lewy safety factor in the time-step calculation |
| $D_{ray}$ | Distance from the ray segment centre to cell centre |
| $D_{edge}$ | Distance from the ray segment centre to cell edge |
| $dP$ | Photon loss from absorption |
| $dP_C$ | Photon loss from Compton scattering |
| $dP_p$ | Momentum change from radiation pressure |
| $E_{ph}$ | Photon energy |
| $E_I$ | Ionization energy of the absorber |
| $f_c$ | Geometric correction factor |
| $f_{shield}$ | Shielding function for $H_2$ |
| $H$ | Bubble constant |
| $I_\nu$ | Intensity |
| $j_\nu$ | Emission coefficient |
| $k_{ph}$ | Photoionization rate |
| $k_{diss}$ | Photodissociation rate of $H_2$ |
| $L_{pix}$ | Linear width of a HEALPix pixel |
| $I_{H_2}$ | HEALPix level |
| $N_{H_2}$ | Column density of $H_2$ |
| $n_{abs}$ | Number density of the absorber |
| $N_{HEAL}(l)$ | HEALPix pixels on level $l$ |
| $N_{ray}$ | Rays per cell |
| $n_p$ | Photon luminosity |
| $n_x$ | Number density of absorber $x$ |
| $P$ | Photon flux |
| $r$ | Radius |
| $r_{cell}$ | Distance from the radiation source to the cell centre |
| $r_{ray}$ | Distance from the radiation source to the next cell boundary crossing |
| $V_{cell}$ | Cell volume |
| $v_{IF}$ | I-front velocity |
| $x_{0,i}$ | Cell centre coordinates |
| $x_{cell,i}$ | Next cell boundary crossing in the $i$th dimension |
| $x_{src,i}$ | Source position in the $i$th dimension |
| $Y_{\nu}$ | Secondary ionization factors |
| $\alpha_B$ | Case B recombination rate |
| $\Gamma_{ph}$ | Photoheating rate |
| $\Delta x$ | Cell width |
| $\theta_{\phi}$ | Angular resolution in units of rays per cell area |
| $\kappa_\nu$ | Absorption coefficient |
| $\lambda_{mfp}$ | Mean free path |
| $\Omega_{ray}$ | Solid angle associated with a ray |
| $\sigma_{abs}$ | Cross-section of the absorber |
| $\theta_{ray}$ | Angle associated with a ray |
| $\tau$ | Optical depth |
We avoid this inefficiency by utilizing adaptive ray tracing (Abel & Wandelt 2002), which progressively splits rays when the sampling becomes too coarse and is based on HEALPix (Hierarchical Equal Area isoLatitude Pixelization; Górski et al. 2005). In this scheme, the rays are traced along normal directions of the centres of HEALPix pixels, which evenly divides a sphere into equal areas. The rays are initialized at each point source with the photon luminosity (photon s\(^{-1}\)) equally spread across \(N_{\text{pix}} = 12 \times 4^2\) rays, where \(l\) is the initial HEALPix level. We usually find \(l = 0\) or 1 is sufficient because these coarse rays will usually be split before traversing the first cell.

The rays are traced through the grid in a typical fashion (e.g. Abel et al. 1999), in which we calculate the next cell boundary crossing. The ray segment length crossing the cell is

\[
dr = R_0 - \min_{i=1}^{n} \left[ \frac{(x_{\text{cell},i} - x_{\text{src},i})}{\hat{n}_{\text{ray},i}} \right],
\]

where \(R_0, \hat{n}_{\text{ray}}, x_{\text{cell},i}\) and \(x_{\text{src},i}\) are the initial distance travelled by the ray, normal direction of the ray, the next cell boundary crossing in the \(i\)th dimension and the position of the point source that emitted the ray, respectively. However, before the ray travels across the cell, we evaluate the ratio of the face area \(A_{\text{cell}}\) of the current cell and the solid angle \(\Omega_{\text{ray}}\) of the ray:

\[
\Phi_x = \frac{A_{\text{cell}}}{\Omega_{\text{ray}}} = \frac{N_{\text{pix}} (\Delta x)^2}{4\pi R_0^2}.
\]

If \(\Phi_x\) is less than a pre-determined value (usually \(>3\)), the ray is split into four child rays. We investigate the variations in solutions with \(\Phi_x\) in Section 7.2. The pixel numbers of the child rays \(p'\) are given by the ‘nested’ scheme of HEALPix at the next level, that is, \(p' = 4 \times p + [0, 1, 2, 3]\), where \(p\) is the original pixel number. The child rays (1) acquire the new normal vectors of the pixels; (2) retain the same radius as of the parent ray; and (3) get a quarter of the photon flux of the parent ray. Afterwards, the parent ray is discontinued.

A ray propagates and splits until

(i) the photon has travelled \(c \times dp_p\), where \(dp_p\) is the radiative transfer time-step;

(ii) its photon flux is almost fully absorbed (\(>99.9\) per cent) in a single cell, which significantly reduces the computational time if the radiation volume filling fraction is small;

(iii) the photon leaves the computational domain with isolated boundary conditions; or

(iv) the photon travels \(\sqrt{3}\) of the simulation box length with periodic boundary conditions.

In the first case, the photon is halted at that position and saved where it will be considered in the solution of \(I_{\nu}\) at the next time-step. In the next time-step, the photon will encounter a different hydrodynamical and ionization state, hence \(\kappa\), in its path. Furthermore, any time-variations in the luminosities will be retained in the radiation field. This is how this method retains the time-derivative of the radiative transfer equation. The last restriction prevents our method from considering sources external to the computational domain, but a uniform radiation background can be used in conjunction with ray tracing in ENZO-MORAY that adds the local radiation field to the background intensity.

2.2 Radiation field

The radiation field is calculated by integrating equation (4) along each ray, which is done by considering the discretization of the ray into segments. In the following section, we assume the rays are monochromatic. For convenience, we express the integration in terms of the optical depth \(\tau = \int \kappa(r, t) \, dr\) and, for a ray segment,

\[
dr = \sigma_{\text{ph}}(\nu) n_{\text{abs}} \, dr.
\]

Here, \(\sigma_{\text{ph}}\) and \(n_{\text{abs}}\) are the cross-section and number density of the absorbing medium, respectively. We use the cell-centred density in our calculations. Using trilinearly interpolated densities (see Mellema et al. 2006) did not produce improved results. In the static case, equation (4) has a simple exponential analytic solution and the photon flux of a ray is reduced by

\[
dP = P \times (1 - e^{-\tau})
\]

as it crosses a cell. We equate the photoionization rate to the absorption rate, resulting in photon conservation (Abel et al. 1999; Mellema et al. 2006). Thus, the photoionization \((k_{\text{ph}}}\) and photoheating \((\Gamma_{\text{ph}})\) rates associated with a single ray are, respectively,

\[
k_{\text{ph}} = \frac{P (1 - e^{-\tau})}{n_{\text{abs}} V_{\text{cell}} \, dr_p}
\]

and

\[
\Gamma_{\text{ph}} = k_{\text{ph}} (E_{\text{ph}} - E_i),
\]

where \(V_{\text{cell}}\) is the cell volume, \(E_{\text{ph}}\) is the photon energy and \(E_i\) is the ionization energy of the absorbing material. In each cell, the photoionization and photoheating rates from each ray in the calculation are summed and after the ray tracing is complete, these rates can be used to update the ionization state and energy of the cells. Considering a system with only hydrogen photoionizations and radiative recombinations, these changes are very straightforward and are useful for illustrative purposes. The change in neutral hydrogen is

\[
\frac{dn_{\text{H}}}{dt} = \sigma_{\text{ph}} n_{\text{H}} - C_{\text{H}} n_{\text{e}} n_{\text{H}} - k_{\text{ph}},
\]

where \(\sigma_{\text{H}} = 2.59 \times 10^{-13} \text{ cm}^2 \text{s}^{-1}\) is the recombination coefficient at \(10^4\) K in the Case B on-the-spot approximation in which all recombinations are locally reabsorbed (Spitzer 1978) and \(C_{\text{H}}\) is the collisional ionization rate. However, for more accurate solutions in calculations that consider several chemical species, the photoionization rates are terms in the relevant chemical networks (e.g. Abel et al. 1997).

2.3 Geometric corrections

For a ray-tracing method to accurately, that is, without non-spherical artefacts, compute the radiation field, the computational grid must be well sampled by the rays. The main source of potential artefacts is the geometrical difference between the cell and the HEALPix pixel relevant in the angular integration of the intensity over the cell. In this section, we devise a correction scheme to account for these differences. Consider the solid angle \(\Omega_{\text{ray}}\) and photon flux \(P\) associated with a single ray and assume the flux is constant across \(\Omega_{\text{ray}}\). There exists a discrepancy between the geometry cell face and HEALPix pixel when the pixel does not cover the entire cell face, which is illustrated in Fig. 1. This mismatch causes non-spherical artefacts and is most apparent in the optically-thin case, where the area of the pixel is dominant over \((1 - e^{-\tau})\) when calculating \(k_{\text{ph}}\). One can avoid these artefacts by increasing the sampling \(\Phi_x\) to high values (>10), but we have formulated a simple geometric correction to the calculation of the radiation field. This correction is not unique to the HEALPix formalism but can be applied to any type of pixelization.
The contribution to $k_{\text{ph}}$ and $\Gamma_{\text{ph}}$ must be corrected by the covering factor $f_c$ of the pixel with respect to the cell. When the pixel is fully contained within the cell face, $f_c = 1$. Because the geometry of the pixel can be complex with curved edges, we approximate $f_c$ by assuming the pixel is square. The covering factor is thus related to the width of a pixel, $L_{\text{pix}} = R_0 L_{\text{pix}}$, and the distance from the ray-segment mid-point to the closest cell boundary $D_{\text{edge}}$, which is depicted in Fig. 1. To estimate $f_c$, we first find the distance $d_{\text{cento},i}$ from the mid-point of the ray segment to the cell centre $x_{0,i}$ in orthogonal directions,

$$D_{\text{edge}} = \left| R_{0,i} + \hat{n}_i \frac{dr}{2} - x_{0,i} \right|, \quad (12)$$

where $R_{0,i}$ is the distance travelled by the ray in each orthogonal direction. The distance to the closest cell boundary is $D_{\text{edge}} = \frac{dr}{2} - \max_{i=1-3}(D_{\text{edge}})$. Thus, the covering factor is related to the square of the ratio between $L_{\text{pix}}$ and $D_{\text{edge}}$

$$f_c = \left(\frac{1}{2} + \frac{D_{\text{edge}}}{L_{\text{pix}}}\right)^2. \quad (13)$$

One half of the pixel is always contained within the cell, which results in the factor of 1/2. Finally, we multiply $k_{\text{ph}}$ and $\Gamma_{\text{ph}}$ by $f_c$ but leave the absorbed radiation $d\mathcal{P}$ untouched because this would underestimate the attenuation of the incoming radiation. Using $f_c$ calculated like above, the method is no longer photon-conserving. In our implementation, we felt that the spherical symmetry obtained outweighed the loss of photon conservation. However, we show that there are no perceptible deviations from photon conservation in Sections 4.1 and 7.1.

Next, we briefly describe how to retain photon conservation with a geometric correction. Note that we compute $f_c$ by only considering the distances in orthogonal directions. A better estimate would consider the distance between the cell boundary and ray-segment mid-point in the direction between the mid-point and cell centre of $x_{\text{mid}} - x_0$. We find that the method outlined here provides a sufficient correction factor to avoid any non-spherical artefacts and deviations from photon conservation. Furthermore, in principle, the ray should also contribute to any neighbouring cells that overlap with $\Omega_{\text{ray}}$, which is the key to be photon conservative with such a geometric correction.

### 2.4 Optically-thin approximation

In an optically-thin medium, radiation is only attenuated by geometric dilution in the local approximation to equation (2), that is, the inverse square law. With such a simple solution, the tracing of rays is wasteful; however, these rays must be propagated because the medium farther away can be optically thick. Here we describe a method that minimizes the computational work of ray tracing in the optically-thin regime by exploiting this fact. Each ray tracks the total column density $N_{\text{abs}}$ and the equivalent total optical depth $\tau$ traversed by the photon. If $\tau < \tau_{\text{abs}} - 0.1$ after the ray exits the cell, we calculate the photoionization and photoheating rates directly from the incoming ray instead of the luminosity of the source:

$$k_{\text{ph}} = \frac{\sigma_{\text{ph}} P_{\text{ray}}}{d\mathcal{P}_{\text{pix}} r_{\text{ray}}}. \quad (14)$$

Note that the photon number $P$ in the ray has already been geometrically diluted by ray splitting. Here $r_{\text{cell}}$ and $r_{\text{ray}}$ are the radii from the radiation source to the cell centre and where the ray exits the cell, respectively. Thus, the last factor corrects the flux to a value appropriate for the cell centre. The photoheating ray is calculated in the same manner as the general case, $\Gamma_{\text{ph}} = k_{\text{ph}}(E_{\text{ph}} - E_0)$. This should only be evaluated once per cell per radiation source. No photons are removed from the ray. With this method, we only require one ray to travel through each cell where the gas is optically thin, thus reducing the computational expense.

We must be careful not to overestimate the radiation when multiple rays enter a single cell. In the case of a single radiation source, the solution is simple – only assign the cell the photoionization and photoheating rates when $k_{\text{ph}} = 0$. However, in the case with multiple sources, this is no longer valid and we must sum the flux from all optically-thin sources. Only one ray per source must contribute to a single cell in this framework. We create a flagging field that marks whether a cell has already been touched by an optically thin photon from a particular radiation source. Naively, we would be restricted to tracing rays from a single source at a time, if we use a boolean flagging field. However, we can trace rays for 32 sources at a time by using bitwise operations on a 32-bit integer field. For example in C, we would check if an optically-thin ray from the nth source has propagated through cell i by evaluating $(\text{MarkerField}[i] \gg n \& 1)$. If false, then we can add the optically-thin approximation [equation (14)] to the cell and set $(\text{MarkerField}[i] |= (1 \gg n))$ to mark the cell.

