A new moment method for continuum radiative transfer in cosmological re-ionization

Kristian Finlator, Feryal Özel and Romeel Davé
The University of Arizona, Tucson, AZ 85721, USA

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ABSTRACT
We introduce a new code for computing time-dependent continuum radiative transfer and non-equilibrium ionization states in static density fields with periodic boundaries. Our code solves the moments of the radiative transfer equation, closed by an Eddington tensor computed using a long characteristics (LC) method. We show that traditional short characteristics and the optically thin approximation are inappropriate for computing Eddington factors for the problem of cosmological re-ionization. We evolve the non-equilibrium ionization field via an efficient and accurate (errors <1 per cent) technique that switches between fully implicit or explicit finite differencing depending on whether the local time-scales are long or short compared to the time-step. We tailor our code for the problem of cosmological re-ionization. In tests, the code conserves photons, accurately treats cosmological effects and reproduces analytic Strömgren sphere solutions. Its chief weakness is that the computation time for the LC calculation scales relatively poorly compared to other techniques ($t_{LC} \propto N_{\text{cells}}^{1.5}$); however, we mitigate this by only recomputing the Eddington tensor when the radiation field changes substantially. Our technique makes almost no physical approximations, so it provides a way to benchmark faster but more approximate techniques. It can readily be extended to evolve multiple frequencies, though we do not do so here. Finally, we note that our method is generally applicable to any problem involving the transfer of continuum radiation through a periodic volume.

Key words: radiative transfer – methods: numerical – galaxies: formation – intergalactic medium – cosmology: theory – diffuse radiation.

1 INTRODUCTION
The epoch of re-ionization is the current frontier in understanding how galaxies form and evolve over cosmic time. After the Universe cooled sufficiently to recombine hydrogen atoms at redshift $z \approx 1088$ (Spergel et al. 2007), the Universe was fully neutral. Gravity grew ever denser structures that, at $z \sim 30–50$, were able to collapse into stars and/or black holes. The radiation emitted from these first objects then began to re-ionize hydrogen. By $z \sim 6$, hydrogen re-ionization appears to be complete (Fan 2007), and the diffuse intergalactic medium (IGM) has a neutral fraction of $\sim 10^{-4}$. Understanding this transition epoch is central to understanding the origin of galaxies and the evolution of the IGM. It is a major science driver for a host of upcoming international telescope facilities, such as the James Webb Space Telescope and the Atacama Large Millimeter Array.

Re-ionization involves a complex interplay between non-linear growth of structure, radiative cooling, star/black hole formation, chemical enrichment and photon transport. Numerical simulations are required to accurately model these highly non-linear processes. However, the large dynamic range and complex physics involved make this an extraordinarily challenging computational problem. To obtain a full picture of re-ionization in the context of currently favoured hierarchical structure formation models, it is imperative that simulations include processes of star formation, galaxy formation and IGM evolution, along with feedback processes that connect all three. Cosmological hydrodynamic simulations accounting for these processes are now achieving maturity, thanks to improving algorithms and computing power. However, the inclusion of radiation transport complicates matters immensely. A cosmological radiative hydrodynamics code that can accurately evolve a representative volume with sufficient dynamic range to study how galaxies re-ionize the Universe would be a major development towards understanding re-ionization. In this paper we provide a step towards that end by introducing a new accurate moment-based method for calculating radiative transfer (RT) in a cosmological context.

Time-dependent RT is one of the most difficult components to treat in any theoretical study of the re-ionization epoch owing to the problem’s well-known high dimensionality. Consequently, over
the past decade, a number of approximate treatments have emerged that seek to render it more tractable through well-motivated physical approximations. The most flexible methods are the fully analytic treatments (for example, Madau, Haardt & Rees 1999; Wyithe & Loeb 2003; Furlanetto, Zaldarriaga & Hernquist 2004; Iliev, Scannapieco & Shapiro 2005; Kramer, Haiman & Oh 2006). These generally involve assuming values for quantities such as the gas clumping factor and the recombination rate that are averaged over all space or, in the case of the excursion-set formalism (Furlanetto et al. 2004), over the volume of an ionized region. In exchange, they readily allow for broad surveys of parameter space to be performed.

The next step in the direction of a full solution is taken by the seminumerical methods (Ciardi et al. 2000; Mesinger & Furlanetto 2007; Choudhury, Haehnelt & Regan 2008; Geil & Wyithe 2008), which combine numerically generated density fields with analytic treatments for RT using techniques such as the excursion-set formalism in order to account more realistically for source bias and the effects of inhomogeneous density fields. These treatments offer a dramatic increase in realism over purely analytic calculations at modest additional computational cost. However, they have some difficulty accounting fully for the consequences of inhomogeneous density fields such as shadowing and the tendency for low-density regions to have a lower neutral fraction during the later stages of re-ionization (Choudhury et al. 2008). These problems arise from the need of seminumerical models to make assumptions regarding the shape of the ionized regions surrounding individual sources and the non-trivial relationship between dark matter and gas densities in the non-linear regime.

Some of these difficulties are avoided in models that actually solve the RT equation on numerically generated density fields but without fully accounting for radiative feedback on the sources (Ciardi et al. 2001; Sokasian, Abel & Hernquist 2001; Mellemma et al. 2006; Iliev et al. 2007a; McQuinn et al. 2007; Pawlik & Schaye 2008; see also Iliev et al. 2006 for a very useful comparison of a number of techniques). None the less, obtaining realistic baryonic density and emissivity fields in such contexts still presents considerable challenges (McQuinn et al. 2007). Additionally, while parametrized treatments for radiative feedback have been introduced in such models in order to study, for example, whether the photoevaporation of minihaloes extends the epoch of re-ionization (Ciardi et al. 2006; McQuinn et al. 2007), the simplified nature of these studies leaves their results open to question (Mesinger & Furlanetto 2007). Hence, while each of these methods has yielded an abundance of insight into re-ionization and warrant continued development, the need is emerging for a complete solution to the RT equation that is merged self-consistently with hydrodynamical calculations.

To date, only the OTVET algorithm (Gnedin & Abel 2001) has been consistently deployed for radiative hydrodynamic calculations of re-ionization. While this technique is realistic, efficient and has broken a great deal of ground in theoretical studies of re-ionization, the possible consequences of its physical approximations remain poorly understood owing to the lack of complementary techniques.

In this work, we present a moment method solution to the RT equation (Auer & Mihalas 1970) and test it on static density fields. Our technique is highly flexible, involves a minimum of physical approximations and can readily be combined with existing hydrodynamical calculations. It is similar to the method presented by Stone, Mihalas & Norman (1992), but with several differences. First, we optimize our code only for cubical simulation volumes with periodic boundaries, as this is typical of cosmological simulations. Secondly, we derive our Eddington tensors from a long characteristic (LC) calculation in order to minimize artefacts owing to poor angular and spatial resolution. Finally, we include a treatment for non-equilibrium ionizations and account for the cosmological terms in the RT equation. In a follow-up paper, we will present its implementation within a cosmological galaxy formation code.

We do not solve for the hydrodynamic response to the radiation field, hence the temperature field is constant in time (but not necessarily in space) for all of our present calculations. For our cosmological applications (Sections 3.3.1–3.3.3 and 7), we obtain the mass-weighted baryon temperature field directly from the same simulation snapshots that are used to generate the baryon density and emissivity fields. In all other tests, the temperature is set to a uniform value of $10^4$ K unless otherwise specified.

We begin in Section 2 by casting the RT equation into the form in which we solve it and summarizing our numerical method. In Section 3, we compare the performance of LC versus two other time-independent RT techniques in order to select a method for deriving the Eddington tensor, which we need in order to close our moment hierarchy. After demonstrating that LC introduces the fewest unphysical artefacts, we optimize it for computing re-ionization using a suite of realistic albeit low-resolution integrations. In Section 4, we discuss our technique for evolving the non-equilibrium ionization field. In Section 5, we summarize our iterative scheme for weaving these ingredients into a self-consistent calculation. In Section 6, we subject our code to a number of standard tests. In Section 7, we apply our code to the problem of re-ionizing a static cosmological density field. Finally, we summarize our method and results in Section 8.

2 SOLVING THE RADIATIVE TRANSFER EQUATION

We begin this section by writing down the RT equation in comoving coordinates including emission, absorption and cosmological effects. Next, we recast the RT equation in the form that our code computes and discuss our treatment of the various terms. Finally, we discuss our approach to solving these equations numerically.

2.1 The moments of the radiative transfer equation

The RT equation in comoving coordinates is (for a derivation, see Gnedin & Ostriker 1997)

$$\begin{align*}
\frac{1}{c} \frac{\partial N_\nu(\mathbf{n})}{\partial t} + \frac{\mathbf{\hat{h}}}{a} \cdot \nabla N_\nu(\mathbf{\hat{h}}) + H \left( 2N_\nu - \nu \frac{\partial N_\nu}{\partial \nu} \right) &= c\eta_\nu - c\chi_\nu N_\nu(\mathbf{\hat{h}}).
\end{align*}$$

Here, $N_\nu(\mathbf{\hat{h}})$ represents the number of photons with frequency between $\nu$ and $\nu + d\nu$ crossing an area $dA$ in the direction $\mathbf{\hat{h}}$ into a solid angle $d\Omega$ during a time interval $dt$; $H$ is the Hubble constant; $a$ is the cosmological expansion factor; $\nabla$ denotes a gradient in comoving coordinates; $\eta_\nu$ is the local number of photons emitted per unit time per unit solid angle with frequency between $\nu$ and $\nu + d\nu$; $c$ is the speed of light and the absorption mean opacity $\chi_\nu = \sum_i \sigma_{\nu,i}$ is the sum of the opacities due to the various absorbing species. All emissivities and opacities are taken as isotropic because equation (1) is written in the cosmological comoving frame. Here and throughout our work, we compute the radiation field in terms of photon number densities rather than energy densities. For simplicity of notation, we will generally omit the $\mathbf{\hat{h}}$ dependence of $N_\nu$ from now on.

The left-hand side of equation (1) is the convective derivative of the photon phase-space density but written in terms of $N_\nu$. The
first two terms are the classical convective derivative modified to apply in comoving spatial coordinates, and the terms proportional to the Hubble constant account for, respectively, the dilution of \(N_c\) and redshifting of the photon frequencies owing to cosmological expansion. The terms on the right-hand side account for photon emission and absorption, respectively.

By integrating over the frequency range \((\nu_1, \nu_2)\), we recast equation (1) in a form appropriate for a multigroup method:

\[
\frac{1}{c} \frac{\partial N}{\partial t} + \frac{\hat{n}}{a} \cdot \nabla N = \eta - (\chi_H + \chi_{abs}) N. \tag{2}
\]

Here, we have defined the photon number density \(N\), the emissivity \(\eta\), the cosmological opacity \(\chi_H\), the spectral slope \((\nu(\partial/\partial\nu))\) and the absorption mean opacity \(\chi_{abs}\) as follows:

\[
\eta \equiv \int_{\nu_1}^{\nu_2} \eta_{\nu} \, d\nu,
\]

\[
\chi_H \equiv \frac{H}{c} \left(2 - \left\langle \nu \frac{\partial}{\partial \nu} \right\rangle \right),
\]

\[
\left\langle \frac{\partial}{\partial \nu} \right\rangle \equiv \int_{\nu_1}^{\nu_2} \frac{\partial \nu N_{\nu}}{\partial \nu} \, d\nu / \int_{\nu_1}^{\nu_2} N_{\nu} \, d\nu,
\]

\[
\chi_{abs} \equiv \int_{\nu_1}^{\nu_2} \chi_{\nu} N_{\nu} \, d\nu / \int_{\nu_1}^{\nu_2} N_{\nu} \, d\nu. \tag{7}
\]

Equation (2) is equivalent to an integral of equation (1) over frequency as long as the frequency-averaged cosmological and absorption mean opacities \(\chi_H\) and \(\chi_{abs}\) can be determined consistently. Both depend on the slope of the spectrum at each frequency bin. The dependence of the absorption mean opacity \(\chi_{abs}\) is clear, and the dependence of the cosmological opacity \(\chi_H\) can be made more intuitive by noting that, for a power-law spectrum \(N_{\nu} \propto \nu^{-a}\), the spectral slope \((\nu(\partial/\partial\nu))\) is given by \(-a\). In this case, the cosmological opacity \(\chi_H\) reduces to \((H/c)(2 + \alpha)\). This term is generically quite small in the problem of cosmological re-ionization: For star-forming galaxies and active galactic nuclei, the slope of the ultraviolet continuum generally falls within the range \(a \sim 0.3-5\), so during the re-ionization epoch \(\chi_H \sim 0.1-3 \times 10^{-26} \text{cm}^{-1}\). By contrast, even for a neutral hydrogen fraction of \(10^{-3}\) at \(z = 6\) (Fan et al. 2006), the opacity at \(912\ \text{Å}\) at the mean density is around \(3-4 \times 10^{-25} \text{cm}^{-1}\). This is simply a statement that, throughout the re-ionization epoch, ionizing photons tend to be absorbed long before they can be diluted or redshifted by the Hubble flow. For this reason, we bring the cosmological term to the right-hand side of equation (2). In multifrequency computations we will allow the spectral slope \(a\) to vary self-consistently with frequency by using the value from the previous time-step. However, in the present work, we neglect it entirely as we consider only monochromatic problems. From now on, we use the opacity \(\chi\) to refer to the sum of the cosmological and absorption mean opacities: \(\chi \equiv \chi_H + \chi_{abs}\).

The first two angle moments of equation (2) are

\[
\frac{\partial \mathcal{J}}{\partial t} = -\frac{1}{\alpha} \nabla_c \cdot \mathcal{F} + 4\pi \eta - c\chi \mathcal{J}, \tag{8}
\]

\[
\frac{\partial \mathcal{F}}{\partial t} = -\frac{c}{\alpha} \nabla_c \cdot (c \mathcal{F}) - c\chi \mathcal{F}, \tag{9}
\]

\[
\int \frac{N \hat{n} \, d\Omega}{\int N \, d\Omega}.
\]

The zeroth and first moments \(\mathcal{J}\) and \(\mathcal{F}\) are the number density and flux of photons in a frequency bin, respectively, and the Eddington tensor \(f\) is used to close the moment hierarchy; we will discuss how we obtain the Eddington tensor in Section 3.

When constructing a solution to equations (8) and (9), it is important to centre the photon number density, flux and the components of the Eddington tensor about each cell spatially in such a way that the resulting finite-difference approximation for the number density at the updated time (equation 11) is cell-centred. This is important not only to improve the solution’s accuracy in space, but also because improper centring can lead to spurious anisotropies in the radiation field or even prevent the solution from converging altogether.

Accordingly, we centre the variables as follows: \(\mathcal{J}\) and diagonal components of \(f\) are positioned at the cell centre, components of \(\mathcal{F}\) are stored at cell faces and off-diagonal elements of \(f\) are stored at cell edges (see Fig. 1).

One ambiguity remains regarding the treatment of off-diagonal elements of \(f\) such as \(f_{ij} \equiv \int \mathcal{N} \hat{n} \, d\Omega / \int \mathcal{N} \, d\Omega\). Proper centring requires that these factors always enter into the partial derivatives of equation (13) via a spatially averaged product with the photon number density \(\mathcal{J}\). For example, the finite-difference approximation for \(\mathcal{J}^{n+1}(i, j, k)\) includes, among other things, the spatial average of the product \(f_{ij} \mathcal{J}\) over the cells \((i, j, k), (i - 1, j, k), (i, j - 1, k)\) and \((i - 1, j - 1, k)\). In such instances, it is possible to use either the ‘average of the products’, \(f(\mathcal{J})\) or the ‘product of the averages’, \(f(\langle \mathcal{J} \rangle)\). Testing suggests that the differences between the two options are small, but inspection shows that the ‘average of the products’ option gives rise to significant cancelling of terms within the full finite-difference expression and hence could lead to less smooth solutions. For this reason, we prefer the ‘product of the averages’ approach.

\subsection{2.2 Solving the radiative transfer equation}

We now discuss our technique for integrating equations (8) and (9) numerically. These equations can be quite stiff when applied to
the problem of cosmological re-ionization, we use an explicit finite-differencing scheme in time. In other words, we use the photon number density and flux at the updated time on the right-hand side of equations (8) and (9). Stone et al. (1992) solved the resulting system using the ‘automatic flux-limiting’ prescription of Mihalas & Weaver (1982). This scheme proceeds by integrating equation (9) over one time-step analytically before plugging the result into an implicitly finite-differenced form of equation (8). However, Hayes & Norman (2003) found that the results from this technique do not differ significantly from the results of simply finite-differencing equation (9). Our own testing also indicates that the latter technique produces accurate results, hence in our code we used the updated flux $F^{n+1}$ and number density $J^{n+1}$ to relate to the previous values $F^n$ and $J^n$ as follows:

$$J^{n+1} = \frac{1}{1 + x^{n+1}} \left\{ F^n + 4 \eta_i \Delta t \frac{\partial}{\partial x} \left( \frac{F^n}{1 + x^{n+1}} \right) + c^2 \Delta t \frac{\partial}{\partial x} \left( \frac{F^{n+1}}{1 + x^{n+1}} \right) \right\},$$

(11)

$$F^{n+1} = \frac{1}{1 + x^{n+1}} \left[ F^n - c^2 \Delta t \frac{\partial}{\partial x} \left( f J^{n+1} \right) \right],$$

(12)

where the index $i$ runs over all source cells and $f$ runs over all source cells and $x^{n+1} \equiv c \kappa_{\lambda}^{n+1} \Delta t$.