### 2.5 Additional physics

Other radiative processes can also be important in some situations, such as the attenuation of the radiation in the Lyman–Werner bands, secondary ionizations from X-ray radiation, Compton heating from scattered photons and radiation pressure. We describe our implementation of these physics next.

#### 2.5.1 Absorption of Lyman–Werner radiation

Molecular hydrogen can absorb photons in the Lyman–Werner bands through the two-step Solomon process, which for the lowest ro-vibrational states already consists of 76 absorption lines ranging from 11.1 to 13.6 eV (Stecher & Williams 1967; Dalgarno & Stephens 1970; Haiman, Abel & Rees 2000). Each of these spectral lines can be modelled with a typical exponential attenuation equation (Ricotti, Gnedin & Shull 2001), but Draine & Bertoldi (1996) showed that this self-shielding is well modelled with the following
relation to the total H$_2$ column density:

\[ f\text{\_shield}(N_{\text{H}_2}) = \begin{cases} 
1 & (N_{\text{H}_2} \leq 10^{14}) \\
(N_{\text{H}_2}/10^{14})^{-0.75} & (N_{\text{H}_2} > 10^{14})
\end{cases} \]

(15)

where \( N_{\text{H}_2} \) is in units of cm$^{-2}$. To incorporate this shielding function into the ray tracer, we store the total H$_2$ column density and calculate the H$_2$ dissociation rate by summing the contribution of all rays:

\[ k_{\text{diss}} = \sum_{\text{rays}} \frac{P \sigma_{\text{LW}} \Omega_{\text{ray}} r^2 \, dr}{A_{\text{cell}} \, dV \, dp}, \]

(16)

where \( \sigma_{\text{LW}} = 3.71 \times 10^{18} \text{ cm}^2 \) is the effective cross-section of H$_2$ (Abel et al. 1997). To account for absorption, we attenuate the photon number flux by

\[ dP = P[f\text{\_shield}(N_{\text{H}_2} + dN_{\text{H}_2}) - f\text{\_shield}(N_{\text{H}_2})], \]

(17)

where \( dN_{\text{H}_2} \) is the H$_2$ column density in the current cell.

2.5.2 Secondary ionizations from X-rays

At the other end of the spectrum, a high-energy (\( E_{\gamma} \gtrsim 100 \text{ eV} \)) photon can ionize multiple neutral hydrogen and helium atoms and this should be considered in such radiation fields. Shull & van Steenberg (1985) studied this effect with Monte Carlo calculations over varying electron fractions and photon energies up to 3 keV. They find that the excitation of hydrogen and helium, and the ionization of He ii are negligible. The number of secondary ionizations of H and He is reduced from the ratio of the photon and ionization energies (\( E_{\gamma}/E_i \)) by a factor of

\[ Y_{\text{H},\text{LH}} = 0.3908(1 - x^{0.4920}x^{1.7592}), \]

(18)

\[ Y_{\text{H},\text{He}} = 0.0554(1 - x^{0.4614}x^{1.6660}), \]

(19)

where \( x \) is the electron fraction. The remainder of the photon energy is deposited into thermal energy that is approximated by

\[ Y_T = 0.9971[1 - (1 - x^{0.2663}x^{1.3163})]\]

(20)

and approaches 1 as \( x \rightarrow 1 \). Thus, in the gas with low electron fractions, most of the energy results in ionizations of hydrogen and helium, and in nearly ionized gas, the energy goes into photoheating.

2.5.3 Compton heating from photon scattering

High-energy photons can also cause Compton heating by the scattering of free electrons. During a scattering, a photon loses \( \Delta E(T_e) = 4kT_e \times (E_{\gamma}/m_e c^2) \) of energy, where \( T_e \) is the electron temperature. For the case of monochromatic energy groups, we model this process by considering that the photons are absorbed by a factor of

\[ dP_c \over P = (1 - e^{-\tau_c})\frac{\Delta E(T_e)}{E_{\gamma}} \]

(21)

which is the equivalent of the photon energy decreasing. Here, \( \tau_c = n_e \sigma_{\text{KN}} dl \) is the optical depth to Compton scattering and \( \sigma_{\text{KN}} \) is the non-relativistic Klein–Nishina cross-section (Rybicki & Lightman 1979). The Compton heating rate is thus

\[ \Gamma_{\text{phot}} = \frac{dP_c}{n_e V_{\text{cell}} dl}, \]

(22)

which has been used in Kim et al. (2011).

2.5.4 Radiation pressure

Another relevant process is radiation pressure, where the absorption of radiation transfers momentum from photons to the absorbing medium. This is easily computed by considering the momentum

\[ dp_{\gamma} = P \frac{E_{\gamma}}{c} \hat{r} \]

(23)

of the absorbed radiation from the incoming ray, where \( \hat{r} \) is the normal direction of the ray. We do not include the radiation pressure on dust currently. The resulting acceleration of the gas because of radiation pressure is

\[ da = \frac{P \delta p_{\gamma}}{dp \rho V_{\text{cell}}}, \]

(24)

where \( \rho \) is the gas density inside the cell. This acceleration is then added to the other forces, for example, gravity, in the calculation in an operator split fashion.

3 NUMERICAL IMPLEMENTATION IN ENZO

In this section, we describe our parallel implementation of the adaptive ray-tracing method into ENZO. ENZO is a parallel block-structured AMR (Berger & Colella 1989) code that is publicly available (Bryan & Norman 1997; O’Shea et al. 2004). First, we explain the programming design of handling the ‘photon packages’ that are traced along the adaptive rays. We use the terms photon packages and rays interchangeably. Next, we focus on the details of the radiation hydrodynamics and then on the importance of correct time-stepping. Finally, we give our parallelization strategy of tracing rays through an AMR hierarchy. This implementation is included in the v2.0 public version of ENZO.

3.1 Programming design

Each photon package is stored in the AMR grid with the finest resolution that contains its current position. The photon packages keep track of the (1) photon flux; (2) photon type; (3) photon energy; (4) time-interval of its emission; (5) emission time; (6) current time; (7) radius; (8) total column density; (9) HEALPix pixel number; (10) HEALPix level; and (11) position of the originating source, totalling 60 (88) bytes for single (double) precision. When ENZO uses double precision for grid and particle positions and time, items (4)–(7) and (11) are double precision.

We only treat point sources of radiation in our implementation; therefore, all base-level photon packages originate from them. As they travel away from the source, they generally pass through many AMR grids, especially if the simulation has a high dynamic range. This is a challenging programming task as rays are constantly entering and exiting grids. Before any computation, the number of rays in a particular grid is highly unpredictable because the intervening medium is unknown. Furthermore, the splitting of parent rays into child rays and a dynamic AMR hierarchy add to the complexity. Because of this, we store the photon packages as a doubly linked list (Abel & Wandelt 2002). Thus, we can freely add and remove them from grids without the concern of allocating enough memory before the tracing commences.

We illustrate the underlying algorithm of the ray-tracing module in ENZO in Fig. 2 and the ray-tracing algorithm is shown in Fig. 3. The module is only called when advancing the finest AMR level. We describe its steps below.
Step 1 – Create $N_{\text{init}}$ new photon packages on the initial HEALPix level from point sources. Place the new rays in the highest-resolution AMR grid that contains the source.

Step 2 – Initialize all radiation fields to zero.

Step 3 – Loop through all AMR grids, tracing any rays that exist in it. For each ray, the following substeps are taken.

Step 3a – Compute the ray normal based on the HEALPix level and pixel number of the photon package with the HEALPix routine `pix2vec_nest`. One strategy to accelerate the computation is to store ray segment paths in memory (Abel & Wandelt 2002; Krumholz et al. 2007b); however, this must be recomputed if the grid structure or point source position changes. We do not restrict these two aspects and cannot employ this acceleration method.

Step 3b – Compute the position of the ray ($r_{\text{cen}} + r \hat{n}$), the current cell coordinates in floating point and its corresponding integer indices. Here $r_{\text{cen}}$ is the position of the point source, $r$ is the distance travelled by the ray and $\hat{n}$ is the ray normal.

Step 3c – Check if a subgrid exists under the current cell. If so, move the ray to a linked list that contains all rays that should be moved to other grids. We call this variable `PhotonMoveList`. Store the destination grid number and level. Continue to the next ray in the grid (Step 3a). We determine whether a subgrid exists by creating a temporary three-dimensional field of pointers that either equal the pointer of the current grid if no subgrid exists under the current cell or equal the child grid pointer that exists under the current cell. This provides a significant speedup when compared to a simple comparison of a photon package position and all of the child grid boundaries. Note that this is the same algorithm used in Enzo when moving collisionless particles to child grids.

Step 3d – Compute the next cell crossing of the ray and the ray segment length across the cell (equation 5).

Step 3e – Compare the solid angle associated with the ray at radius $r + dr$ with a user-defined splitting criterion (equation 6). If the solid angle is larger than the desired minimum sampling, split the ray into four child rays (Section 2.1). These rays are inserted into the linked list after the parent ray, which is subsequently deleted. Continue to the next ray (Step 3a), which will be the first child ray.

Step 3f – Calculate the geometric correction (equation 13), optical depth of the current cell (equation 7) and photoionization and photoheating rates (equations 9 and 10), and add the column density of the cell to the total column density of the ray.

Step 3g – Add the effects of any optional physics modules (Section 2.5) – secondary ionizations from X-rays, Compton heating from scattering and radiation pressure.

Step 3h – Update the current time ($t = t + \Delta t$), photon flux ($P = P + \Delta P$, equation 8) and radius of the ray ($r = r + dr$).

Step 3i – If the photon flux is zero or the total optical depth is large (>20), delete the ray.

Step 3j – Check if the ray has travelled a total distance of $cdP$, in the last time-step. If we are keeping the time-derivative of the radiative transfer equation, halt the photon. If not (i.e. infinite speed of light), delete the photon.

Step 3k – Check if the ray has exited the current grid. If false, continue to the next cell (Step 3b). If true, move the ray to the linked list `PhotonMoveList`, similar to Step 3c. If the ray exits the simulation domain, delete it if the boundary conditions are isolated; otherwise, we change the source position of the ray by a distance $-\text{sign}(n[\text{i}]) \times \text{DomainWidth}[\text{i}]$, where $n$ is the ray normal and $\text{i}$ is the dimension of the outer boundary it has crossed. The radius is kept unchanged. In essence, this creates a ‘virtual source’ outside the box because the ray will be moved to the opposite side of the domain, appearing that it has originated from this virtual source.

Step 4 – If any rays exist in the linked list `PhotonMoveList`, move them to their destination grids and return to Step 3. This requires Message Passing Interface communication if the destination grid exists on another processor.

Figure 2. Flow chart for the overall algorithm of the radiative transfer module in Enzo that illustrates (1) the creation of photon packages; (2) ray tracing; (3) the transport of photon packages between AMR grids; and (4) coupling with the hydrodynamics. The ray-tracing algorithm, which is contained in the 'Trace Rays' is detailed in Fig. 3.
Figure 3. Flow chart for the ray-tracing algorithm for one photon passing through a grid. Note that only one step is needed in the routine to adaptively split rays. The remainder is a typical ray-tracing method.

**Step 5** — If all rays have not been halted (keeping the time-derivative of the radiative transfer equation), absorbed or exited the domain, return to Step 3.

**Step 6** — With the radiation fields updated, call the chemistry and energy solver and update only the cells with radiation, which is discussed further in Section 3.3.

**Step 7** — Advance the time associated with the photons, $t_p$, by the global time-step $\Delta t$ (for its calculation, see Section 3.4). If $t_p$ does not exceed the time on the finest AMR level, return to Step 1.

### 3.2 Energy groups

In our implementation, photon packages are monochromatic, that is, energy groups (Mihalas & Mihalas 1984, chapter 6), and are assigned a photon type that corresponds whether it is a photon that (1) ionizes hydrogen; (2) singly ionizes helium; (3) doubly ionizes helium; (4) has X-ray energy; or (5) dissociates molecular hydrogen (Lyman–Werner radiation). One disadvantage of monochromatic rays is that the number of rays increases with the number of frequency bins. However, this allows for the early termination of rays that are fully absorbed, which are likely to have high-absorption cross-sections (e.g. H I ionizations near 13.6 eV) or a low initial intensity (e.g. He II ionizing photons in typical stellar populations). The other approach used by some groups (e.g. Trac & Cen 2007) is to store all energy groups in a single ray. This reduces the number of the rays generated and the computation associated with the ray tracing. Unless the ray dynamically adjusts its memory allocation for the energy groups as they become depleted, this method is also memory-intensive in the situation where most of the energy groups are completely absorbed but a few groups still have significant flux.

In practice, we have found that one energy group per photon type is sufficient to match expected analytical tests (Section 7.3). For example, when modeling Pop III stellar radiation (e.g. Abel et al. 2007; Wise & Abel 2008b, for hydrogen ionizing radiation only), we have three energy groups – H I, He I and He II – each with energy that equals the average photon energy above the ionization threshold.

### 3.3 Coupling with hydrodynamics

Solving the radiative transfer equation is already an intensive task, but coupling the effects of radiation to the gas dynamics is even more difficult because the radiation fields must be updated on a time-scale such that it can react to radiative heating, that is, the sound-crossing time. The frequency of its evaluation will be discussed in the next section.