These equations can be combined and rearranged into the form

$$A \cdot J^{n+1} = b,$$

(13)

where the vector notation indicates that we are solving a coupled system of algebraic equations with dimension equal to the number of computational cells. The update matrix $A$ is a function of $J^n$ and $F^n$ but not $J^{n+1}$, hence the photon number densities may be updated via a simple matrix inversion. The photon number density in each cell couples only to 18 of its neighbouring cells. Consequently, only 19 elements in each row of $A$ are non-zero, making it a sparse matrix.

Linear systems of equations for which the coefficient matrix is sparse but not both symmetric and positive definite can be solved via the biconjugate gradient method. We have found that the preconditioned biconjugate gradient routine LINBCG in Numerical Recipes (Press et al. 1992) solves the problem rapidly. We use the diagonal of $A$ as the preconditioner and halt the iteration when the residual $|A \cdot J^{n+1} - b|/|b|$ is less than $10^{-6}$.

We generalize this technique to multifrequency problems by solving equations (11) and (12) independently for a number of multi-group frequency bins. We compute the Eddington tensor $f$, absorption mean opacity and cosmological opacity fields separately for each frequency bin. When evaluating equations (5)–(7), we use the spectrum $J(\nu)$ from the previous time-step.

### 3 Computing the Eddington Factors

As is well known, the primary difficulty in solving the RT equation lies in its high dimensionality. Treating the moments of the equation does not suppress this dimensionality unless the photon mean free path is short compared to all length scales of interest, in which case one can close the moment hierarchy with analytical flux limiters (e.g. Hayes et al. 2006). This is not the case in the problem of cosmological re-ionization, hence an accurate solution depends critically on an accurate derivation of the Eddington tensor $f$. This in turn requires knowing how the photon density $N$ varies as a function of direction $\hat{n}$ (see equation 10). A fully consistent treatment would obtain $N(\hat{n})$ via a time-dependent integration of the RT equation; however, if this was easily done then of course the entire problem would already be solved. Here, we derive the Eddington tensor $f$ from a time-independent formal solution to the RT equation (that is, a solution in which $\partial N / \partial t = 0$; see also Auer & Mihalas 1970; Stone et al. 1992). We note that this is our only approximation.

Previous efforts have approached this problem through computationally efficient techniques such as source characteristics (SC; Stone et al. 1992, Hayes & Norman 2003) or the optically thin approximation (Gnedin & Abel 2001). While these techniques have their strengths and have led to a great deal of insight into re-ionization, the associated compromises in accuracy are poorly understood. For this reason, we undertake an accurate calculation of the Eddington tensor, even though this degrades our computational efficiency, in order to study its impact on cosmological problems. In this section, we begin by reviewing the LC technique for computing the Eddington tensor $f$. We then compare it to SC and the optically thin approximation in order to highlight the strengths of LC. Finally, we optimize LC for calculations of cosmological re-ionization.

### 3.1 Long characteristics

The LC approach to computing $N(\hat{n})$ at a target cell consists of integrating the (time-independent) RT equation along characteristics that run in the directions $\hat{n}_i$ from the target cell to the source cells $i$. The photon density at the target cell is then given by the sum

$$N(\hat{n}) = \sum_i \frac{n_i}{c_i} e^{-\tau_i} \delta(\hat{n} - \hat{n}_i),$$

(14)

where the index $i$ runs over all source cells and $\tau_i$ is the total optical depth between the target cell and the source cell $i$. The problem of computing $N(\hat{n})$ at a target cell hence reduces to one of determining the total optical depth $\tau_i$ to each source cell. Here, we outline our approach to computing $\tau_i$ (see also Fig. 2). We note that this treatment is similar to the ray-tracing technique of Abel, Norman & Madau (1999).

Consider the contribution to the Eddington tensor in a target cell whose centre is located at $r_T \equiv (x_T, y_T, z_T)$ owing to a source cell $i$ whose centre is located at $r_i \equiv (x_i, y_i, z_i)$. We compute the optical depth between the two cells by integrating along a ray that points in the direction $\hat{n} = (n_x, n_y, n_z) = (r_i - r_T)/(|r_i - r_T|)$. Starting at $r_T$, the direction in the distance $\Delta z$ to the nearest $y$–$z$ plane $\Delta r_z$ is given

![Figure 2. A sketch of our LC method in two dimensions. LC from the bottom-left cell to sources 1 and 2 are shown; the line integral to source 3 is halted when it encounters an intervening optically thick cell.](https://academic.oup.com/mnras/article-abstract/393/4/1090/1004335)
by

\[ \Delta r_i = \left[ \frac{\Delta x}{2} - \text{sign}(x_i - x) \right] \sqrt{1 + \left( \frac{n_y}{n_x} \right)^2 + \left( \frac{n_z}{n_x} \right)^2}, \]

(15)

where \( \text{sign}(x) \) equals \(-1\) or \(+1\) if \( x \) is negative or positive, respectively. Analogous relations exist for the distance to the next \( x-z \) boundary \( \Delta r_i \) and the next \( x-y \) boundary \( \Delta r_j \). We determine which cell the ray enters next by evaluating which of the three distances is shortest; for example, if \( \Delta r_i < \Delta r_j \) and \( \Delta r_i < \Delta r_j \), then the ray will next encounter a \( y-z \) plane. We then add the contribution \( \chi \Delta r_i \) to the optical depth from the cell that the ray just traversed assuming that \( \chi \) is uniform throughout the cell. Repeating this procedure, we continue adding contributions to the line integral until either the ray enters the source cell or the accumulated optical depth exceeds a maximum value \( \tau_{\text{max}} \) that will be determined from convergence testing. If the accumulated optical depth exceeds \( \tau_{\text{max}} \) before the ray enters the source cell \( i \), then we consider the source to be completely obscured and halt the line integral. Otherwise, we add the contribution of the source cell to the Eddington tensor at the target cell and proceed to the next source cell.

If the cell is itself a source, then we account for the contribution of its self-illumination to its Eddington tensor \( f \) by adding \( (4 \pi \Delta N_0 / 3) \mathbf{I} \) to the numerator and \( 4 \pi N_0 \) to the denominator in equation (10), where \( \mathbf{I} \) indicates the unit tensor and \( N_0 \) is given by

\[ N_0 = \frac{\eta}{\chi}(1 - e^{-\tau_i}), \]

\[ r_i = \left( \frac{\Delta x \Delta y \Delta z}{(4/3) \pi} \right)^{1/3}. \]

### 3.2 Comparison of techniques

#### 3.2.1 Short characteristics

A well-known difficulty with cosmological re-ionization is the large number of sources involved. The computation time for SC in its original form (Kunasz & Auer 1988; Stone et al. 1992) does not scale with the number of sources, hence we considered whether it would be an appropriate method for computing the Eddington tensor field. Here we compare the performance of SC versus LC for the simple case of an isolated point source in a homogeneous medium. Note that different flavours of SC (Mellama et al. 2006; Rijkhorst et al. 2006), which do scale with the number of sources, perform much better in this scenario, hence our conclusions apply only to SC as described by Kunasz & Auer (1988).

SC involves solving the RT equation within each cell along characteristics that run from the cell’s faces to its centre using boundary conditions at the cell faces that are obtained through interpolation. Given the boundary conditions on the computational volume, one simply marches downstream from one side of the volume to the other so that, at each cell, the upstream boundary conditions are always known. SC is an efficient technique for computing a time-independent formal solution to the RT equation (or even a time-dependent one; see Hayes & Norman 2003): in three dimensions, the computation time-scales with the number of cells on each side of the computational grid \( n_{\text{grid}} \) as \( O(n_{\text{grid}}^3) \). Unfortunately, if the emissivity or opacity varies significantly on the scale of the computational grid, then the interpolations can give rise to dramatic numerical artefacts in the spatial distribution of the photon number density. In the problem of cosmological re-ionization, sources are generally point-like and there are sharp transitions between optically thick and thin regions (for example, at ionization fronts), hence such artefacts are expected. Additionally, in the presence of point sources, the number of angles that must be sampled in order to yield smooth ionization fronts can scale as poorly as \( O(n_{\text{grid}}^3) \), yielding a less favourable overall scaling of \( O(n_{\text{grid}}^5) \) (Razoumov & Scott 1999; Nakamoto, Umemura & Susa 2001).

In order to demonstrate the anisotropies that arise around point sources in SC, we consider the idealized case of a galaxy consisting of \( 10^8 \, M_\odot \) of young stars at \( z = 20 \) with an ionizing escape fraction of 10 per cent. We locate the galaxy at the centre of a homogeneous region 0.5 (proper) Mpc on a side in which pure hydrogen of total number density \( 1.5 \times 10^{-3} \, \text{cm}^{-3} \) and temperature \( 10^4 \, K \) is ionized to a neutral fraction of \( 10^{-3} \). We solve the time-independent RT equation for this scenario using both SC and LC. In the SC case we sample the unit sphere with 320 uniformly distributed unit vectors. In both cases we use a grid resolution of 64\(^3\) cells.

In Fig. 3 we show contours of photon number density versus position in a plane that contains the source as calculated using SC (black solid) and LC (red dotted).

The strong anisotropies resulting from the interpolations that are inherent to SC compare unfavourably to LC, which does not involve interpolations.

#### 3.2.2 Optically thin approximation

The optically thin approximation (Gnedin & Abel 2001) involves evaluating equation (10) via a time-independent formal solution to the RT equation in which the opacity is neglected. Specifically, \( \chi \) is calculated from the sum total of all photons emitted in the volume, with no attenuation. This approach conserves photons, does not suffer from some of the grid-induced artefacts that can occur in the SC approach, and yields results that are qualitatively reasonable.
Moreover, the computation time scales as $O(N^3)$. These desirable characteristics motivate us to evaluate the benefits of accurately accounting for the optical depth, and the most direct way to do so is simply to compare the results of using optically thin versus accurate Eddington tensors within our moment method. Our LC code is well suited for performing such a comparison. For this reason, we revisit the problem of multiple sources embedded in an initially optically thick medium. In the optically thin approximation, a source can affect the Eddington tensor in the vicinity of a neighbouring source even before their respective H\textsc{ii} regions have overlapped. This can potentially lead to errors in the shape of the resulting ionization fronts even before they overlap (see also Gnedin & Abel 2001).

We consider the problem of a bright source with a monochromatic ionizing luminosity of $5 \times 10^{48} \text{s}^{-1}$ located 2.2 kpc from a faint source whose luminosity is $5 \times 10^{47} \text{s}^{-1}$. Both sources are embedded in a homogeneous medium of pure hydrogen with number density $10^{-3} \text{cm}^{-3}$ and temperature $10^4 \text{K}$. The medium is initially entirely neutral. In this arrangement, the flux from the bright source dominates that of the faint source at a distance from the faint source equal to one quarter of the faint source’s Strömgren radius. We evolve this system with Eddington tensors obtained from LC and the optically thin approximation until the sources’ H\textsc{ii} regions overlap at $t \approx 5 \text{Myr}$. We use a grid of $80^3$ computational cells and disable periodic boundary conditions.

In Fig. 4, we compare the resulting neutral fractions along the line passing through the source centres before, during and after overlap. At $t = 0.5 \text{Myr}$, the two H\textsc{ii} regions are evolving approximately correctly in the optically thin approximation although there is a suggestion that photons stream too rapidly along the direction connecting the two sources. By $t = 1.5 \text{Myr}$, there is a noticeable tendency for the ionization fronts to advance too rapidly between the two sources in the optically thin case. This tendency oversuppresses the neutral fraction in this region. By $t = 2.5 \text{Myr}$, it is clear that overlap has occurred too soon in the optically thin approximation. Finally, after overlap has occurred ($t = 5 \text{Myr}$) the optically thin approximation performs well again because, at least within the ionized region, it is no longer a strong approximation.

In Fig. 5, we compare the morphologies of the H\textsc{ii} regions at $t = 2.1 \text{Myr}$. The left- and right-hand panels show the results of using the optically thin approximation and LC, respectively. Looking at the right-hand panel first, we see that the H\textsc{ii} regions show slight departures from spherical symmetry even with accurate Eddington tensors, appearing slightly boxy in this projection owing to low spatial resolution. In addition to this asymmetry, however, the smaller H\textsc{ii} region appears dramatically elongated prior to overlap when we use the optically thin approximation to compute the Eddington tensors. In fact, the optically thin approximation causes both H\textsc{ii} regions to elongate along the axis that connects the two sources, leading to the early overlap seen in Fig. 4.

What effect do morphological errors and a tendency towards early overlap have on galaxy evolution during the recombination epoch? Figs 4 and 5 suggest that the errors will be small on scales that are larger than the largest ionized regions at any given time. The fact that moment methods automatically conserve photons irrespective of the Eddington tensors reinforces this view. However, at smaller scales it is possible that galaxy evolution in satellite haloes will be oversuppressed, especially in regions between larger haloes. Such an error could in turn lead to an underestimate of the number density of smaller ionized regions, which may dominate the photon budget of overdense regions (Iliev et al. 2007b). The only way to settle this question will be through full-scale simulations of re-ionization in which the two techniques can be compared.

### 3.3 Optimizing the long characteristics calculation

Our LC calculation of the Eddington tensors is time consuming. To optimize the calculation, we introduce some numerical approximations. Because these approximations are numerical and not physical, it is possible to rigorously assess the errors introduced through convergence tests. The key optimization is that we only recompute the Eddington tensor field when the radiation field has changed significantly, and not at every time-step of the moment solver. Since in typical cosmological situations the radiation field evolves relatively slowly over much of the volume, this results in many fewer LC calculations. In this section we discuss our optimizations and quantify the errors.

The first problem that we must address is the way that we smooth the Eddington tensor field. Smoothing is necessary because discontinuities in the opacity field (for example, around isolated sources or at ionization fronts) give rise to discontinuities in the Eddington tensor field, which in turn imprint numerical artefacts on to the morphology of the radiation and ionization fields. In extreme cases, these discontinuities can prevent the code from converging altogether (as also noted by Razoumov & Scott 1999). While the optimal solution to these problems would be to enforce a spatial resolution at which no cell is optically thick, this condition is computationally prohibitive. We have found that smoothing the Eddington tensor field largely removes the numerical effects (see, however, Fig. 5). We employ a ‘cubical tophat’ smoothing filter whose length is three times the length of a single computational cell; in other words, the filter subtends 27 cells and weights them equally. This smoothing prevents the radiative pressure tensor $c f \mathcal{J}$ from varying too rapidly on the scale of our finite-difference stencil (equation 11). It does not degrade the quality of our solution for two reasons: (1) it does not impact photon conservation, and (2) it
does not reduce the solution’s spatial resolution because the moment method is already second order in space; that is, we smooth over the same spatial scales used to compute the spatial derivatives.

Next, we turn to the choice of numerical parameters. Our implementation of LC introduces three parameters: (1) the maximum optical depth from a target cell to a source cell $\tau_{\text{max}}$ beyond which we consider the source to be obscured and halt its LC line integral; (2) the depth $n_d$ of periodic replicas that we use to mimic periodic boundaries and (3) the minimum fractional change in photon number density $f_j$ required to trigger an update to a cell’s Eddington tensor. We select optimal values for each of these parameters by running parameter convergence tests: For each parameter, we compute the re-ionization of a cosmological density field at moderate spatial resolution assuming a range of values for the parameter while holding the other parameters constant. We then determine what parameter value leads to a 10 per cent median accuracy in the photon number density $J$. Note that (as we have directly verified) this is equivalent to requiring a 10 per cent median accuracy in the neutral fraction $x_{\text{HI}}$.

We obtain the initial conditions for these convergence tests by dividing the gas and stellar densities from the $z = 9$ snapshot of an $8 \, h^{-1}$ Mpc cosmological volume (the w8n256vzw simulation of Oppenheimer & Davé 2006) on to a $16^3$ grid. We divide the total mass associated with smoothed particle hydrodynamics (SPH) particles that lie near cell boundaries between the cells by summing incomplete gamma functions to their equivalent Plummer SPH smoothing kernels. We assume that all gas is completely neutral at $z = 9$. We compute the cell emissivities by convolving the stellar populations in each cell with the Bruzual & Charlot (2003) stellar population synthesis models and assuming a 10 per cent escape fraction for ionizing photons. During the integration, we account for cosmological expansion by assuming ($\Omega, \Lambda, H_0) = (0.3, 0.7, 70)$. With this set-up, we find that the volume-averaged neutral fraction drops to roughly $x_{\text{HI}} = 10^{-3}$ at $z = 6$ (Fig. 16), in good agreement with available constraints (Fan et al. 2006), hence our convergence tests are realistic.

3.3.1 Optimizing the maximum optical depth

We look for an optimal maximum optical depth $\tau_{\text{max}}$ beyond which the effect of terminating the LC line integrals is small. To do so, we compute the re-ionization of our cosmological test case assuming $\tau_{\text{max}} = 1, 5, 6$ and 1000 and using the hybrid treatment for the periodic depth $n_d$ (see Section 3.3.2). We compare in Fig. 6 the resulting errors.

The top panel shows how the median fractional error in the local photon number density $J$ varies with integration time, where we compute the fractional errors by comparing against the $\tau_{\text{max}} = 1000$ test case. At early times $[\log(x_{\text{HI}}) > -0.5]$ the fractional errors are small regardless of the choice of $\tau_{\text{max}}$. This simply reflects the fact that, at this epoch, re-ionization is dominated by scales below...
our spatial resolution so that RT between cells is subdominant to self-ionization of individual cells. As \( \log(x_{\text{HI}}) \) drops below \(-0.5\), however, the transport of photons between cells becomes more important and the errors in the LC calculation become noticeable. The errors reach a maximum at the point when the individual \( \text{H} \text{\textsc{i}} \) regions begin to overlap \( \log(x_{\text{HI}}) \sim -1 \), and then begin to decline slowly as the universe becomes increasingly optically thin. The slow decline in errors at late times owes to the fact that cells can ‘see’ more sources and the Eddington tensors become more nearly isotropic irrespective of \( \tau_{\text{max}} \). Comparing the error trends for different values of \( \tau_{\text{max}} \), we find that the accuracy errors seem nearly converged even for \( \tau_{\text{max}} = 1 \).