**ENZO** solves the physical equations in an operator-split fashion over a loop of AMR grids. On the finest AMR level, we call our radiation transport solver before this main grid loop in the following sequence:
(i) All grids:

(a) Solve for the radiation field with the adaptive ray tracer
(b) Update species fractions and energies for cells with radiation with a non-equilibrium chemistry solver on subcycles (equation 25)

(ii) For each grid:

(a) Solve for the gravitational potential with the particle mesh method
(b) Solve hydrodynamics
(c) Update species fractions and energies for cells without radiation with a non-equilibrium chemistry solver on subcycles (equation 25)
(d) Update particle positions
(e) Star particle formation

(iii) All grids: Update the solution from children grids

Since the solver must be called many times, the efficiency of the radiation solver is paramount. After every radiation time-step, we call the non-equilibrium chemistry and energy solver in ENZO. This solves both the energy equation and the network of stiff chemical equations on small time-steps, that is, subcycles (Anninos et al. 1997). The time-step is

\[
dt = \min \left( \frac{0.1n_e}{|dn_e/dr|}, \frac{0.1n_{hi}}{|dn_{hi}/dr|}, \frac{0.1e}{|de/dr|}, \frac{d_{hydro}}{2} \right),
\]

where \(n_e\) is the electron number density, \(e\) is the specific energy, and \(d_{hydro}\) is the hydrodynamic time-step. This limits the subcycle time-step to a 10 per cent change in either electron density, neutral hydrogen density or specific energy. In simulations without radiation, ENZO calls this solver in an operation-split manner after the hydrodynamics module for grids only on the AMR level that is being solved. In simulations with radiative transfer, the radiation field can change on much faster time-scales than the normal hydrodynamical time-steps.

For example, a grid on level \(L\) might have no radiation in its initial evaluation, but the I-front exists just outside its boundary. Then radiation permeates the grid in the time between \(t_h\) to \(t_h + d_{hi}\), and the energy and chemical state of the cells must be updated with each radiation update to advance the I-front accurately. If one does not update these cells, it will appear that the I-front does not enter the grid until the next hydrodynamical time-step! Visually, this appears as discontinuities in the temperature and electron fraction on grid boundaries. One may avert this problem by solving the chemistry and energy equations for every cell on every radiative transfer time-step, but this is very time-consuming and unnecessary, especially if the radiation filling factor is small.

We choose to dynamically split the problem by cells with and without radiation. In every radiation time-step, the chemothermal state of only the cells with radiation is updated. For the solver subcycling, we replace \(d_{hydro}\) with \(d_r\) in equation (25) in this case. Once the radiative transfer solver is finished with its time-steps, the hydrodynamic module is called and then the chemothermal state of the cells without radiation is updated on a subcycle time-step stated in equation (25).

For cells that transition from zero to non-zero photoionization rates, the initial state that enters into the chemistry and energy solver does not correspond to the current time of the radiation transport solver \(t_{rg}\), but either time \(t_h\) if the grid level is the finest level because its chemothermal state has not been updated or time \(t_h + d_{hi}\) on all other levels. In principle, one could first revert the cell back to time \(t_h\) and then update to \(t_{rg}\) with the chemistry and energy solver if the cell is on the finest level. However in practice, the time-scales in the gas without radiation are small compared to the ionization and heating time-scales when radiation is introduced. Therefore, we do not perform this correction and find that this does not introduce any inaccuracies in both test problems (see Section 4) and real-world applications.

3.4 Temporal evolution

There have been several methods of choosing a maximal time-step to solve the radiation transfer equation while retaining stability and accuracy. We describe several methods to calculate the radiative transfer time-step in this section. With a small enough time-step, the solution is accurate (ignoring any systematic ones), but the solver is slow. Furthermore, for very small time-steps, the photon packages only advance a short distance and they will exist in every \(dx/dp\) cell with radiation and are stored between time-steps, excessively consuming memory. On the shortest time-scale, one can safely set the time-step to the light-crossing time of a cell (Abel et al. 1999; Trac & Cen 2007) but encounters the problems stated above.

If the time-step is too large, the solution will become inaccurate; specifically, I-fronts will advance too slowly, as radiation intensity exponentially drops with a scalelength of the mean free path

\[
\lambda_{mfp} = \frac{1}{n_{abs}a_{abs}}
\]

past the I-front. For example, in our implementation, the chemothermal state of the system remains constant as the rays are traced through the cells. In the case of a single \(H\) region, the speed of the I-front is limited to approximately \(\lambda_{mfp}/d_r\).

3.4.1 Minimizing the neutral fraction change

Another strategy is restricting the neutral fraction to change a small amount, that is, for a single cell,

\[
dr_{P,cell} = \epsilon_{ion} \frac{n_{hi}}{|dn_{hi}/dr|} = \frac{\epsilon_{ion}}{\left| k_{ph} + \sigma_{abs}(C_{H} + \sigma_{B}) \right|}
\]

where \(\epsilon_{ion}\) is the maximum fraction change in the neutral fraction. Shapiro, Iliev & Raga (2004) found that this limited the speed of the I-front. We can investigate this further by evaluating the I-front velocity in a growing Strömgren sphere without recombinations:

\[
N_f = 4\pi R^2 n_{hi} \gamma_{hi} \gamma_{hi}
\]

Using \(k_{ph} = N_f \sigma/4\pi R^2 A_{cell}\) and \(k_{ph} \propto n_{hi}/n_{hi}\), we can make substitutions, respectively, on the left- and right-hand sides of equation (28) to arrive at the I-front velocity \(v_{hi} \propto n_{hi}/R_{hi}\).

We have implemented this method but we only consider cells within the I-front (by experiment, we choose \(\tau > 0.5\)), because we are interested in evolving I-fronts at the correct speed. In the ionized region, the absolute changes in the neutral fraction are small and will not significantly affect the I-front evolution. In other words, \(n_{hi}/(dn_{hi}/dr)\) may be large but \((dn_{hi}/dr) \sim 0\); thus, we can safely ignore these cells when determining the time-step without sacrificing accuracy.

We search for the cell with the smallest \(d_r\) based on equation (27). In principle, one could use this value without modifications as the time-step, but there is considerable noise both spatially and temporally. In order to stabilize this technique, we first spatially smooth the values of \(d_r\) with a Gaussian filter over a 3D cube. Because we only consider the cells within the I-front, we set \(d_r\) on the hydrodynamical time-step outside the front during the smoothing. After we have smoothed \(d_r\), we select the minimum value as \(d_r\). Significant noise in \(d_r\) can exist between time-steps as well.
Because the solution can become inaccurate if the time-step is allowed to be too large, we restrict the next time-step to be less than twice the previous time-step,

$$d_{t+1} = \min(2d_{t}, d_{\text{max}}).$$

(29)

Fig. 4 shows the smooth evolution of $d_p$ in a growing Strömgren sphere when compared to the values of $\min(d_{P,\text{con}})$.

3.4.2 Time-averaged quantities within a time-step

Mellema et al. (2006) devised an iterative scheme that allows for large time-steps while retaining accuracy by considering the time-averaged values $(T, k_{\text{abs}}, n_e, n_{\text{HII}})$ during the time-step. Starting with the cells closest to the source, they first calculate the column density to the cell. Then they compute the time-averaged neutral density for the cell and its associated optical depth, which is added to the total time-averaged optical depth. With these quantities, one can compute a photoionization rate and update the electron density. This process is repeated until convergence is found in the neutral number density. In a test with a Strömgren sphere, they found analytical agreement with $10^{-3}$ less time-steps than a method without time-averaging. Another advantage of this method is the use of pre-calculated tables for the photoionization rates as a function of the optical depth, based on a given spectrum. This minimizes the energy groups needed to accurately sample a spectrum. We are currently implementing this method into ENZO+MORAY.

3.4.3 Physically motivated

A constant time-step is necessary when solving the time-dependent radiative transfer equation in ENZO+MORAY. It should be small enough to evolve I-fronts accurately, as discussed earlier. The time-step can be based on physical arguments, for example, the sound-crossing time of an ionized region at $T > 10^4$ K. To be conservative, one may choose the sound-crossing time of a cell (e.g. Abel et al. 2007; Wise & Abel 2008b). Alternatively, the diameter of the smallest relevant system (e.g. an accretion radius, transition radius to a D-type I-front, etc.) in the simulation may be chosen to calculate the sound-crossing time.

If the time-step is too large, the I-front will propagate too slowly, but it eventually approaches the correct radius at late times (see Section 7.4). This does not prevent one from using a large time-step, particularly if the system is not critically affected by a slower I-front velocity. One example is an expanding H II region in a power-law density gradient. After a brief, initial R-type phase, the I-front becomes a D-type phase, where the ionization and shock fronts progress jointly at the sound speed of the ionized region. A moderately large (0.1 Myr) time-step can accurately follow its evolution. However, after the I-front passes a critical radius (Franco, Tenorio-Tagle & Bodenheimer 1990), the I-front detaches from the shock front, accelerates and transitions back to an R-type front. This can also occur in champagne flows when the I-front passes a density discontinuity. The I-front velocities in these two stages differ by up to a factor of ~10. Although the solution is accurate with a large time-step in the D-type phase, the I-front may lag behind because of the constant time-step. After a few recombination times, the numerical solution eventually approaches the analytical solution. If such a simulation focuses on the density core expansion and any small-scale structures, such as cometary structures and photodissociation regions, one can cautiously sacrifice the temporal accuracy at large scales for computational savings.

3.4.4 Change in incident radiation

I-front velocities can approach significant fractions of the speed of light in steep density gradients and in the early expansion of the H II region. If the I-front position is critical to the calculation, the radiation transport time-step can be derived from a non-relativistic estimate of the I-front velocity

$$v_{\text{I}}(r) \approx \frac{F(r)}{n_{\text{abs}}(r)^{\frac{1}{2}}}$$

(30)

based on the incident radiation field at a particular position. Alternatively, the propagation of the I-front can be restricted by limiting the change in the specific intensity $I$ to a safety factor $C_{\text{RT,ct}}$, resulting in a time-step of

$$d_{t+1} = C_{\text{RT,ct}} \frac{1}{|dI/dr|}.$$  

(31)

See Shapiro et al. (2006) for the exact calculation of a relativistic I-front. Neglecting relativistic terms does not affect the solution because the front velocity is only considered in the time-step calculation.
We consider the specific intensity after the ray travels through the cell, so \( I = I_0 \exp(-\tau) \), where \( \tau = n_H \sigma d l \) is the optical depth through the cell. The time-derivative of \( I \) is

\[
\frac{dI}{dt} = I_0 \exp(-\tau)(-n_H \sigma d l),
\]

which can be expressed in terms of the local optical depth and neutral fraction,

\[
\frac{dI}{dt} = -I \frac{\tau n_H}{n_H}.
\]

\( n_H \) is computed with the same formula as equation (27). Substituting in equation (31) gives

\[
dt = \frac{C_{RT} \varv d \sigma n_H}{\tau n_H}.
\]

In practice, we have found that a ceiling of 3 can be placed on the optical depth, so optically-thick cells do not create a very small time-step. We still find excellent agreement with analytical solutions with this approximation. We show the accuracy using this time-step method in Section 7.4.

### 3.5 Parallelization strategy

Parallelization of the ray-tracing code is essential when exploring problems that require high resolution and thus large memory requirements. Furthermore, ENZO is already parallelized and scalable to \( O(10^5) \) processors in AMR simulations and to \( O(10^3) \) processors in unigrid calculations. ENZO stores the AMR grid structure on every processor, but only one processor contains the actual grid and particle data and photon packages. All other processors contain an empty-grid container. As discussed in Step 4 in Section 3.1, we store the photon packages that need to be transferred to other grids in the linked list PhotonMoveList. In a single-processor (serial) run, moving the rays is trivial by inserting these photons into the linked list of the destination grid. For multiprocessor runs, we must send these photons through MPI communication to the processors that host the data of the destination grids. We describe our strategy below.

The easiest case is when the destination grid exists on the same processor as the source grid, where we move the ray as in the serial case. For all other rays, we organize the rays by destination processors and send them in groups. We also send the destination grid level and ID number along with the ray information that is listed at the beginning of Section 3.1.

For the maximum overlap of communication and computation, which enables scaling to a large numbers of processors, we must employ ‘non-blocking’ MPI communication, where each processor does not wait for synchronization with other processors. We use this technique for the sending and receiving of rays. Here we desire to minimize the idle time of each processor when it is waiting to receive data. In the loop shown in Fig. 2 with the condition that checks whether we have traced all of the rays, we aggressively transport rays that are local on the processor and process any MPI receive calls as they arrive, not waiting for their completion in order to continue to the next iteration. Next, we describe the steps in this algorithm.

**Step 1** – Before any communication occurs, we count the number of rays that will be sent to each processor. The MPI receive calls (MPI_Irecv) must have a data buffer that is greater than or equal to the size of the message. We choose to send a maximum of \( N_{\text{msg}} \) (=10^6 in ENZO v2.0) rays per MPI message. Therefore, we allocate a buffer of this size for each MPI_Irecv call. We then determine the number of MPI messages, \( N_{\text{msg}} \), and send this number in a non-blocking fashion, that is, MPI_Isend.

**Step 2** – Pack the photon packages into a contiguous array for MPI communication while the messages from Step 1 complete.

**Step 3** – Process the number of photon messages that we are expecting from each processor, sent in Step 1. Then post this number of MPI_Irecv calls for the photon data. Because we strive to make the ray-tracing routine to be totally non-blocking, the processors will most likely not be synchronized on the same loop (Steps 3–5 in Section 3.1). Therefore, there might be additional \( N_{\text{msg}} \) MPI messages waiting to be processed. We check for these messages and aggressively drain the message stack to determine the total number of photon messages that we are expecting and post their associated MPI_Irecv calls for the photon data.

**Step 4** – Send the grouped photon data with MPI_Isend with a maximum size of \( N_{\text{max}} \) photons.

**Step 5** – Place any received photon data into the destination grids. We monitor whether the processor has any rays that were moved to grids on the same processor. If so, this processor has rays to transport and we do not necessarily have to wait for any MPI receive messages and thus use MPI_Testsome to receive any messages that have already arrived. If not, we call MPI_Waitsome to wait for any MPI receive messages.

**Step 6** – If all processors have exhausted their workload, then all rays have been either absorbed, exited the domain or halted after travelling a distance \( cdp \). We check this in a similar non-blocking manner to the \( N_{\text{msg}} \) calls in Step 1.

Finally, we have experimented with a hybrid OpenMP/MPI version of ENZO, where workload is partitioned over grids on each MPI process. We found that the parallelization over grids for photon transport does not scale well and the threading over the rays in each grid is a better approach. Because the rays are stored in a linked list in each grid, we must manually split the list into separate lists and let each thread work on each list.

### 4 Radiative Transfer Tests

Tests play an important role in creating and maintaining computational tools. In this section, we present tests drawn from the Cosmological Radiative Transfer Codes Comparison Project (RT06), where results from 11 different radiative transfer codes compared results in four test problems. The codes use various methods for radiation transport: ray tracing with short, long and hybrid characteristics; Monte Carlo casting; I-front tracking (Alvarez, Bromm & Shapiro 2006b); and variable Eddington Tensor formalism (Gnedin & Abel 2001). They conducted tests that investigated (1) the growth of a single Str"omgren sphere enforcing isothermal conditions; (2) the same test with an evolving temperature field; (3) the shadowing created by a dense, optically-thick clump; and (4) multiple H\(_{\text{II}}\) regions in a cosmological density field. In all of the tests presented here, we use the method of restricted neutral fraction changes (Section 3.4.1) for choosing a radiative transfer timestep. We cast 48 rays (HEALPix level 1) from the point source and require a sampling of at least \( \Phi = 5.1 \) rays per cell.

#### 4.1 Test 1 – pure hydrogen isothermal H\(_{\text{II}}\) region expansion

The expansion of an ionising region with a central source in a uniform medium is a classic problem first studied by Str"omgren (1939). This simple but useful test can uncover any asymmetries or artefacts that may arise from deficiencies in the method or newly
introduced bugs in the development process. In this problem, the ionized region grows until recombinations balance photoionizations [equation (1)]. The evolution of the radius $r_i$ and velocity $v_i$ of the I-front has an exact solution of

$$r_i(t) = R_i[1 - \exp(-t/t_{rec})]^{1/3},$$

$$v_i(t) = \frac{R_i}{3t_{rec}} \exp(-t/t_{rec}) \left[1 - \exp(-t/t_{rec})\right]^{2/3},$$

where $t_{rec} = (\alpha_B n_H)^{-1}$ is the recombination time.

We adopt the problem parameters used in RT06. The ionizing source emits $5 \times 10^{48}$ photon s$^{-1}$ of monochromatic radiation at 13.6 eV and is located at the origin in a simulation box of 6.6 kpc. The ambient medium is initially set at $T = 10^4$ K, $n_H = 10^{-3}$ cm$^{-3}$ and $x = 1.2 \times 10^{-3}$, resulting in $R_i = 5.4$ kpc and $t_{rec} = 122.4$ Myr. The problem is run for 500 Myr. In the original tests, the temperature is fixed at $10^4$ K; however, our solver is inherently tied to the chemistry and energy solver. To mimic an isothermal behaviour, we set the adiabatic index $\gamma = 1.0001$, which ensures an isothermal state but not a fixed ionization fraction outside of the Str"omgren sphere.

In Fig. 5, we show (a) the evolution of the neutral and ionization fractions as a function of the radius at $t = 10, 30, 100$ and 500 Myr; and (b) the growth of the I-front radius as a function of time and its ratio with the analytical Str"omgren radius [equation (35)]. The I-front has a width of $\sim 0.7$ kpc, which is in agreement with the inherent thickness of $\sim 18\lambda_{mon} = 0.74$ kpc, given a 13.6-eV monochromatic spectrum. There are small kinks in the neutral fraction at 1.5 and 3 kpc that corresponds to artefacts created by the photon-package splitting at these radii. However, these do not affect the overall solution. One difference between our results and the codes presented in RT06 is the increasing neutral fraction outside the H$\ii$ region. This occurs because the initial ionized fraction and temperature is set to $1.2 \times 10^{-3}$ and $10^4$ K, respectively, which are not the equilibrium values. Over the 500 Myr in the calculation, the neutral fraction increases to 0.2, which is close to its equilibrium value. In the right-hand panel of Fig. 5, the I-front radius exceeds $R_i$ by a few per cent for most of the calculation. This difference happens because the analytical solution [equation (35)] assumes the H$\ii$ region has a constant ionised fraction. The evolution of the ionized fraction as a function of the radius can be analytically calculated (e.g. Osterbrock 1989; Petkova & Springel 2009), causing the I-front radius to be slightly larger, increasing from 0 to 3 per cent in the interval 80–350 Myr. Our results are in excellent agreement with this more accurate analytical solution. We show the distribution of the neutral fraction in the domain for $t = 10, 100$ and 500 Myr in Fig. 6 that agrees well with the results in RT06. In Fig. 7, we show a slice of the neutral fraction through the origin. Other than the ray-splitting artefacts that generate the plateaus at 1.5 and 3 kpc, one sees spherical symmetry without any noise in our solution.

![Figure 5](image-url)

**Figure 5.** Test 1 – H$\ii$ region expansion with a monochromatic spectrum of 13.6 eV. Top panel: radially averaged profile of the neutral (solid line) and ionized (dashed line) fraction at 10, 30, 100 and 500 Myr. Bottom panel: evolution of the calculated (top panel, dashed line) and analytical (top panel, solid line) Str"omgren radius. The ratio of these radii is plotted in the bottom panel.

![Figure 6](image-url)

**Figure 6.** Test 1 – H$\ii$ region expansion with a monochromatic spectrum of 13.6 eV. Probability distribution function for the neutral fraction at 10 Myr (solid line), 100 Myr (dashed line) and 500 Myr (dotted line). The recombination of hydrogen at $T = 10^4$ K causes the maximum neutral fraction to decrease from 1 to 0.75.

### 4.2 Test 2 – H$\ii$ region expansion: temperature evolution

This test is similar to Test 1, but the temperature is allowed to evolve. The radiation source now has a blackbody spectrum with a $T = 10^4$ K. The initial temperature is set at 100 K. The higher energy photons have a longer mean free path than the photons at the ionization threshold in Test 1. Thus, the I-front is thicker as the photons can penetrate deeper into the neutral medium. Here, we use four energy groups with the following mean energies and relative luminosities: $E_i = (16.74, 24.65, 34.49, 52.06)$, $L_i/L = (0.277, 0.335, 0.2, 0.188)$.

In Fig. 8, we show the radially averaged neutral and ionized fractions at $t = 10, 30, 100$ and 500 Myr, and the total neutral
fraction of the domain in Fig. 9. Compared with Test 1, the I-front is thicker, as expected with the harder spectrum. Artefacts originating from ray splitting, similar to Test 1, appear at $r \sim 1$ and 3 kpc as kinks in the neutral fraction. The total neutral fraction decreases to 0.67 over $4t_{\text{rec}} = 500$ Myr, which is in agreement with the analytical expectation and other codes in RT06. Fig. 10 shows the distribution of the ionized fraction and temperature in Test 2. The overall trends agree with the codes presented in RT06 with the exception of the ray-splitting artefacts that appear as slight rises in the distribution at $\log{N_e} \sim -1$ and $\log{T} \sim 3$. In Fig. 11, we show slices of the neutral fraction and temperature through the origin at $t = 10$ and 100 Myr. Here one sees the spherically symmetric H II regions and a smooth temperature transition to the neutral ambient medium. In Fig. 12, we show the ratio of the I-front radius $r_{\text{IF}}$ in our simulation and $R_e$. Before $1.5t_{\text{rec}}$, $r_{\text{IF}}$ lags behind $R_e$, initially by 10 per cent and then increases to $R_e$; however, afterwards, this ratio asymptotes to a solution that is 4 per cent greater than $R_e$. This behaviour is approximately the median result in RT06, where this ratio varies between 1 and 1.1, and the early evolution of $r_{\text{IF}}$ is underpredicted by almost all of the codes. If we use one energy group with the mean energy (29.6 eV) of a $T = 10^5$ K blackbody, we find that $r_{\text{IF}}/R_e = 1.08$, which is representative of the codes in the upper range of RT06.

### 4.3 Test 3 – I-front trapping in a dense clump and the formation of a shadow

The diffusivity and angular resolution of a radiative transport method can be tested with the trapping of an I-front by a dense, neutral clump. In this situation, the I-front will uniformly propagate until it reaches the clump surface. Then the radiation in the line of sight of the clump will be absorbed more than the ambient medium. If the clump is optically thick, a shadow will form behind the clump. The sharpness of the I-front at the shadow surface can be used to determine the diffusivity of the method. Furthermore, the shadow surface should be aligned with the outermost neutral regions of the clump, which can visually assess the angular resolution of the method.

The problem for this test is contained in a 6.6-kpc box with an ambient medium of $n_H = 2 \times 10^{-4}$ cm$^{-3}$ and $T = 8000$ K. The clump is in pressure equilibrium with $n_H = 0.04$ cm$^{-3}$ and $T = 40$ K.
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Figure 11. Test 2 – \text{H} \text{II} region expansion with a $T = 10^5$ K blackbody spectrum. Top panel: slices through the origin of the neutral fraction at 10 and 100 Myr. Bottom panel: slices of the temperature at 10 and 100 Myr.

Figure 12. Test 2 – \text{H} \text{II} region expansion with a $T = 10^5$ K blackbody spectrum. Top panel: evolution of the radius of the simulated I-front (dashed line) and analytical (solid line) Strömgren radii. Bottom panel: the ratio of the calculated and analytical Strömgren radii.

It has a radius of $r_c = 0.8$ kpc and is centred at $(x, y, z) = (5, 3.3, 3.3)$ kpc. The ionized fraction of the entire domain is zero. In RT06, the test considered a plane-parallel radiation field with a flux $F_0 = 10^6$ photon s$^{-1}$ cm$^{-2}$ originating from the $y = 0$ plane. Our code can only consider point sources, so we use a single radiation source located in the centre of the $y = 0$ boundary. The luminosity of $N_\gamma = 3 \times 10^{51}$ photon s$^{-1}$ corresponds to the same flux $F_0$ at 5 kpc, the location where the I-front trapping can be calculated analytically (Shapiro et al. 2004) and with these parameters, it should halt at approximately the centre of the clump. We use the same four energy groups as in Test 2.

In Fig. 13, we show the neutral fraction and temperature of a one-dimensional cut through the centre of the dense clump at $z = 0.5$ at $t = 1, 3, 5$ and 15 Myr. The I-front is halted at a little more than halfway through the clump, which is consistent with the analytical expectation. The hardness of the $T = 10^5$ K blackbody spectrum allows the gas outside the I-front to be photoheated. Where the gas is ionized, the temperature is between $10^4$ and $20^4$ K, but decreases sharply with the ionized fraction. Fig. 14 depicts the average ionized fraction and temperature inside the dense clump, both of which gradually increase as the I-front propagates through.
4.4 Test 4 – multiple sources in a cosmological density field

The last test in RT06 involves a static cosmological density field at \( z = 9 \). The simulation comoving box size is 0.5 \( h^{-1} \) Mpc and has a resolution of 128\(^3\). There are 16 point sources that are centred in the 16 most-massive haloes. They emit \( f_{\gamma} = 250 \) ionizing photons per baryon in a blackbody spectrum with an effective temperature \( T = 10^5 \) K and they live for \( t_s = 3 \) Myr. Thus, the luminosity of each source is

\[
N_{\gamma} = f_{\gamma} \frac{M \Omega_{\text{b}}}{\Omega_{\text{m}0} M_{\text{HI}} t_s} \tag{37}
\]

where \( M \) is the halo mass, \( \Omega_{\text{m}0} = 0.27 \) and \( \Omega_{\text{b}} = 0.043 \). The radiation boundaries are isolated so that the radiation leaves the box instead of being shifted periodically. The simulation is evolved for 0.4 Myr.

Fig. 17 depicts the distribution of the neutral fraction and temperature of the entire domain and shows good agreement with the codes presented in RT06. We show the growth of the \( \text{H} \, \text{II} \) regions by computing the mass-averaged \( x_m \) and volume-averaged \( x_v \) ionized fraction in Fig. 18. Initially, \( x_m \) is larger than \( x_v \) and at \( t \approx 170 \) kyr, \( x_v \) becomes larger. This is indicative of inside-out reionization (e.g. Gnedin 2000; Miralda-Escudé, Haehnelt & Rees 2000; Sokasian et al. 2003), where the dense regions around haloes are ionized first and then the voids are ionized last. At the end of the simulation, 65 per cent of the simulation is ionized. However, by visual inspection in the slices of the electron fraction (Fig. 19), there appears to be very good agreement with the codes \( \text{C}^{2}\text{RAY} \) and \( \text{FTTE} \). At first glance, our results appear to be different from those of RT06 because of the colour-mapping. Our results are also in good agreement with the multifrequency version of TRAPHIC [see also Pawlik & Schaye (2011) for a better representation of the electron fraction slices]. In the slices of the electron fraction and temperature (Fig. 19), the photoheated regions are larger than the ionized regions by a factor of 2–3 because of the hardness of the \( T = 10^5 \) K blackbody spectrum.