The bottom panel shows the distribution of accumulated fractional errors in local photon number density at the point where the neutral fraction \( x_{\text{HI}} \) has dropped to 7 per cent. There is a peak in the error distribution near 10–20 per cent, with significant tails out to low errors and a few regions with errors of order unity. We find no correlation between the magnitude and fractional error in \( J \); in other words, bright regions are equally as likely as faint ones to suffer large fractional errors. As in the top panel, the solution seems generally converged even for \( \tau_{\text{max}} = 1 \) although the errors for \( \tau_{\text{max}} = 5 \) and 6 are slightly lower systematically. Evidently, choosing \( \tau_{\text{max}} = 1 \) would be sufficient to guarantee a median accuracy better than 10 per cent at all times; however, in order to be conservative, we choose \( \tau_{\text{max}} = 6 \).

### 3.3.2 Optimizing the periodic depth

Hydrodynamical simulations of cosmological volumes assume periodic boundaries. We are thus faced with the problem of accounting for periodic boundaries in our LC calculations. Unfortunately, an analytic treatment is impossible as it cannot be determined a priori whether a cell can ‘see’ a source in a periodic replica of the volume. The only obvious treatment is the brute-force approach of mimicking periodic boundaries by positioning periodic replicas around the simulation volume. Each source is then reproduced in each replica, and the LC line integrals must be computed from each cell in the central volume to each copy of each source. We use the periodic depth parameter \( n_{\text{g}} \) to indicate the depth of the periodic replicas. For example, \( n_{\text{g}} = 1 \) corresponds to positioning 26 replica volumes about the simulation. Clearly, accuracy and computation time both grow with \( n_{\text{g}} \). Our problem thus reduces to determining the minimal value of \( n_{\text{g}} \) that allows for better than 10 per cent accuracy at all times.

It is tempting to suppose that, since the universe is optically thick until the neutral fraction \( x_{\text{HI}} \) drops below \( \sim 10^{-3} \), using \( n_{\text{g}} = 1 \) should be adequate until then. However, straightforward testing indicates that this leads to median errors in photon number density that approach 10 per cent even when \( x_{\text{HI}} > 5 \) per cent. In order to determine what value of \( n_{\text{g}} \) leads to converged behaviour, we have computed the re-ionization of a static density field from \( z = 9 \) to 6 using \( n_{\text{g}} = 1, 2, 5 \). We also introduce a hybrid scheme in which \( n_{\text{g}} \) changes from 1 to 2 when the mean neutral fraction drops below 0.5, which, as we will show, is the best alternative.

In Fig. 7, we show how the resulting fractional errors vary with time. The top panel shows the median fractional error in local photon number density as a function of time. We compute the fractional error by comparing with the \( n_{\text{g}} = 5 \) result, which yields a very nearly converged solution for low neutral fractions and completely converged solutions for \( x_{\text{HI}} > 50 \) per cent. At early times \( (x_{\text{HI}} > 0.6) \), the universe is so optically thick that few cells are affected by sources in replica volumes. In this regime, using \( n_{\text{g}} = 1 \) leads to negligible errors. As \( x_{\text{HI}} \) approaches 0.5, however, some of the \( \text{H} \text{\textsc{i}} \) regions grow to substantial fractions of the simulation volume and cross its boundaries so that the median fractional error begins to rise. By the time \( x_{\text{HI}} = 0.01 \) (\( z \approx 6.3 \)), the median fractional error exceeds 1 per cent even if \( n_{\text{g}} = 2 \). Not surprisingly, the errors from \( n_{\text{g}} = 1 \) are larger at all time-steps.

The bottom panel shows the distribution of accumulated fractional errors in local photon number density at the point where the neutral fraction has dropped to 7 per cent. There is a peak in the error distribution near 10–20 per cent, with significant tails out to low errors and a few regions with fractional errors of order unity. The errors in the hybrid scheme are comparable to the errors for \( n_{\text{g}} = 2 \), with a median error of 3 per cent. Noting that the errors generally increase with time-step, we conclude that the hybrid scheme leads to median errors that are always \( \leq 10 \) per cent.

The hybrid \( n_{\text{g}} \) scheme speeds up our code significantly. We have verified through direct testing that the LC computation time varies with the periodic depth roughly as \((2n_{\text{g}} + 1)^3\) (that is, proportional to the total number of volumes), regardless of both the spatial resolution and the ionization state of the universe. It follows that, for a calculation in which \( x_{\text{HI}} \) drops below 50 per cent after roughly half of the total integration time has elapsed, using hybrid \( n_{\text{g}} \) rather than using \( n_{\text{g}} = 2 \) reduces the computation time by up to \( \approx 40 \) per cent without affecting the accuracy.

Finally, it is possible that the accuracy of the hybrid \( n_{\text{g}} \) scheme varies with the age of the universe, the baryonic clumping factor and the length of the computational volume in addition to \( x_{\text{HI}} \) because each of these factors potentially impacts the number of optically
thin lines of sight through a cosmological volume. Of these, the dependence on the length is the strongest since, for representative cosmological volumes, the relationship between $x_{\text{HI}}$, baryonic clumping factor and the age of the universe is unique. The present scheme achieves the required 10 per cent accuracy for any volume whose length is $\geq 8\, h^{-1}\, \text{Mpc}$ because larger volumes are pierced by fewer optically thin lines of sight at given $x_{\text{HI}}$.

3.3.3 Optimizing the Eddington tensor update criterion

Our technique involves periodically updating the Eddington tensor field in order to maintain consistency with the time-dependent integration. Naturally, more frequent Eddington tensor updates lead to a more accurate solution; in fact, Auer & Mihalas (1970) recommend iterating to convergence between the radiation and Eddington tensor fields. Unfortunately, this approach would be prohibitively time-consuming for our problem. Instead, we opt to update the Eddington tensor in a given computational cell only when the radiation field has changed significantly in that cell; this technique has been shown to be an excellent approximation in other contexts (for example, Hubeny & Burrows 2007). In particular, after each time-step, we recompute the Eddington tensor in those cells where the photon number density has undergone a fractional change greater than $f_J$ in at least one frequency bin since the last update to its Eddington tensors. In order to determine how the resulting errors vary with $f_J$, we compute the re-ionization of a static density field from $z = 9$ to 6 using $f_J = 0, 0.01, 0.05, 0.1$ and 0.5.

In Fig. 8, we show how the resulting fractional errors vary with time. This figure demonstrates the power and flexibility of the moment method: even if we only compute the full angular dependence of the radiation field when it has changed by more than a factor of 2 ($f_J = 0.5$), the typical local errors are better than 20 per cent at all times. Most importantly, because setting $f_J > 0$ results in less-frequent updates to the Eddington tensor field, it speeds up the computation considerably. Through direct testing, we find that the computation time $t$ for our re-ionization calculation varies with $f_J$ as $t \propto f_J^{-0.5}$.

We now examine the top panel of Fig. 8 in more detail. At early times ($x_{\text{HI}} > 0.5$), errors are small because re-ionization is dominated by the self-ionization of small, overdense regions rather than by radiation transport. Eddington tensor updates are frequent in overdense regions owing to the rapidly evolving $J$, but they are also fast because, in an optically thick universe, the $\tau_{\text{max}}$ parameter insures that most of the LC line integrals terminate well before they arrive at the source. After $x_{\text{HI}}$ drops below 0.5, the errors begin to grow. However, rather than growing without bound, they level off at a characteristic value that in turn grows with $f_J$. This is the regime in which setting $f_J > 0$ yields the biggest savings in computation time because, on average, the LC line integrals traverse more cells before reaching $\tau_{\text{max}}$. On the other hand, the radiation field evolves more slowly because the rapidly evolving overdense regions are already largely re-ionized. Hence setting $f_J > 0$ corresponds to culling the most expensive Eddington tensor updates aggressively while preserving the overall accuracy.

The bottom panel of Fig. 8 indicates that the distribution of errors shifts to smaller errors with decreasing $f_J$, with values of $f_J$ less than 0.1 leading to median errors $\leq 10$ per cent. In practice, errors may be slightly larger as the median error at a given time-step and $f_J$ increases slightly with increasing spatial resolution. Moreover, Fig. 8 does not address errors in the topology of the ionization field, which may vary differently with $f_J$ (although McQuinn et al. 2007 argue that the topology of re-ionization is dominated by the emissivity field and $x_{\text{HI}}$ and does not vary strongly with other parameters). The appropriate choice of $f_J$, therefore, depends on the problem. However, for reference, we note that choosing $f_J = 0.05$ generally leads to median errors that are better than 10 per cent while speeding up the calculation by roughly a factor of 3.