5 RADIATION HYDRODYNAMICS TESTS

We next show results from radiation hydrodynamics test problems presented in RT09. They involve (1) the expansion of an \( \text{H} \, \text{II} \) region in a uniform medium, similar to Test 2; (2) an \( \text{H} \, \text{II} \) region in an isothermal sphere; and (3) the photoevaporation of a dense, cold clump, similar to Test 3. We turn off self-gravity and AMR in accordance with RT09.

5.1 Test 5 – classical \( \text{H} \, \text{II} \) region expansion

Here we consider the expansion of an \( \text{H} \, \text{II} \) region into a uniform neutral medium including the hydrodynamical response to the heated
Figure 16. Test 3 – I-front trapping in a dense clump and shadowing. Clockwise from the upper left-hand side: slices through the origin of the neutral fraction (1 Myr), temperature (1 Myr), temperature (15 Myr) and neutral fraction (15 Myr).

Figure 17. Test 4 – multiple cosmological sources. Probability distribution function for the neutral fraction (left-hand panel) and temperature (right-hand panel) at 50 kyr (solid line) and 200 kyr (dashed line).

Figure 18. Test 4 – multiple cosmological sources. Evolution of the mass-averaged (dashed line) and volume-averaged (solid line) ionized fractions.
gas. The ionized region has a greater pressure than the ambient medium, causing it to expand. This is a well-studied problem (Spitzer 1978) with an analytical solution, where the I-front moves as

\[ r_s(t) = r_s,0 \left( 1 + \frac{7c_s}{4R_s} \right)^{4/7}, \]  

(38)

where \( c_s \) is the sound speed of the ionized gas and \( r_s,0 \) is \( r_s \) in equation (35). The bubble eventually reaches pressure equilibrium with the ambient medium at a radius

\[ r_t = R_s \left( \frac{2T}{T_0} \right)^{2/3}, \]  

(39)

where \( T \) and \( T_0 \) are the ionized and ambient temperatures, respectively. These solutions only describe the evolution at late times and not the fast transition from R-type to D-type at early times.

The simulation setup is similar to Test 2 with the exception of the domain size \( L = 15 \text{kpc} \). Here pressure equilibrium occurs at \( r_t = 185 \text{kpc} \), which is not captured by this test. However, more interestingly, the transition from R-type to D-type is captured and occurs around \( R_s = 5.4 \text{kpc} \). The test is run for 500 Myr.

The growth of the I-front radius is shown in Fig. 20, using both \( T = 10^4 \text{K} \) and \( x_e = 0.5 \) as I-front definitions, compared to the analytical solution [equation (39)]. We define this alternative measure because the I-front becomes broad as the D-type front creates a shock. Densities in this shock, as seen in Fig. 21, are high enough for the gas to recombine but not radiatively cool. Before \( 2t_{\text{rec}} \approx 250 \text{Myr} \), the temperature cut-off overestimates \( r_s \) by over 10 per cent; however, at later times, it provides a good match to the \( t^{4/7} \) growth at late times. With the \( x_e = 0.5 \) criterion for the I-front, the radius is always underestimated by \( \sim 20 \text{ per cent} \). This behaviour was also seen in RT09.

Fig. 21 shows the progression of the I-front at times \( t = 10, 200 \) and 500 Myr in radial profiles of the density, temperature, pressure and ionized fraction. The initial H II region is overpressurized and creates a forward shock wave. The high-energy photons can penetrate through the shock and partially ionizes and heats the exterior gas, clearly seen in the profiles. As noted in RT09, this heated exterior gas creates a photoevaporative flow that flows inwards. This interacts with the primary shock and creates the double-peaked features in the density profiles at 200 and 500 Myr. Fig. 22 shows slices through the origin of the same quantities, including the neutral...
ionized and photoheated, the density gradient provides the pressure imbalance to drive the gas outwards.

This test is constructed to study the transition from R-type to D-type in the core and back to R-type in the density gradient. Thus, the simulation focuses on the small-scale, not long-term, behaviour of the I-front. The simulation box has a side length $L = 0.8\ kpc$ with the core density $n_0 = 3.2\ cm^{-3}$, core radius $r_0 = 91.5\ pc$ (15 cells) and temperature $T = 100\ K$ throughout the box. The ionization fraction is initially zero and the point source is located at the origin with a luminosity of $10^{50}\ photon\ s^{-1}\ cm^{-3}$. The simulation is run for 75 Myr.

Because this problem does not have an analytical solution, we compare our calculated I-front radius and velocity, shown in Fig. 23, to the RT09 results. Their evolution is in agreement within 5 per cent of RT09. As in Test 5, we use an extra definition of $T = 10^4\ K$ for the I-front. We compute the I-front velocity from the radii at 50 outputs, which causes the noise shown in Fig. 23.

For the first Myr, the radiation source creates a weak R-type front where the medium is heated and ionized but does not expand because $v_{IF} > c_s$. When $v_{IF}$ becomes subsonic, the medium can react to the passing I-front and creates a shock, leaving behind a heated rarefied medium. This behaviour is clearly seen in the radial profiles of the density, temperature, ionized fraction and pressure in Fig. 24. The inner density decreases over two orders of magnitude after 25 Myr. To illustrate any deviations in spherical symmetry, we show in Fig. 25 slices of the density, temperature, neutral fraction and ionized fraction at the final time. The only artefact apparent to us is the slight broadening of the shock near the $x = 0$ and $y = 0$ planes. This causes the I-front radius to be slightly smaller in those directions. In the diagonal direction, the neutral column density through the shock is slightly smaller, allowing the high-energy photons to photoionize and photoheat the gas to $x = 5 \times 10^{-3}$ and $T = 2000\ K$ out to $\sim 50\ pc$ from the shock. The reflecting boundaries are responsible for this artefact because this is not seen when the problem is centred in the domain, removing any boundary effects.

5.3 Test 7 – photoevaporation of a dense clump

The photoevaporation of a dense clump in a uniform medium proceeds very differently when radiation hydrodynamics are considered instead of a static density field. The I-front first proceeds as a very fast R-type front and then it slows down to a D-type front when it encounters the dense clump. As the clump is gradually photoionized and heated, it expands into the ambient medium. The test presented here is exactly like Test 3 but with gas dynamics. In this setup, the I-front overtakes the entire clump, which is then completely photoevaporated.

Fig. 26 shows cuts of the density, temperature, neutral fraction and pressure in a line connecting the source and the clump centre at $t = 1$, 10 and 50 Myr. At 1 Myr, the I-front has propagated through the leftmost 500 pc of the clump. This heated gas is now overpressurized, as seen in the pressure plot in Fig. 26 and then expands into the ambient medium. This expansion creates a photoevaporative flow seen in many star-forming regions (e.g. M16; Hester et al. 1996) as stars irradiate nearby cold, dense overdensities. These flows become evident in the density at 10 Myr, seen both in the line cuts and in the slices (Fig. 27). They have temperatures of up to 50 000 K. At this time, the front has progressed about halfway through the clump, if one inspects the neutral fraction. However, the high-energy photons have heated all but the rear surface of the clump. At the end of the test ($t = 50\ Myr$), only the core and its associated shadow is

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Figure 20. Test 5 – H II region in a uniform medium. Top panel: growth of the computed I-front radius at an ionized fraction $x_i = 0.5$ (dashed line) and at a temperature $T = 10^{4}\ K$ (dotted line) compared to the analytical estimate [solid line; equation (38)]. Bottom panel: the ratio of the computed I-front radii to the analytical estimate.

Figure 21. Test 5 – H II region in a uniform medium. Clockwise from the upper left-hand side: radial profiles of the density, temperature, ionized fraction and pressure at times $t = 10$, 200 and 500 Myr.

fraction. These depict the very good spherical symmetry of our method. The only apparent artefact is a very slight diagonal line, which is caused by the HEALPix pixelization differences between the polar and equatorial regions. This artefact diminishes as the ray-to-cell sampling is increased.

5.2 Test 6 – H II region expansion in an isothermal sphere

A more physically motivated scenario is an isothermal sphere with a constant-density $n_c$ core, which is applicable to collapsing molecular clouds and cosmological haloes. The radial density profile is described by

$$n(r) = \begin{cases} n_c & \text{(} r \leq r_0) \\ n_c(r/r_0)^{-2} & \text{(} r > r_0) \end{cases},$$

where $r_0$ is the radius of the core. If the Strömgren radius is smaller than the core radius, then the resulting H II region never escapes into the steep density slope. When the I-front propagates out of the core, it accelerates as it travels down the density gradient. There exists no analytical solution for this problem with full gas dynamics but was extensively studied by Franco et al. (1990). After the gas is

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neutral, as shown in Fig. 28. The core has been compressed by the surrounding warm medium, thus causing the higher densities seen at \( t = 50 \) Myr. The non-spherical artefacts on the inner boundary of the warm outermost shell are caused by the initial discretization of the sphere, as discussed in Section 4.3. Next, Fig. 29 shows the distributions of the temperature and flow Mach number in the entire domain at 10 and 50 Myr, showing similar behaviour to the codes in RTO9. Finally, in Fig. 30, we show slices of the flow Mach number at 10 and 50 Myr, showing the supersonic photoevaporative flows that originate from the clump.

Figure 22. Test 5 – H\textsc{ii} region in a uniform medium. Clockwise from the upper left-hand side: slices through the origin of the ionized fraction, neutral fraction, temperature and density at time \( t = 500 \) Myr.

Figure 23. Test 6 – H\textsc{ii} region in a \( 1/r^2 \) density profile. Top panel: growth of the computed I-front radius as \( T = 10^4 \) K and \( x_0 = 0.5 \) as definitions for the front. Bottom panel: velocity of the I-front, computed from outputs at 0.5 Myr intervals. The velocity is calculated from \( r_{IF} \), whose coarse time-resolution causes the noise seen in \( v_{IF} \). It is smooth within the calculation itself.

Figure 24. Test 6 – H\textsc{ii} region in a \( 1/r^2 \) density profile. Clockwise from the upper left-hand side: radial profiles of the density, temperature, ionized fraction and pressure at times \( t = 3, 10 \) and 25 Myr.
Figure 25. Test 6 – H II region in a $1/r^2$ density profile. Clockwise from the upper left-hand side: slices through the origin of the ionized fraction, neutral fraction, temperature and density at time $t = 25$ Myr.

Figure 26. Test 7 – photoevaporation of a dense clump. Line cuts from the point source through the middle of the dense clump at $t = 1$, 10 and 50 Myr (clockwise from the upper left-hand side) of the density, temperature, pressure and neutral fraction.

6 RADIATION HYDRODYNAMICS APPLICATIONS

We have completed presenting results from the RT06 and RT09 test suites. We expand on these test suites to include more complex situations, such as a Rayleigh–Taylor problem illuminated by a radiation source, champagne flows, an irradiated blastwave, collimated radiation and an H II region with a variable source that further demonstrate its capabilities and accuracy. Finally, we use the new MHD implementation in enzo v2.0 in the problem of a growing H II region in a magnetic field.

6.1 Application 1 – champagne flow from a dense clump

Radiation-driven outflows from overdensities, known as champagne flows, are a long-studied problem (e.g. Yorke 1986, section 3.3). To study this, we use the same setup as Bisbas et al. (2009) – a spherical tophat with an overdensity of 10 and radius of 1 pc in a simulation box of 8 pc. The ambient medium has $\rho = 290 \, \text{cm}^{-3}$ and $T = 100 \, \text{K}$. The radiation source is offset from the overdensity centre by 0.4 pc. It has a luminosity of $10^{49} \, \text{photon s}^{-1}$ and a $T = 10^5 \, \text{K}$ blackbody spectrum. The resulting Strömgren radius is 0.33 pc, just inside the overdense clump. These parameters are the same as used in Bisbas et al. (2009). The entire domain initially has an ionized fraction of $10^{-6}$. We do not consider self-gravity. The simulation has a resolution of $128^3$ on the base grid and we refine the grid up to four times if a cell has an overdensity of $1.5 \times 2^l$, where $l$ is the AMR level. The simulation is run for 150 kyr.

We show slices in the $x$–$y$ and $x$–$z$ planes of the density in Fig. 31 at $t = 10, 40, 100$ and 150 kyr. In the direction of the clump centre, the I-front shape transitions from spherical to parabolic after it escapes from the clump in the opposite direction. At $t = 10$ kyr, the surface of the H II region is just contained within the overdensity. In the $x$–$z$ plane, there are density perturbations only above a latitude of $45\degree$. We believe that these are caused by the mismatch between
HEALPix pixels and the Cartesian grid, even with our geometric correction. After the I-front escapes from the clump in the negative \(x\)-direction, these perturbations grow from Rayleigh–Taylor instabilities as the gas is accelerated when it exits the clump. As the shock propagates through the ambient medium, it is no longer accelerated and has a nearly constant velocity, as seen in Test 6. Thus, these perturbations are not as vulnerable to Rayleigh–Taylor instabilities at this point. The ambient medium and shock are always optically thick, even in the directions of the bubbles. Bisbas et al. found that the shock fragmented and formed globules; however, we find that the density shell is stable against such fragmentation. To investigate this scenario further, our next tests involve radiation-driven Rayleigh–Taylor instabilities.

\[ v_z(x, y, z) = 0.01[1 + \cos(2\pi x/L_x)] \times [1 + \cos(2\pi y/L_y)] \times [1 + \cos(2\pi z/L_z)]/8. \]  

We run two cases, an optically-thick and an optically-thin case. In the former, we take the parameter choices from the past literature (e.g. Liska & Wendroff 2003; Stone et al. 2008) by setting the top and bottom halves of the domain to a density \(\rho_1 = 2\) and \(\rho_0 = 1\), respectively. The velocity perturbation is set in the \(z\)-direction by

\[ v_z(x, y, z) = 0.01[1 + \cos(2\pi x/L_x)] \times [1 + \cos(2\pi y/L_y)] \times [1 + \cos(2\pi z/L_z)]/8. \]  

6.2 Application 2 – irradiated Rayleigh–Taylor instability

Here we combine the classic case of a Rayleigh–Taylor instability and an expanding \(\text{H} \text{II}\) region. The Rayleigh–Taylor instability occurs when a dense fluid is being supported by a lighter fluid, initially in hydrostatic equilibrium, in the presence of a constant acceleration field. This classic test alone evaluates how subsonic perturbations evolve. We consider the case of a single-mode perturbation. The system evolves without any radiation until the perturbation grows considerably and then turns on the radiation source. These tests demonstrate that \textsc{enzo+moray} can follow a highly dynamic system and resolve fine density structures.