3.3.4 Full error budget

In Fig. 9, we summarize the results of these convergence tests by comparing the distributions of errors in accuracy at $t = 285$ that result from our fiducial choice of numerical parameters. The median errors for $\tau_{\text{max}} = 6$, hybrid $n_S$ and $f_J = 0.05$ are 8.0, 2.1 and 2.2 per cent, respectively. Hence our fiducial choice of parameters leads to a typical numerical accuracy of 10 per cent in $J$.

3.4 Computational scaling

The computation time for LC, $t_{\text{LC}}$, is proportional to the number of cells $n_{\text{grid}}^3$, the number of cells containing sources $n_S$ and the average length of a line integral in cells $n_l$: $t_{\text{LC}} \propto n_{\text{grid}}^3 n_S n_l$.

Both $n_S$ and $n_{\text{grid}}$ generally vary with spatial resolution as well as with the mean opacity. In the limit of an optically thin volume ($n_l \sim n_{\text{grid}}$) with non-zero emissivity everywhere ($n_S = n_{\text{grid}}$), $t_{\text{LC}} \propto n_{\text{grid}}^3$, while in the limit of an optically thick medium ($n_l$ constant) and highly clustered sources ($n_S$ constant) the scaling flattens to $t_{\text{LC}} \propto n_{\text{grid}}$. Because $t_{\text{LC}}$ potentially scales quite unfavourably with $n_{\text{grid}}$, we expect that it will ultimately dominate our spatial resolution limit. Hence, it is of interest to determine where the scaling falls for our problem. To do so, we gridded the same cosmological snapshot used in Section 3.3 on to grids of increasing spatial resolution assuming...
n−6 to n−7. On the other hand, the generally longer computation times and steeper scaling at low xHI indicate that our code will slow down considerably as the mean neutral fraction drops below 0.01. In future work we plan to study how to transition to the much faster optically thin approximation at this epoch without introducing significant inaccuracies.

4 SOLVING FOR THE NON-EQUILIBRIUM IONIZATION STATES

In order to compute cosmological re-ionization, we must integrate the non-equilibrium equations for ionization and recombination of hydrogen and helium. A thorough discussion of the relevant chemical processes including analytic fits for the cross-sections and reaction rates is provided by Abel et al. (1997) and Anninos et al. (1997). Here, we focus on deriving a technique for integrating these equations. We neglect H+ and H2 because we do not anticipate being able to resolve the mass scales at which these species are expected to dominate (≪106 M⊙; see e.g. Couchman & Rees 1986). However, it would be trivial to extend our technique to account for these species as well.

Following Anninos et al. (1997), we write the equation that governs the abundance of species i schematically as

\[ \frac{\partial n_i}{\partial t} = C_i(T, n_j) - D_i(T, n_j)n_i, \]  

where \( C_i \) and \( D_i \), respectively, represent source and destruction terms summed over all species \( j \) that can convert to or result from species \( i \). Equation (16) can be modified to hold in an expanding universe by redefining \( n_i \) as the comoving number density and normalizing the reaction rate coefficients by \( a^2 \).

Equation (16) can be quite stiff; that is, its terms can evolve on very different time-scales from each other. This property has led many authors to adopt unconditionally stable integration techniques (see e.g. Anninos et al. 1997; Mellema et al. 2006). Unfortunately, stable techniques are not necessarily accurate. Moreover, within cosmological density fields the time-scales of the terms in equation (16) can vary rapidly with position. For example, we have found that the time-scales encountered during a typical re-ionization calculation at our expected spatial resolution can vary between 10^2 and 10^4 Myr at a given time. We have explored the stability and accuracy of a number of integration techniques when applied to a range of gas densities and ionization time-scales. Here we discuss two techniques, a fully implicit (FI) backwards differencing formula and second-order Runge–Kutta (RK2).

Figure 9. The distributions of accuracy error at \( t = 285 \) for our fiducial choice of numerical parameters (\( \tau_{\text{max}}, n_3, f_J \)) = (6, ‘hybrid’, 0.05). For this set of parameters, the error is dominated by the error owing to our choice of \( \tau_{\text{max}} \). Adding the median errors in quadrature, we expect a typical error of 9 per cent in \( J \).

Figure 10. LC computation time versus number of grid cells to a side in the case of a mostly neutral (solid, black) and highly ionized (dashed, red) universe. The scaling flattens to \( n_{\text{grid}}^{3.4} \) at high resolution, depending on the neutral fraction xHI.
where all densities on the right-hand side are evaluated at the updated time. This fully implicit technique is accurate to first order in time and is stably stable (Gear 1971). We solve the resulting set of algebraic equations using Newton–Raphson iteration. For 1-Myr time-steps, we have found that the iterative solution converges to within a tolerance of $10^{-3}$ in fewer than four iterations, hence it is also reasonably efficient. However, evaluating and inverting the Jacobian is time-consuming. Moreover, in regimes where the shortest time-scale is comparable to the time-step, its accuracy suffers because the rate coefficients at the end of the time-step are not a good approximation for their time-step-averaged values.

Second-order explicit Runge–Kutta methods are accurate to second order in time and can be computed rapidly, but they become unstable if the time-step is comparable to or longer than the shortest relevant time-scale. We have implemented the standard form of RK2 (e.g. Press et al. 1992). In addition, we have implemented a hybrid technique that combines the accuracy of RK2 around long time-scales with the stability of implicit methods at short time-scales. To do so, the hybrid technique simply checks all relevant time-scales before each time-step and uses RK2 whenever the time-step is shorter than the shortest relevant time-scale.

We test these techniques by solving equation (16) for a single zone composed of pure hydrogen. The zone has a uniform, constant total number density and is initially entirely neutral. The ionizing radiation field is time independent, and we refer to its intensity by its associated ionization time-scale $t_I$. The relevant processes are radiative ionization, collisional ionization owing to collisions with electrons and radiative recombination assuming case-B recombination rates. We evolve the ionization state using 0.5-Myr time-steps for 50 Myr and then determine the accumulated fractional error in the numerical result by comparing to the analytical solution. The temperature of the gas is fixed at $10^4$ K, the total number density is $1.66 \times 10^{-3} \text{cm}^{-3}$, roughly the cosmological mean density at $z = 9$, and we ignore Hubble expansion for simplicity.

In Fig. 11, we compare the results of performing the test integration with our three schemes versus the analytical solution. In the top panel, we find that the accumulated fractional error varies non-trivially with $t_I$. For small $t_I$ (i.e. intense ionizing backgrounds) the solution reaches ionization equilibrium well before the integration ends. In this ‘equilibrium regime’ the error grows with decreasing $t_I$. We have found that the accuracy here cannot be further improved by integrating with smaller time-steps or switching to a higher order finite differencing scheme in time [for example, note that the second-order accurate RK2 scheme yields the same magnitude of error as the first-order accurate FI scheme for $\log(t_I) = -0.5–1$]. The ‘error floor’ owes directly to roundoff error: if the machine accuracy is $\epsilon_m$ and if the solution is close enough to equilibrium that the change in the next time-step is small compared to the current solution, $|n_n| \Delta t < \epsilon_m n_i$, then the error cannot decay.

For large enough $t_I$ (weak ionizing backgrounds), the solution does not reach ionization equilibrium and roundoff error becomes subdominant. In this ‘non-equilibrium regime’ the error is dominated by the usual truncation error in the finite-differencing scheme with the result that using shorter time-steps or switching to a higher order finite differencing scheme improves the accuracy, as can immediately be seen from Fig. 11. We repeated this test integration with a range of densities, time-steps and integration times. In the non-equilibrium regime, we find that RK2 consistently yields accuracies better than 1 per cent while FI often yields fractional errors of order unity.

To evaluate how much computation time we save through our hybrid technique, we tracked the number of calls to each of the two ionization routines throughout a test calculation of re-ionization similar to that in Section 7 but with only 8$^3$ computational cells. Before re-ionization ($x_{HI} > 50$ per cent) RK2 is chosen 91 per cent of the time, while after re-ionization it is chosen 38 per cent of the time. Overall, RK2 is called 52 per cent of the time. Noting that RK2 is 4 times faster than FI, our use of a hybrid technique rather than relying only on FI roughly halves the time required for evolving the ionization state. In other words, it simultaneously improves both the accuracy and the efficiency of our technique.

The bottom panel can be used to determine whether our tests span the domain of physical conditions that arise in cosmological calculations. At our anticipated spatial resolution (>50 $h^{-1}$ kpc), $t_I$ ranges between $10^{-4}$ and $10^2$ Myr while the final (that is, post-recombination) hydrogen neutral fraction ranges between $10^{-7}$ and 1. Our test calculations clearly span this domain, hence we conclude that our hybrid integration technique stably and efficiently yields fractional errors of $\leq 1$ per cent throughout our problem’s domain.
5 PUTTING IT ALL TOGETHER

Having discussed our techniques for updating the Eddington tensor, radiation and ionization fields, we now turn to our method for combining these ingredients into a single code. Fig. 12 illustrates our algorithm for computing a single time-step. At the beginning, we solve self-consistently for the updated photon number densities $J^{n+1}$ and ionization states $n^{i+1}$ in terms of the previous values $(J^n, F^n, n^i)$ through iteration. Schematically, we loop through the following calculations until the solutions have converged:

$$J^{n+1} = J^{n+1}(J^n, n^{i+1}, F^n),$$
$$n^{i+1} = n^{i+1}(J^{n+1}, n^i).$$

During the first iteration of each time-step, we use the values from the previous time-step as the initial guess for the updated values.