We set the acceleration field \(g_z = 0.1\) and the adiabatic index \(\gamma = 1.4\). We use a domain size of \((L_x, L_y, L_z) = (0.5, 0.5, 1.5)\) with a resolution of \((64, 64, 192)\). For hydrostatic equilibrium, we set \(P = P_0 - g\rho(z)z\) with \(P_0 = 2.5\). In order to consider a radiation source with a ionizing photon luminosity of \(10^{42}\) photon s\(^{-1}\), we scale the domain to a physical size of \((0.5, 0.5, 1.5)\) pc; time is in units of Myr; density is in units of \(m_\odot\), resulting in an initial temperature of \((T_0, T_1) = (363, 726)\) K. The radiation source is placed at the centre of the lower \(z\)-boundary face and starts to shine at \(t = 10\) Myr.

The optically-thin case is set up similarly but with three changes: (1) a density contrast of 10; (2) a luminosity of \(10^{43}\) photon s\(^{-1}\); and (3) the source is born at 6.5 Myr. The time units are decreased to 200 kyr so that \((T_0, T_1) = (1.8 \times 10^3, 1.8 \times 10^4)\) K. Note that in code units, the pressure is unchanged. We adjust the physical unit scaling because we desire an optically-thin bottom medium with \(T > 10^4\) K and \(x_e \sim 1\). Furthermore, the I-front remains...
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Figure 28. Test 7 – photoevaporation of a dense clump. Same as Fig. 26 but at $t = 50$ Myr.

Figure 29. Test 7 – photoevaporation of a dense clump. Probability distribution function for the temperature (left-hand panel) and flow Mach number (right-hand panel) at $t = 10$ Myr (solid line) and 50 Myr (dashed line).

R-type before interacting with the instability. A possible physical analogue could be a radiation source heating and rarefying the medium below.

The $x$- and $y$-boundaries are periodic, and the $z$-boundaries are reflecting. These will cause artificial features, in particular, because of the top reflecting boundary; nevertheless, these tests provide a stress test on a radiation hydrodynamics solver. We show the evolution of

the density, temperature and ionized fraction of the optically-thick and optically-thin cases in Figs 32 and 33, respectively. The initial state of the Rayleigh–Taylor instability is shown in the left-hand panels.

In the optically-thick case, a D-type front is created, which is clearly illustrated by the spherical density enhancement at 0.02 Myr. The shock then passes through the instability at $\sim 0.25$ Myr and reflects off the upper $z$-boundary. This and complex shock reflections create Richtmyer–Meshkov instability (see Brouillette 2002, for a review), driving a chaotic jet-like structure downwards. The radiation source photoevaporates the outer parts of this structure. The interaction between the dense cool ‘jet’ and the hot medium further drives instabilities along the surface, which can be seen when comparing $t = 0.59$ and 0.91 Myr slices. At a later time, the jet can-
Figure 31. Application 1 – champagne flow from a dense clump. Slices of the density through the initial clump centre in the $x$–$y$ plane (top panel) and $x$–$z$ plane (bottom panel) at $t = 10$, 40, 100 and 150 kyr. Note the instabilities that grow from perturbations created while the HII region is contained in the dense clump.

Figure 32. Application 2 – irradiated Rayleigh–Taylor instability; optically-thick case. Slices at $y = 0$ of the density (top panel), temperature (middle panel) and electron fraction (bottom panel). The source turns on at $t = 0$. The radiation source provides further buoyancy in the already $T = 10^4$ K gas. The volumes that are first ionized and photoevaporated are the outer regions of the instability. The enhanced heating also drives the upper regions of the instability, making the top interface turbulent. It then reflects off the upper not reach the bottom of the domain before being photoevaporated. Eventually, this structure is completely destroyed, leaving behind a turbulent medium between the hot and cold regions.

The optically-thin problem is less violent than the optically-thick case because the R-type front does not interact with the initial instability as strongly.
z-boundary and creates a warm, $T = 5 \times 10^3$ K, partially ionized ($x_e \sim 10^{-2}$), turbulent medium seen in the slices at $t \geq 0.67$ Myr. The slices of the electron fraction also show that the dense gas is optically thick.

6.3 Application 3 – photoevaporation of a blastwave

A SN blastwave being irradiated by a nearby star is a likely occurrence in massive-star-forming regions. In this test, we set up an idealized test that mimics this scenario. The ambient medium has a density $\rho_0 = 0.1$ cm$^{-3}$ and temperature $T_0 = 10$ K. The domain size is 1 kpc. We use two levels of AMR with a base grid of $64^3$ that is refined if the density or total energy slope is greater than 0.4. The blastwave is initialized at the beginning of the Sedov–Taylor phase when the mass of the swept-up material equals the ejected material. It has a radius of 21.5 pc, a total energy of $10^{50}$ erg and a total mass of 100 $M_\odot$, corresponding to $E = 315$ eV per particle or $E/k_B = 3.66 \times 10^6$ K. The radiation source is located at the centre of the left-hand $x$-boundary and has a luminosity of $10^{46}$ erg s$^{-1}$. We use a $T = 10^3$ K blackbody spectrum with two energy groups (16.0 and 22.8 eV). The source turns on at 2.5 Myr at which point the blastwave has a radius of 200 pc. The simulation is run for 7.5 Myr.

Fig. 34 shows the I-front overtaking and disrupting the blastwave. We show the blastwave before the source is born at 2.5 Myr. The interior is rarefied ($\rho \sim 10^{-3}$ cm$^{-3}$) and is heated to $T \sim 5 \times 10^3$ K by the reverse shock. At $t = 3$ Myr, the I-front is still R-type and it ionizes the rear side of the dense shell. Because the interior is ionized and diffuse, the I-front rapidly propagates through it until it reaches the opposite shell surface. Shortly afterwards, the I-front transitions from R-type to D-type at a radius of 0.5 kpc, seen in the formation of a shock in the 5-Myr density panel. This transition occurs by the construction of the problem not by the interaction with the blastwave. The surfaces of the blastwave that are perpendicular to the I-front have the highest column density and thus are last to be fully ionized. The pressure forces from the warm ambient medium and blastwave interior compress these surfaces, photoevaporating them in the process, similar to Test 7. They survive until the final time $t = 7.5$ Myr. As the R-type I-front interacts with the blastwave interior, the density perturbations create I-front instabilities (Whalen & Norman 2008) that are seen on the HII region surface at the coordinate $z = 0.5$. Behind the I-front, the dense shell of the blastwave is photoevaporated and a smooth overdensity is left in the initial blastwave centre.

6.4 Application 4 – collimated radiation from a dense clump

Some astrophysical systems produce collimated radiation either intrinsically by relativistic beaming or by an optically-thick torus absorbing radiation in the equatorial plane. The latter case would be applicable in a subgrid model of active galactic nuclei (AGNs) or protostars, for example. Simulating collimated radiation with ray tracing is trivially accomplished by only initializing rays that are within some opening angle $\theta_c$.

We use a domain that is 2 kpc wide and has an ambient medium with $\rho_0 = 10^{-3}$ cm$^{-3}$, $T = 10^4$ K and $x_e = 0.99$. We place a dense clump with $\rho/\rho_0 = 100$, $T = 100$ K, $x_e = 10^{-3}$ and $r = 250$ pc, at the centre of the box. Radiation is emitted in two polar cones with $\theta_c = \pi/6$ with 768 (HEALPix level 3) initial rays, a total luminosity of $10^{46}$ erg s$^{-1}$ and a 17.6-eV monochromatic spectrum. This results in $t_{\text{rec}} = 1.22$ Myr and $R_r = 315$ pc, just outside the sphere. The base grid has a resolution of $64^3$ and it is refined with the same overdensity criterion as Application 1. We run this test for 25 Myr.

We illustrate the expansion of the HII region created by the beamed radiation in Fig. 35. Before $t = 3$ Myr, the HII region is conical and contained within the dense clump, depicted in the $t = 0.1$ Myr snapshot of the system. At this time, the I-front is transitioning from R-type to D-type in the transverse direction of the cone. This can be seen in the minute overdensities on the HII transverse surface. When it breaks out of the overdensity, a champagne flow develops, where the I-front transitions back to a weak R-type front. The cloud surface is a constant-pressure contact discontinuity (CD) with a density jump of 100. After the front heats the gas at the CD, there exists a pressure difference of $\sim 100$. In response, the high-density gas accelerates into the ambient medium and heats it to $3 \times 10^4$ K. Additionally, a rarefaction wave travels towards the...
A dense clump centre. At later times, the transverse D-type front continues through the clump, eventually forming a disc-like structure at the final time. The polar champagne flows proceed to flow outwards and produces a dense shell with a diffuse \((10^{-28} \text{ cm}^{-3})\) and warm \((5000 \text{ K})\) medium in its wake.

### 6.5 Application 5 – time-variations in the source luminosity

Our implementation retains the time-derivative of the radiative transfer equation \((\text{equation (2)})\) if we choose a constant ray-tracing time-step, which saves the photon packages between time-steps if \(c dt_p < L_{\text{box}}\). This effect only becomes apparent when the variation time-scale of the point source is smaller than the light crossing time of the simulation. Furthermore, the time-step should resolve the variation time-scale by at least a few times. This property might be important in large box simulations with variable sources, for example, AGN radiative feedback. To test this, we can use an exponentially varying source with some duty cycle \(t_0\). In a functional form, this can be described as

\[
L(t) = L_{\text{max}} \times \exp[A(t_t / t_0 - 1)],
\]

where \(t_t = 2 \times |t - t_0 - \text{round}(d(t_0))|\) and \(A = 4\) controls the width of the radiation pulse. To illustrate the effects of source variability, we remove any dependence on the medium by considering an optically-thin uniform density \(\rho = 10^{-4} \text{ cm}^{-3}\). We take \(L_{\text{box}} = 1 \text{ Mpc}\), which has a light crossing time of 3.3 Myr. A source is placed at the origin with \(L_{\text{max}} = 10^{55} \text{ photon s}^{-1}\) and \(t_0 = 0.5\) Myr. We use a radiative transfer time-step of 50 kyr to resolve the duty cycle by 10 time-steps. The simulation is run for 6 Myr, so the radiation propagates throughout the box.

The variability in the source is clearly illustrated in the photoionization rates, shown in Fig. 36. The shells of the relative maximum \(k_{\text{ph}}\) correspond to the radiation that was emitted when the source was at its peak luminosity. They are separated by \(c t_0\) Mpc and are geometrically diluted with increasing radius. Averaged over shells of the same width, photoionization rates decrease as \(1/r^2\).

Next we test the hydrodynamical response to a varying source by repeating Test 5. We set the peak luminosity \(L_{\text{max}} = 2 \times 10^{46} \text{ erg s}^{-1}\) that is a factor of 4 more luminous than Test 5, so the average luminosity is \(\sim 5 \times 10^{46} \text{ erg s}^{-1}\). The spectrum is monochromatic with an energy of 29.6 eV. We set the variation time-scale \(t_t = c L_{\text{box}}/3 = 16.3\) kyr and use a constant radiative transfer time-step \(t_p = t_t/4 = 4.07\) kyr. The simulation is run for 200 Myr. We show the radial profiles of the density, temperature, ionized fraction and pressure in Fig. 37. The variable source has little effect on the overall growth of the \(\text{HII}\) region. It has approximately the same radius as Test 5 at \(t = 200\) Myr when run with a monochromatic spectrum (see Section 7.3). At early times, the variable source creates density perturbations with an average size of 500 pc inside the ionized region, seen in the \(t = 50\) Myr profiles. They do not create any instabilities and are smoothed out over its sound crossing time of \(\sim 50\) Myr.

### 6.6 Application 6 – \(\text{HII}\) region with MHD

Another prevalent physical component in astrophysics is a magnetic field. We utilize the new MHD framework (Wang & Abel 2009) in ENZO v2.0 that uses an unsplit conservative hydrodynamics solver and the hyperbolic \(\nabla \cdot \mathbf{B} = 0\) cleaning method of Dedner et al. (2002). We show a test problem with an expanding \(\text{HII}\) region in an initially uniform density field and constant magnetic field. We use the same problem setup as Krumholz et al. (2007b) – \(\rho = 100 \text{ cm}^{-3}\), \(T = 11\) K and \(L_{\text{box}} = 20\) pc with a resolution of 256. This ambient medium is threaded by a magnetic field \(B = 14.2\mu \text{G}\). The Alfvén speed is \(2.6\) km s\(^{-1}\). The radiation source is located in the centre of the box with a luminosity \(L = 4 \times 10^{46} \text{ photon s}^{-1}\) with a 17.6-eV monochromatic spectrum, resulting in a Strömgren radius \(R_s = 0.5\) pc. The simulation is run for 1.58 Myr. The hydrodynamics solver uses an HLL Riemann solver (Harten, Lax & van Leer 1983) and piecewise linear method (PLM) reconstruction (van Leer 1977) for the left- and right-hand states in this problem.

As the \(\text{HII}\) region grows in the magnetized medium, shown in Figs 38 and 39, it transforms from spherical to oblate as it is magnetically confined to directions perpendicular to the magnetic field. This occurs at \(t > 0.5\) Myr because the magnetic pressure exceeds the thermal pressure, and the gas can only flow along field lines.
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7 RESOLUTION TESTS

Resolution tests are important in validating the accuracy of the code in most circumstances, especially in production simulations where the initial environments surrounding radiation sources are unpredictable. In this section, we show how our adaptive ray-tracing implementation behaves when varying spatial, angular, frequency and temporal resolutions.

7.1 Spatial resolution

Here we use Test 1 (Section 4.1) as a test bed to investigate how the evolution of the Strömgren radius changes with the resolution.

Krumholz et al. observed some carbuncle artefacts along the I-front, whereas we see smooth density gradients, which is most likely caused by both the geometric correction to the ray tracing (Section 2.3) and the diffusivity of the HLL Riemann solver when compared to Roe’s Riemann solver used in Krumholz et al. (2007b), who also use PLM as a reconstruction method. The magnetic field lines evolve in a similar manner to their results.

7.2 Angular resolution

The Cartesian grid must be sampled with sufficient rays in order to calculate a smooth radiation field. To determine the dependence on the angular resolution, we consider the propagation of radiation through an optically-thin, uniform medium. The radiation field should follow a $1/r^2$ profile. As the grid is less sampled by rays, the deviation from $1/r^2$ should increase. This test is similar to Test 1, but the medium has $\rho = 10^{-3} \text{ cm}^{-3}$, $T = 10^4 \text{ K}$ and $\epsilon = 10^{-4}$. The simulation is only run for one time-step because the radiation field should be static in this optically-thin test.

We keep all aspects of the test the same, but use resolutions of $16^3$, $32^3$, $64^3$ and $128^3$. In Fig. 40, we show the ratio $r_{\text{IF}}/r_{\text{anyl}}$, similar to Fig. 5, using these different resolutions. The radii in the $64^3$ and $128^3$ runs evolve almost identically. Compared to these resolutions, the lower $16^3$ and $32^3$ resolution runs only lag behind by 1 per cent until 300 Myr and afterwards it is larger by 0.5 per cent than the higher resolution cases. This shows that our method gives accurate results, even in marginally resolved cases, which is expected with a photon-conserving method. Furthermore, this demonstrates that the geometric correction does not significantly affect photon conservation.

7.3 Frequency resolution

The frequency dependence of the radiation field is important for the accuracy of the code. In our tests, we consider a uniform medium with $\rho = 10^{-3} \text{ cm}^{-3}$, $T = 10^4 \text{ K}$ and $\epsilon = 10^{-4}$. We vary the frequency resolution by changing the number of frequency bins. In Fig. 42, we show the ratio of the calculated photon number density to the exact value as a function of frequency. We see that for a frequency resolution of $10^3$, the results are accurate to within 1 per cent.

7.4 Temporal resolution

The temporal resolution of the radiation field is important for the accuracy of the code. In our tests, we consider a uniform medium with $\rho = 10^{-3} \text{ cm}^{-3}$, $T = 10^4 \text{ K}$ and $\epsilon = 10^{-4}$. We vary the temporal resolution by changing the number of time-steps. In Fig. 43, we show the ratio of the calculated photon number density to the exact value as a function of time. We see that for a temporal resolution of $10^3$, the results are accurate to within 1 per cent.
photoionization rate and a $1/r^2$ field, and then plot the standard deviation of this difference field versus angular resolution in Fig. 42. We plot this relation for resolutions of $32^3, 64^3$ and $128^3$ and find no dependence on the spatial resolution, which is expected because we control the angular resolution in terms of cell widths, not in absolute solid angles. We find that the deviation from an inverse square law decreases as $\sigma \propto \Phi^{-0.6}$.

7.3 Frequency resolution

The I-front radius is within 5–10 per cent of analytical solutions in Tests 1, 2 and 5 with only one energy group; however, a multifrequency spectrum can create differences in the reactive flows. We use Test 5 (Section 5.1; an expanding H II region with hydrodynamics) to probe any differences in the solution when varying the resolution of the spectrum. In RT09, ZEUS-MP was used to demonstrate the effect of a multifrequency spectrum on the dynamics of the I-front in this test. Instead of a single shock seen in the monochromatic spectrum, the shock obtains a double-peaked structure in the density and radial velocity. We rerun Test 5 with a $T = 10^5$ K blackbody spectrum sampled by $n_\nu = 1, 2, 4, 8$ and 16 frequency bins. We use the following energies:

(i) $n_\nu = 1$: mean energy of 29.6 eV
(ii) $n_\nu = 2$: mean energies in bins 13.6–30 and > 30 eV–21.1, 43.0 eV
(iii) $n_\nu = 4$: mean energies in bins 13.6–20, 20–30 and 30–40 and > 40 eV–16.7, 24.6, 34.5, 52.1 eV

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Figure 38. Application 6 – H II region with MHD. Left- to right-hand side: slices of the density at $t = 0.18, 0.53$ and 1.58 Myr in the $x$–$y$ plane. The streamlines show the magnetic field.

Figure 39. Application 6 – H II region with MHD. Slices of the density (top panels) and the $x$-component of the magnetic field (bottom panels) in the $y$–$z$ plane at $t = 0.18, 0.53$ and 1.58 Myr (left- to right-hand side).
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Figure 40. Growth of the I-front radius, compared to the analytical radius, in Test 1 with varying spatial resolutions. At the resolutions of $16^3$ and $32^3$, the I-front is underestimated for the first $\sim 25$ Myr but converges within 0.5 per cent of the higher resolution runs.

Figure 41. Variations in the photoionization rates for different ray-to-cell samplings $\Phi_c$. The colour map only spans a factor of 3 to enhance the contrast. In comparison, the photoionization rate actually spans four orders of magnitude in this test.

(iv) $n_\nu = 8$ and 16: logarithmically spaced between 13.6 and 50 eV for the first $n_\nu - 1$ bins, and the last bin is the mean energy above 50 eV.

Fig. 43 shows the radial profiles of the density, temperature, ionized fraction and radial velocity at $t = 200$ and 500 Myr. All of the runs with $n_\nu > 1$ show the double-peaked features in the density and radial velocities. The monochromatic spectrum misses this feature completely because all of the radiation is absorbed at a characteristic column density. In the multifrequency spectra, the higher energy photons are absorbed at larger column densities and photoheat this gas. This heated gas creates a photoevaporative flow that collides with the innermost shock, forming the double-peaked density profile. The $n_\nu \geq 4$ runs are indistinguishable and the $n_\nu = 2$ spectrum only leads to a marginally higher density in the outer shock and lower ionized fractions and temperatures in the ambient medium.

In effect, a monochromatic spectrum can be sufficient if the problem focuses on large-scale quantities, for example, ionized filling fractions in reionization calculations. Conversely, these effects may be important when studying the details of small-scale processes, for example, photoevaporation.

Figure 42. Standard deviations of the difference between the computed photoionization rates and an inverse square law as a function of ray-to-cell samplings $\Phi_c$ for different spatial resolutions. There is no dependence on the spatial resolution and the accuracy increases as $\sigma \propto \Phi_c^{-0.6}$.

Figure 43. Radial profiles (clockwise from the upper left-hand side) of the density, temperature, radial velocity and ionized fraction for Test 5 with $n_\nu = 1, 2, 4, 8$ and 16 frequency bins sampling the $T = 10^5$ K blackbody spectrum. The data are shown at $t = 200$ Myr (top panel) and $t = 500$ Myr (bottom panel). The double-peaked structure in the shock only appears with a multifrequency spectrum. The solution converges at $n_\nu \geq 4$. 
7.4 Temporal resolution

The previous three dependencies did not affect the propagation of the I-front greatly. However, in our and others’ past experience (e.g. Shapiro et al. 2004; Mellema et al. 2006; Petkova & Springel 2009), the time-step, especially a too small one, can drastically underestimate the I-front velocity. Here we use Test 1 but with the 64\(^2\) resolution to compare different time-stepping methods – restricted changes in H\(\|\) (\(dn/dt\) based; Section 3.4.1), constant time-steps of 0.1, 0.5, 1 and 5 Myr (Section 3.4.3) and based on the incident radiation (\(dl/dt\) based; Section 3.4.4). The growth of the I-front radius is shown in Fig. 44. Both the H\(\|\)-restricted and the incident radiation variable time-stepping methods agree within a few per cent throughout the entire simulation, as does the run with constant \(dt_p = 0.1\) Myr time-steps. With the larger constant time-steps, the numerical solution lags behind the analytical one, but they converge to an accurate H\(\|\) radius at late times. Even a \(dt_p = 5\) Myr time-step, which underestimated it by 35 per cent at 50 Myr, is within a per cent of the analytical solution.

The larger constant time-steps deviate from these more accurate solutions at early times because the photon energy gradient is large and thus so is the I-front velocity. To understand this, the I-front can be considered static in a given time-step. Here the ionizing radiation can only penetrate into the neutral gas by roughly a photon mean path \(\lambda_{\text{mfp}}\). Only in the next time-step, the I-front can advance. If the time-step is larger than \(\lambda_{\text{mfp}}/d_{\text{IF}}\), then the numerical solution may fall behind.

The variable time-stepping of the \(dn/dt\) and \(dl/dt\) methods adjust accordingly to the physical situation, as seen in the plot of time-step versus time (Fig. 45). They provide high accuracy when the source first starts to shine. At later times, the I-front slows down as it approaches the Strömgren radius and large time-steps are no longer necessary. The \(dl/dt\) method has a similar time-step to the \(dn/dt\) method. It is larger by a factor of \(\sim 2\) because of our choice of the safety factor \(C_{\text{RT,eff}} = 0.5\). This causes its calculated radius to be smaller by 1 per cent at \(t < t_{\text{rec}}\), which is still in good agreement with the analytical value.

Figure 44. Growth of the I-front radius, compared to the analytical radius, in Test 1 with varying radiative transfer time-steps. The \(dn/dt\) and \(dl/dt\) based time-steps provide the best accuracy, combined with computational efficiency because they take short time-steps when H\(\|\) is expanding rapidly but take long time-steps when the photon gradients are small when \(\tau_{\text{IF}}\) is large. At the final time, all but the \(t = 5\) Myr constant time-step produces identical I-front radii.

Figure 45. Variable time-stepping for the methods that limit the change in the neutral fraction (solid line) and specific intensity (dotted line). The horizontal lines show the constant time-steps that were used in the tests. The crossing time of a mean free path by the I-front is plotted for reference.

8 METHODOLOGY TESTS

Here we show tests that evaluate new features in ENZO+MORAY, such as the improvements from the geometric correction factor, optically-thin approximations, treatment of X-ray radiation and radiation pressure. Finally, we test for any non-spherical artefacts in the case of two sources.

8.1 Improvements from the covering factor correction

As discussed in Section 2.3, non-spherical artefacts are created by a mismatch between the HEALPix pixelization and the Cartesian grid. This is especially apparent in optically-thin regions, where the area of the pixel is greater than the \((1 - e^{-\tau})\) absorption factor. In this section, we repeat the angular resolution tests described in Section 7.2 with \(\Phi_c = 5.1\). Slices of the photoionization rates through the origin are shown in Fig. 46, depicting the improvements in spherical symmetry and a closer agreement to a smooth \(1/r^2\) profile. Previous attempts to reduce these artefacts involve either introducing a random rotation of the HEALPix pixelization (e.g. Abel & Wandelt 2002; Trac & Cen 2007; Krumholz et al. 2007b) or increasing the ray-to-cell sampling.

In the \(x-y\) plane without the correction, there exist shell artefacts where the photoionization rates abruptly drop when the rays are split. This occurs because the photon flux in the rays are constant, so \(k_{\text{ph}}\) is purely dependent on the ray segment length through each cell. Geometric dilution mainly occurs when the number of rays passing through a cell decreases. With the correction, geometric dilution also occurs when the ray’s solid angle only partially covers the cell. This by itself alleviates these shell artefacts. In the \(x-z\) plane without the correction, there is a non-spherical artefact delineated at a 45\(^\circ\) angle. In the lower region, the rays are associated with equatorial HEALPix pixels and in the upper region, they are polar HEALPix pixels. This artefact is not seen in the \(x-y\) plane because all rays are of equatorial type. The geometric correction smooths this artefact but does not completely remove it.

8.2 Optically-thin approximation

In practice, we have found it difficult to transition from the optically-thin approximation to the optically-thick regime without producing
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Figure 46. Slices of the photoionization rate in the \(x-y\) plane (top row) and \(x-z\) plane (bottom row) with (left-hand column) and without (right-hand column) the geometric correction. The slices are through the origin. In the \(x-y\) plane, it reduces the shell artefacts. In the \(x-z\) plane, it reduces the severity of a non-spherical artefact delineated at a 45° angle, where the HEALPix scheme switches from polar to equatorial-type pixels.