Because this scheme does not converge for general initial conditions and time-step $\Delta t$, we must include a treatment for reducing the time-step whenever necessary. We have implemented an adaptive stepsize scheme that is designed to collapse the time-step rapidly during the first iteration of each time-step, we use the values from the previous time-step as the initial guess for the updated values.

(i) If the maximum fractional change in $J$ between iterations drops below $10^{-4}$, then we consider the solution to have converged. We halve the integration and advance the time-step.

(ii) If the fractional changes in $J$ do not reach $10^{-4}$ in 15 iterations, we divide $\Delta t$ by 4 and restart the iteration.

(iii) If four consecutive substepped iterations converge, then we multiply $\Delta t$ by 2.

(iv) If the substepped time-step becomes smaller than $10^{-5}$ of the original time-step, then we consider the computation to have diverged. In this case, we terminate the integration.

After updating the radiation and ionization fields, we compute the updated fluxes $F^{i+1}$. We then compute the fractional change in each cell’s $J$ since the last update to its Eddington tensor and update the Eddington tensors wherever the fractional change exceeds $f_J$. This marks the end of a single time-step.

6 TESTS

6.1 Strömgren spheres

We now demonstrate that our code accurately computes the growth of $\mathrm{H}$ regions in both static and expanding media. For the static case, we locate a single O star of monochromatic ionizing luminosity $5 \times 10^{48} \, \text{s}^{-1}$ in a homogeneous medium of pure hydrogen with total density $10^{-3} \, \text{cm}^{-3}$, temperature $10^4 \, \text{K}$ and initial ionized fraction 0.0012 (Test 1 from Iliev et al. 2006). The simulation volume has a side length of 10.5 kpc and is divided into 483 cells. We evolve the non-equilibrium radiation and ionization fields for 500 Myr. In the bottom left-hand panel of Fig. 13, we compare how the radius of the resulting ionization front grows with time in our code (solid) versus the analytical solution (dashed; Iliev et al. 2006). In the numerical case, we define the radius of the ionized region as the radius at which the neutral hydrogen fraction drops to 50 per cent.

There is a slight tendency for the numerical radius to exceed the analytical one. In order to put this effect into context, we include an error bar that spans twice the width of a single computational cell; this is our true spatial resolution. Evidently, the solutions agree to within the spatial resolution. In the top panel we show the ratio of the numerical to the analytical solutions as a function of time. At all times, they agree to within 5 per cent. The majority of the codes that are compared in Iliev et al. (2006) also yield ionization front radii that exceed the analytical solution by 1–5 per cent (fig. 7 of Iliev et al. 2006). In fact, Pawlik & Schaye (2008) recently demonstrated that the analytical solution is expected to underpredict the radius of the ionized region (by roughly 5 per cent in their test) owing to the assumption that the ionized region remains fully ionized. Hence we conclude that our method’s accuracy is comparable to the other codes in Iliev et al. (2006).

For the expanding case, we consider a protogalaxy that ‘turns on’ at $z = 20$ with an ionizing luminosity $5 \times 10^{49} \, \text{s}^{-1}$ (this is roughly what is expected for $10^4 \, \text{M}_\odot$ of young Population II stars assuming an ionizing escape fraction of 5 per cent). The protogalaxy lives in a homogeneous medium of pure hydrogen with comoving density $1.66 \times 10^{-27} \, \text{cm}^{-3}$ and temperature $10^4 \, \text{K}$. We evolve the test from $z = 20$ to 10 in an Einstein–de Sitter universe with $h = 0.7$ using 483 computational cells. In the bottom right-hand panel of Fig. 13, we compare the comoving radius of the ionized region as a function of time in our numerical model (solid) against the analytical solution of Shapiro & Giroux (1987) (dashed). As before, the numerical solution tracks the analytical one to within the size of a grid cell at all times. In the top right-hand panel we show the ratio of the numerical to the analytical solutions as a function of time. Once again, our numerical solution is accurate to within 5 per cent at all times.

Combining the results of these tests, we conclude that our code conserves photons, accurately determines the non-equilibrium ionization states and accounts for the relevant cosmological terms.
Figure 13. Test of classical (left) and cosmological (right) Strömgren spheres. In the bottom panels we show the numerical (solid) and analytical (dashed) solutions as a function of time. The error bars in the bottom panel are included for reference and span twice the width of a computational cell. In the top panels we show the ratio of the numerical to the analytical solutions. In both test cases, the numerical and analytical solutions agree to within one cell width at all times.

6.2 Shadowing

We now discuss how well our code is able to produce shadows. Our goal is to run a test case whose results can be compared to Test 3 of Iliev et al. (2006). However, this test involves irradiating a dense clump with a plane-parallel wavefront, a situation that is difficult to impose in our method. Instead, we consider the case of a dense clump of cold hydrogen irradiated by a bright disc located sufficiently far away that the flux from the disc at the clump is approximately plane-parallel. We calibrate the disc’s (isotropic) emissivity to the simulation resolution so that, if it were an infinite plane, the flux would be $2 \times 10^6$ s$^{-1}$ cm$^{-2}$. The radius of the clump and the disc is 0.8 kpc, they are separated by 3.75 kpc and the plane of the disc is oriented perpendicular to the line connecting the disc and the clump. The ambient hydrogen number density and temperature are $2 \times 10^{-4}$ cm$^{-3}$ and 8000 K, while inside the clump they are 0.04 cm$^{-3}$ and 40 K. The box size is 6.6 kpc and contains $64^3$ computational cells. We evolve the simulation for 15 Myr.

Fig. 14 shows the neutral hydrogen fraction and photon number density in the simulation mid-plane after 1 Myr (top panels) and 15 Myr (bottom panels). In these figures the dense clump is on the right and the source disc, seen edge on, is on the left. Looking at the top panels first, we see that after 1 Myr the region behind the clump remains largely neutral although the rest of the volume is completely ionized, suggesting that our technique shadows well, with the photon density at this time four–five orders of magnitude fainter in the shadowed region than in the unshadowed one. The small amount of diffusion results from the fact that our LC module sets the Eddington tensors in the shadowed region to the isotropic case because no sources are visible there. Consequently, photons are free to diffuse into the shadowed region, as is expected in any moment formalism. After 15 Myr, the ionizing field behind the clump has strengthened to a photon number density of roughly 1 per cent of the value in the unshadowed region, driving the neutral hydrogen fraction down to $10^{-3}$. At this point, the volume is in equilibrium; in fact, the radiation and ionization fields do not change appreciably between 5 and 15 Myr.

Comparing Fig. 14 to figs 22 and 24 of Iliev et al. (2006), we find that our technique shadows as well as ray tracing and Monte Carlo codes at $t = 1$ Myr. However, at $t = 15$ Myr our code performs more poorly owing to the diffusion of photons into the shadowed region. Fig. 14 can also be compared with Hayes & Norman (2003), who introduced a moment method that is similar to ours. They demonstrated that incorporating Eddington factors from a time-dependent SC integration results in incomplete shadowing (see their figs 6–9). They also found that increasing the spatial resolution did not resolve the problem. Instead, they concluded that the incomplete shadowing results from the fourth term in equation (11), which involves the Laplacian of the product $f J$. Evaluating this term couples non-adjacent computational cells and gives rise to numerical diffusion in space. This might be expected to present even more of a problem in our technique given that we find it necessary to smooth our Eddington tensors whereas they did not. Despite this, Fig. 14 demonstrates that our technique can shadow reasonably well.

7 COSMOLOGICAL APPLICATION

As a sample application, we compute the re-ionization of a cosmological density field in which we account for Hubble expansion but hold the emissivity and baryon density fields constant. We derive the initial conditions using the same output and the same gridding technique as in Section 3, but here we divide the volume into $64^3$ rather than $16^3$ computational cells so that each computational cell spans a comoving width of $125 h^{-1}$ kpc. Given that the parent simulation...
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begins with $256^3$ baryon particles, this implies that, on average, 64 baryon particles contribute to each cell, hence systematic errors associated with the gridding are dominated by effects related to low spatial resolution rather than to Poisson statistics. We do not attempt a detailed treatment of subgrid physics as our focus is on our RT technique (for a careful treatment of these issues see McQuinn et al. 2007). We evolve the ionization and radiation fields from $z = 9$ to 6 with outputs spaced 1 Myr apart assuming $(\Omega, \Lambda, H_0) = (0.3, 0.7, 70)$. We set $n_{\text{q}} = 1$ and update the full Eddington tensor field whenever the photon number density has changed by more than a factor of 2 in at least 20 per cent of the volume, and after $x_{\text{HI}}$ drops below 0.5 per cent we use the optically thin approximation (tests indicate that this yields better than 20 per cent accuracy in $J$). This computation required roughly 10000 CPU hours using 32 1.6-GHz Itanium2 processors in a shared-memory environment. Note that, although this computation is only intended as a proof-of-concept for our method, it is already quite realistic in the sense that the gas density and emissivity fields derive from a cosmological hydrodynamic simulation that simultaneously reproduces a wide array of observations of galaxies (Davé, Finlator & Oppenheimer 2006; Bouwens et al. 2007; Finlator & Davé 2008) and the IGM (Oppenheimer & Davé 2006) in the post-re-ionization universe.