Figure 47. Optically-thin approximation to the radiation field with one ray per cell in optically-thin regions. The angular artefacts result from the transition to optically-thick regions (white line) at an optical depth \(\tau = 0.1\). We use the optically-thin problem used in the angular resolution test (Section 7.2) with \(\Phi_t = 5.1\) to show these artefacts in \(k_{\text{ph}}\) in Fig. 47. The radiation field strictly follows a \(1/r^2\) profile until it reaches \(\tau_{\text{thin}} = 0.1\), which is denoted by the white quarter circle in the figure. Within this radius, only \(\Phi_t = 1\) is required. Then at this radius, the rays are then split until a sampling of \(\Phi_t\) is satisfied. Angular spike artefacts beyond this radius arise because of the interface between the optically-thin approximation and full ray-tracing treatment. They originate in cells that intersect the \(\tau_{\text{thin}}\) surface, which are split into the optically-thin and optically-thick definitions. Unfortunately, we have not determined a good technique to avoid such artefacts. They occur because of the following reason. When the first ray with \(\tau < 0.1\) exits such a cell, it applies the optically-thin approximation and marks the cell so no other ray from the same source contributes to its \(k_{\text{ph}}\) and \(\Gamma\) field. However, other rays may exit the cell with \(\tau > 0.1\) because the maximum distance between the far cell faces and the source is not always \(\tau < 0.1\). Then these rays will split in this cell and add to \(k_{\text{ph}}\) and become attenuated, reducing its photon fluxes. When the rays continue to the next cell after this transition, the photon fluxes are not necessarily equal to each other, creating the angular artefacts seen in Fig. 47. We are continuing to formulate a scheme that avoids these artefacts because this approximation will be very advantageous in simulations with large ionized filling factors.

8.3 X-ray secondary ionizations and reduced photoheating

Here we test our implementation of secondary ionizations from high-energy photons above 100 eV, described in Section 2.5.2 and used in Alvarez et al. (2009) in the context of accreting black holes. We use the same setup as Test 5 but with an increased luminosity \(L = 10^{50}\) erg s\(^{-1}\) and a mono-chromatic spectrum of 1 keV. Fig. 48 compares the density, temperature, ionized fraction and neutral fraction of the expanding H\(_n\) region, considering secondary ionizations and reduced photoheating and considering only one ionization per photon and the remaining energy being thermalized.

Fig. 48 shows the main effects of secondary ionizations from the 1-keV spectrum on the ionization and thermal state of the system. Without secondary ionizations, each absorption results in one ionization with the remaining energy transferred into thermal energy. However, with secondary ionizations, recall that most of the radiation energy goes into hydrogen and helium ionizations in neutral gas, whereas in ionized gas, most of the energy is thermalized. In this test, only the inner 300 pc is completely ionized because of the

Figure 48. Radial profiles of the temperature and ionized fraction showing the effects of secondary ionizations from a monochromatic 1-keV spectrum. The discontinuity at \(r \sim 0.4\) is caused by artefacts in the ray tracing, which is described in Test 1. The high-energy photons can ionize multiple hydrogen atoms, increasing the ionized fraction. In part, less radiation goes into thermal energy, lowering the temperature.
small cross-section of hydrogen at $E_{ph} = 1\text{ keV}$. Beyond this core, the medium is only partially ionized. This process expands the hot $T = 10^5\text{ K}$ core by a factor of 2. In the outer neutral regions, the ionization fraction is larger by a factor of $\sim 10$, which in turn results in less photoheating, lowering the temperature by a factor of 2–3.

### 8.4 Radiation pressure

Radiation pressure affects gas dynamics in an $\text{H} \text{\II}$ region when its force is comparable to the acceleration created by the gas pressure of the heated region. The imparted acceleration on a hydrogen atom $a_{\text{g}} = E_{ph}/c$. This is especially important when the I-front is in its initial R-type phase, where the gas has not reacted to the thermal pressure yet. Thus, we construct a test that focuses on a small scale, compared to the Strömgren radius. The domain has a size of 8pc with a uniform density $\rho = 2900\text{ cm}^{-3}$ and initial temperature $T = 10^5\text{ K}$. The source is located at the origin with a luminosity $L = 10^{50}\text{ photon s}^{-1}$ and a $T = 10^5\text{ K}$ blackbody spectrum. We use one energy group $E_{ph} = 29.6\text{ eV}$. The grid is adaptively refined on overdensity with the same criterion as Test 8. The simulation is run for 140 kyr.

We compare nearly identical simulations but one with radiation pressure and one without radiation pressure to quantify its effects. Radial profiles of the density, temperature, neutral fraction and radial velocity are shown in Fig. 49 for both simulations at several times. Without radiation pressure, the evolution of $\text{H} \text{\II}$ matches the analytical expectations described in Section 5.1. At $t = 140\text{ kyr}$ with radiation pressure, the I-front radius is increased by $\sim 5$ per cent = 0.16 pc. However, radiation pressure impacts the system the greatest inside the I-front. At $t = 40\text{ kyr}$, the central density is smaller by a factor of 20 with radiation pressure, but the temperatures are almost equal. A rarefaction wave thus propagates towards the centre, depicted by the negative radial velocities at $t = 60\text{ kyr}$. This raises the central density to $10^{-21}\text{ g cm}^{-3}$ at $t = 80\text{ kyr}$. Afterwards, the radiation continues to force gas outwards. From $t = 100$ to $140\text{ kyr}$, the maximum radial velocity of the ionized gas increases from 10 to 50 km s$^{-1}$. This leaves behind an even more diffuse medium, lowering the gas density by a factor of 10 at $t = 140\text{ kyr}$. Thus, the recombination rates are lower, resulting in increased ionization fractions and temperatures in the $\text{H} \text{\II}$ region.

### 8.5 Consolidated $\text{H} \text{\II}$ region with two sources

Here we test for any inaccuracies in the case of multiple sources. We use the same test problem as Petkova & Springel (2009, section 5.1.2), which has two sources with luminosities of $5 \times 10^{48}\text{ photon s}^{-1}$ and are separated by 8 kpc. The ambient medium is static with a uniform density of $10^{-3}\text{ cm}^{-3}$ and $T = 10^4\text{ K}$. This setup is similar to Test 1. The domain has a resolution of $128 \times 64 \times 64$. It is 20 kpc in width and is 10 kpc in height and depth. The problem is run for 500 Myr.

The $\text{H} \text{\II}$ regions grow to $r = 4\text{ kpc}$ where they overlap. Then the two sources are enveloped in a common, elongated $\text{H} \text{\II}$ region. To illustrate this, we show the neutral fraction in Fig. 50. Our method keeps spherical symmetry close to the individual sources and there are no perceptible artefacts from having multiple sources.

### 9 PARALLEL PERFORMANCE

Finally, we demonstrate the parallel performance of $\text{ENZO-}\text{MORAY}$ in weak- and strong-scaling tests. For large simulations to consider radiative transfer, it is imperative that the code scales to a large number of processors.

#### 9.1 Weak scaling

Weak-scaling tests demonstrate how the code scales with the number of processors with a constant amount of work per processor. Here we construct a test problem with a 64$^3$ block per core. The grid is not adaptively refined. The physical setup of the problem is nearly the same as Test 5 with a uniform density $\rho = 10^{-3}\text{ cm}^{-3}$.
Figure 51. Weak-scaling test with one $64^3$ block per process. Each block has one source and is set up similar to the radiation hydrodynamics Test 5. Above eight processes, all parts of the code exhibit good weak scaling except for the interprocessor ray communication. The radiation module timing includes the ray tracing, communication, chemistry and energy solver, and all other overheads associated with the radiation transport. The cache locality of the data causes the decrease in performance from one to eight processes.

and initial temperature $T = 100 \text{K}$. Each block has the same size of 15 kpc as Test 5. At the centre of each grid, there exists a radiation source with a luminosity $L = 5 \times 10^{48}$ photon s$^{-1}$ and a 17-eV monochromatic spectrum. The problem is run for 250 Myr. We run this test with $N_p = 2^n$ cores with $n = [0, 1, \ldots, 10, 11]$. The domain has $(N_x, N_y, N_z)$ blocks that is determined with the MPI routine MPI_Dims_create. For example, with $n = 7$, the problem is decomposed into $(N_x, N_y, N_z) = (4, 4, 8)$ blocks, producing a $256 \times 256 \times 512$ grid. We have run these on the original (Harpertown CPUs) nodes of the NASA NAS machine, Pleiades, with eight cores per node. Fig. 51 shows the performance timings of various parts of the code. From one to two cores, the total time only increases by $\sim 1$ per cent due to the overhead associated with the interprocessor message passing. From two to eight cores, the performance decreases in the hydrodynamics solver, chemistry and energy solver, and obtaining the hydrodynamic boundary conditions because of cache locality problems of the data being passed to the CPU. This occurs because of the CPU architecture, specifically the L1 cache and core connectivity. We see less of a penalty in newer processors, for example, Intel Nehalam and Westmere CPUs. Above eight processes, these routines exhibit near-perfect weak scaling to 2048 cores. Unfortunately, there exists an $N_p^{1/3}$ dependence in the ray communication routines. It becomes the dominant process above 512 processes. We are actively pursuing a solution to this scaling problem. The other parts of the code exhibit excellent weak scaling. Overall, it scales well to 512 processes and there is room to enhance the weak scalability of ENZO+MORAY in the near future.

9.2 Strong scaling

Strong scaling tests show how the problem scales with the number of processors for the same problem. The overhead associated with the structured AMR framework in ENZO can limit the strong scalability. One key property of strong scaling is that each processor must have sufficient work to compute, compared to the communication involved. In our experience, non-AMR calculations exhibit much better strong scaling than AMR ones because of reduced interprocessor communication. We use an AMR simulation to demonstrate the scalability of ENZO+MORAY in a demanding, research application. Here we use a small-box reionization calculation with $L_{\text{box}} = 3 \text{ Mpc} h^{-1}$, a resolution of $256^3$ and six levels of refinement. We measure the time spent on the hydrodynamics, non-equilibrium chemistry, ray tracing and radiation transport communication in a time-step lasting 1 Myr, at $z = 10$. There are nine radiative transfer time-steps in this period. The box has 675 point sources, 15 943 AMR grids and $6.01 \times 10^7 \approx 392^3$ computational cells in this calculation at this redshift. On average, $4.6 \times 10^8$ ray segments are traced each time-step. The ionized volume fraction is 0.10. The calculations are performed on the Nehalam nodes on Pleiades on 2$^n$ cores, where $n = [2, \ldots, 9]$.

Fig. 52 shows the strong-scaling results of this calculation. The hydrodynamics and non-equilibrium chemistry routines scale very well in this range because they depend on local phenomena. Note that the dominant process is the radiation transport instead of the hydrodynamics when compared to the weak-scaling tests. The error bars in the figure represent the deviations across all cores and it shows that load balancing becomes an issue at 128 and 256 cores. This is an even larger problem for the ray tracing because the grids that host multiple radiation sources will have significantly more work than a distant grid. For example, if a few central grids host several point sources, the exterior grids must wait until those grids are finished with ray tracing in order to receive the rays. This idle time constitutes the majority of the time spent in the ray communication routines despite our efforts (see Section 3.5) to minimize idle time. For this reason, the communication of rays does not scale in this problem. One solution is to split the AMR grids into smaller blocks based on the ray-tracing work. This could impact the performance of the rest of ENZO by increasing the number of boundaries and thus communication. Nevertheless, in simulations that are dominated by radiation transport, it will be advantageous to construct such a scheme to increase the feasibility of running larger problems.

10 SUMMARY

In this paper, we have presented our implementation, ENZO+MORAY, of adaptive ray tracing (Abel & Wandelt 2002) and its coupling to the hydrodynamics in the cosmology AMR code ENZO, making it...
a fully functional radiation hydrodynamics code. As this method is photon-conserving, accurate solutions are possible with coarse spatial resolutions. A new geometric correction factor to ray tracing on a Cartesian grid was described and it is general to any implementation. We have exhaustively tested the code to problems with known analytical solutions and the problems presented in the RT06 and RT09 radiative transfer comparison papers. Additionally, we have tested our code with more dynamical problems — champagne flows, Rayleigh–Taylor instabilities, photoevaporation of a blastwave, beamed radiation, a time-varying source and an \textsc{H} II region with MHD — to demonstrate the flexibility and fidelity of \textsc{Enzo-MORAY}. Because production simulations may not have the resolution afforded in these test problems, we have tested the dependence on the spatial, angular, frequency and temporal resolution. It provides accurate solutions even at low resolution, except for the large constant time-steps. However, we have described two methods to determine the radiative transfer time-step that are based on the variations in the specific intensity or changes in the neutral density on the spatial, angular, frequency and temporal resolution. It provides accurate solutions even at low resolution, except for the constant time-steps. Moreover, we have described a method to calculate the radiation field in the optically-thin limit with ray tracing.

Being a ray-tracing code, it scales with the number of radiation sources; nevertheless, it scales well to \(O(10^3)\) processors for problems with \(\sim10^6\) computational cells and \(\sim10^8\) sources, such as reionization calculations. We have also shown that the code shows good strong scaling in AMR calculations, given a large enough problem. The combination of AMR and adaptive ray tracing allows for high-resolution and high dynamical range problems, e.g. present-day star formation, molecular cloud resolving cosmological galaxy formation, and \textsc{H} II regions of Pop III stars. Furthermore, we have included Lyman–Werner absorption, secondary ionizations from X-ray radiation, Compton heating from photon scattering and radiation pressure into the code, which extends the reach of \textsc{Enzo-MORAY} to study AGN feedback, stellar winds and local star formation. Coupling the radiative transfer with MHD further broadens the applicability of our code. The full implementation is included in the latest public version of \textsc{Enzo}, providing the community with a full-featured radiation hydrodynamics AMR code.

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\(^3\) http://enzo.googlecode.com

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