In Fig. 15, we show the neutral fraction as a function of position in a two-dimensional slice through the computational volume at four representative redshifts. Re-ionization proceeds in the familiar way: at early times, individual ionized bubbles grow around the brightest sources, which are strongly clustered. As re-ionization proceeds, the individual ionized regions begin to overlap; this process can be seen to be well underway by $z \approx 8$. The volume-averaged neutral hydrogen fraction dips below 50 per cent at $z \approx 7.75$. Around this time, the mean free path of ionizing photons grows comparable to the length of the simulation volume and the ionization field becomes a network of simply connected regions that are largely ionized and isolated regions that are largely neutral. As this topology emerges, the ionizing background continues to strengthen and the remaining neutral regions continue to shrink. Finally, in the post-overlap universe only regions with high recombination rates and low emissivities remain neutral.

In Fig. 16, we give a more quantitative view of how re-ionization proceeds in our calculation. In the top panel, we compare the neutral hydrogen fraction $x_{\text{HI}}$ averaged over the entire computational volume with the average over underdense and overdense regions. At the beginning of our computation, overdense regions are more rapidly ionized because they host the bulk of the ionizing sources. Meanwhile, underdense regions remain more neutral because they have not yet been penetrated by ionization fronts. As re-ionization proceeds, the filaments channel the ionization fronts into the voids (Ciardi et al. 2001), which rapidly become more highly ionized than the overdense regions. $x_{\text{HI}}$ continues to shrink in all three density bins until $z \sim 6$, by which point most of the universe has arrived at
ionization equilibrium with a fairly uniform ionizing background. At this time, $x_{\text{HI}}$ has dropped to $x_{\text{HI}} \sim 10^{-3}$, in good agreement with observations (Fan et al. 2006).

We show how the relation between density and ionization fraction evolves in a different way in Fig. 17. Here, the different curves show the median relation at five representative ionization fractions as indicated. At early times, highly overdense regions ionize to a neutral fraction below $<10^{-4}$ even when the cosmological mean neutral fraction remains at 99 per cent owing to their high emissivities. Regions that are at and below the mean density ionize next owing to their low recombination rates. Mildly overdense regions ionize last owing to their blend of relatively high recombination rates and low emissivities.

The reversal in the trend of ionization fraction versus overdensity that we find at $z \sim 8$ has recently been discussed in the seminumerical study of Choudhury et al. (2008). In this work, it is argued that underdense regions should be more strongly ionized than overdense regions at late stages in re-ionization owing to their lower recombination rates. Our computation, which (automatically) treats recombination rates realistically, supports their results while making far fewer assumptions regarding baryonic physics. Unfortunately, this calculation cannot be used to study the most overdense regions before $z > 8$ because, in these regions, $J_{21}$ becomes smoother and consequently more accurate. By contrast, the ionizing background in underdense regions tracks the volume average at all times, supporting the idea that underdense regions remain more highly ionized at late times owing to their lower recombination rates rather than a stronger $J_{21}$.

The right axis converts $J_{21}$ into its associated hydrogen ionization rate $\Gamma_{-12} \equiv \Gamma_{\text{HI}}/10^{-12}$. The open triangle indicates the observed upper limit on $\Gamma_{-12}$ at $z = 6$ from Bolton & Haehnelt (2007). The arrow’s length combines the uncertainties in cosmology, the observed Lyman $\alpha$ forest effective optical depths used to derive $\Gamma_{-12}$ and the thermal state of the IGM. This observation is representative of other constraints from the literature. Comparing the Bolton & Haehnelt (2007) constraint against our simulation suggests that the simulated $\Gamma_{-12}$ is a factor of $\sim 20$ too high. This is surprising for several reasons. First, our emissivity field corresponds to the galaxy population at $z = 9$ and does not account for the rise in the star formation rate.
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8 SUMMARY

In this paper, we introduced a method that accurately and efficiently computes continuum RT in static density fields. The code uses a moment-based approach to solve the equation of comoving RT, with the Eddington tensors obtained using a LC method. We compared several techniques for computing the Eddington tensors that are needed to close the moment hierarchy and demonstrated that, of the three methods that we investigated, only the method of LC has the ability to compute highly inhomogeneous radiation fields without introducing numerical artefacts. We found through direct measurement that the computation times for our LC and moments modules scale with the number of computational cells $N_{\text{cells}}$ as $N_{\text{cells}}^{1.5}$ and $N_{\text{cells}}^{1.0}$, respectively. Next, we introduced a hybrid method for computing the evolution of non-equilibrium ionization fields and demonstrated that it is accurate to 1 per cent throughout our computational domain. We combined this with our RT code via an efficient iterative algorithm. The final code is regulated by a number of parameters, and we characterized how these parameters impact computation time and accuracy using a suite of low-resolution convergence tests.

We subjected our method to a number of standard problems in continuum RT. First, we verified that our code accurately computes the growth of an $\text{H} \, \text{II}$ region about a source in the classical (static) case as well as in the case of an expanding medium. We found that, in both cases, the radius of the resulting ionized region agrees with analytic expectations to within the computation’s spatial resolution. However, further investigation into this discrepancy is beyond the scope of this work.

Figure 16. Volume-averaged neutral hydrogen fraction (top) and the ionizing background mean intensity $J_{21}$ (bottom) as a function of the age of the universe (bottom axis) and redshift (top axis). The right axis in the bottom panel indicates the hydrogen ionization rate in units of $10^{-12}$ s$^{-1}$. In both panels, the solid line is the average over all space whereas the dotted and dashed lines are averaged over underdense and overdense regions, respectively. The red dot–dashed curve in the bottom panel shows how the volume-averaged $J_{21}$ varies at half our spatial resolution. The arrow in the top panel indicates the observed limit on $x_{\text{H} \, \text{I}}$ at $z = 6.4$ (Fan et al. 2006), while the limit in the bottom panel is representative of observed limits on the ionization rate at $z = 6$ (Bolton & Haehnelt 2007).

Figure 17. Median neutral fraction as a function of normalized density at five hydrogen neutral fractions as indicated. The curves correspond to redshifts of (top to bottom) 8.9, 7.0, 6.7, 6.3 and 6.0 in our simulation.

formation rate density that occurs between $z = 9$ and 6 (Oppenheimer & Davé 2006). Secondly, we assume an ionizing escape fraction of 10 per cent, whereas Bolton & Haehnelt (2007) suggest that an escape fraction of up to 20 per cent may be required in order to maintain the observed ionization state of the IGM at $z = 6$. Thirdly, we start our calculation at $z = 9$ whereas observations from Wilkinson Microwave Anisotropy Probe five-year data (WMAP-5) are best fit by an instantaneous re-ionization redshift of $11.0 \pm 1.4$ (Dunkley et al. 2008), which suggests that re-ionization was already well underway by $z = 9$. Finally, we do not include active galactic nuclei. All of our assumptions, therefore, tend to underestimate the value of $\Gamma_{-12}$. The source of the discrepancy could lie in cosmic variance, low spatial resolution or the uncertainty in the choice of ionizing escape fraction. As a quick test, we have plotted the evolution of $J_{21}$ in a separate integration in which the same density field was divided into $32^3$ rather than $64^3$ cells (red dot–dashed curve). The resulting curve suggests that some, but not all, of the discrepancy owes to poor spatial resolution. However, further investigation into this discrepancy is beyond the scope of this work.
cosmological volume and found qualitative agreement with other work in the literature. Our code currently accounts for radiative and collisional ionization of hydrogen and helium as well as radiative recombination. It does not account for recombination radiation. Additionally, it does not follow the evolution of the temperature field, hence it does not account for photoionization suppression of star formation in low-mass haloes, photoionization heating, recombination cooling or shock formation.

In the future we plan to expand on our code in several ways. First, we have found that the computation time increases dramatically as the universe becomes optically thin because the LC line integrals traverse more cells before terminating either because they arrive at the source or because they reach $\tau_{\text{max}}$. However, in this regime, the optically thin approximation, which is roughly 10 times faster than LC, becomes increasingly valid. For this reason, we plan to study how to transition smoothly from LC to the optically thin approximation without introducing accuracy errors. Secondly, we will generalize our method to multifrequency RT, which is necessary for studying, for example, ionization front hardening or He II reionization. Finally, we plan to merge our RT scheme with our version of the cosmological galaxy formation code GADGET-2.

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