PHOTON-CONSERVING RADIATIVE TRANSFER AROUND POINT SOURCES IN MULTIDIMENSIONAL NUMERICAL COSMOLOGY

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ABSTRACT

Many questions in physical cosmology regarding the thermal and ionization history of the intergalactic medium are now being successfully studied with the help of cosmological hydrodynamical simulations. Here we present a numerical method that solves for the radiative transfer around point sources within a three-dimensional Cartesian grid. The method is energy-conserving independent of resolution; this ensures correct propagation speeds for ionization fronts. We describe the details of the algorithm and compute as a first numerical application the ionized region surrounding a mini-quasar in a cosmological density field at $z = 7$.

Subject headings: cosmology: theory — galaxies: formation — galaxies: ISM — intergalactic medium — radiative transfer

1. INTRODUCTION

The incorporation of radiation processes and radiative transfer into cosmological hydrodynamical simulations is essential for modeling the structure and evolution of the Lyman forest (Cen et al. 1994; Zhang, Anninos, & Norman 1995; Hernquist et al. 1996; Haehnelt & Steinmetz 1997), interpreting the observations of helium and metal-line absorbers at high redshift (Reimers et al. 1997; Hellsten et al. 1997; Songaila 1998), and for simulating the early reheating and reionization of the intergalactic medium (IGM) (Ostriker & Gnedin 1996; Gnedin & Ostriker 1997). In the last case, the large computational effort is justified by the hope that the study of the transition from a neutral IGM to one that is almost fully ionized could provide some hints about the first generation of stars and quasars in the universe. Until now, radiative transfer effects have either been ignored in such simulations or treated as a self-shielding correction to an optically thin approximation (Katz et al. 1996; Gnedin & Ostriker 1997). Typically, radiation fields are treated as isotropic backgrounds, $J_{\nu}(z)$, which are either specified as an external function computed by other means (e.g., Haardt & Madau 1996) or computed by averaging over all sources within the computational volume (Cen 1994; Gnedin & Ostriker 1997). Only approximate treatments exist for the reprocessing of radiation via absorptions internal to the sources as well as by the IGM, an effect that can significantly influence the spectrum of the metagalactic flux (Haardt & Madau 1996). Moreover, at $z \geq 3$ (5) the IGM itself is opaque in the helium (hydrogen) Lyman continuum, and radiation backgrounds become increasingly inhomogeneous and anisotropic (Reimers et al. 1997; Madau, Haardt, & Rees 1999). Recent analytic work has attempted to forge a closer connection between sources, transport, and sinks of cosmic radiation, albeit in a spatial- and angle-averaged way (Giroux & Shapiro 1996; Haiman & Loeb 1998a, 1998b; Madau et al. 1999).

In this paper we describe an approach to cosmological radiative transfer that relaxes these assumptions and is appropriate on scales comparable to the separation of individual sources of radiation. Our method has the property that energy is conserved independent of numerical resolution, ensuring, for example, that ionization fronts (I-fronts) propagate at the correct speed. The radiation-driven front surrounding a mini-quasar in a cosmological density field at $z = 7$ is computed as a first application of the technique.

2. COSMOLOGICAL RADIATIVE TRANSFER

The equation of cosmological radiative transfer in comoving coordinates (cosmological, not fluid) is (Norman, Paschos, & Abel 1998)

$$\frac{1}{c} \frac{\partial I_{\nu}}{\partial t} + \hat{n} \cdot \nabla I_{\nu} - \frac{H(t)}{c} \left( \nu \frac{\partial I_{\nu}}{\partial \nu} - 3I_{\nu} \right) = \eta_{\nu} - \chi_{\nu} I_{\nu}, \quad (1)$$

where $I_{\nu} \equiv I(t, x, \hat{n}, \nu)$ is the monochromatic specific intensity of the radiation field, $\hat{n}$ is a unit vector along the direction of propagation of the ray, $H(t) \equiv \dot{a}/a$ is the (time-dependent) Hubble constant, and $\dot{a} \equiv (1 + z_{em})/(1 + z)$ is the ratio of cosmic scale factors between photon emission at frequency $\nu$ and the present time $t$. Here $\eta_{\nu}, \chi_{\nu},$ and $c$ denote the emission coefficient, the absorption coefficient, and the speed of light, respectively. Equation (1) will be recognized as the standard equation of radiative transfer with two modifications: the denominator $\dot{a}/a$ in the second term, which accounts for the changes in path length along the ray due to cosmic expansion, and the third term, which accounts for cosmological redshift and dilution. In principle, one could solve equation (1) directly for the intensity at every point in $(t, x, \hat{n}, \nu)$ space given $\eta$ and $\chi$. However, the high dimensionality of the problem, not to mention the high spatial and angular resolution needed in cosmological simulations, make this approach impractical. Therefore, we proceed through a sequence of well-motivated approximations that reduce the complexity to a tractable level.

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Comparing the third with the second term in equation (1), the classical transfer equation (Kirchhoff 1860),

\[
\frac{1}{c} \frac{\partial I_v}{\partial t} + \hat{n} \cdot \nabla \chi_v = \eta_v - \chi_v I_v ,
\]  

(2)

is recovered if the scale of interest, \( L_c \) is much smaller than the horizon, \( c/H(t) \). (Note that this is only true if \( |v(\partial I_v/\partial \nu)| \leq I_v \), i.e., for continuum radiation. However, we can nonetheless still use eq. [2] for line transfer, provided that we Doppler shift the absorption cross section in \( \chi_v \) due to Hubble expansion.) In the case of constant absorption and emission coefficients, the time derivative can also be dropped, and one is left with the static transfer equation

\[
\hat{n} \cdot \nabla \chi_v = \eta_v - \chi_v I_v .
\]  

(3)

This equation is also adequate for problems in which the absorption and emission coefficients change on timescales much longer than the light crossing time, \( L/c \). This will always be the case in the volumes we will be able to simulate in the near future, and we thus adopt this approximation. At small distances from the source, however, this simplification will always break down, allowing I-fronts to expand faster than the speed of light. This can be easily dealt with, as we will show in the subsequent section.

An extensive literature exists on methods of solving equation (3) (e.g., Mihalas & Mihalas 1984) depending on the symmetry of the problem and the properties of \( \eta_v \) and \( \chi_v \).

A direct solution of equation (3) is impractical because of the high dimensionality of the problem. Our approach is approximate, and is based on decomposing the radiation field into point-source and diffuse components, \( I_v = I_v^{\text{ps}} + I_v^{\text{diff}} \). The motivation for doing this is that whereas \( I_v^{\text{ps}} \) is highly anisotropic, we expect \( I_v^{\text{diff}} \) to be nearly isotropic, and accordingly we can employ the best methods tailored for each component.

Utilizing the linearity of the radiation field, we can write

\[
\hat{n} \cdot \nabla I_v^{\text{diff}} = \chi_v (S_v - I_v^{\text{diff}}) ,
\]  

(4)

\[
\hat{n} \cdot \nabla I_v^{\text{ps}} = -\chi_v I_v^{\text{ps}} ,
\]  

(5)

where diffuse emission (e.g., due to recombination radiation) appears only in the transport equation for the diffuse radiation field via the source function \( S_v \). The advantage of equation (5) can now be solved by ray in a completely decoupled fashion. For \( \chi_v(x) = \text{const} \), equation (5) has the simple analytic solution

\[
I_v(x_t) = I_v(x_0) e^{-\tau} = I_v(x_0) \exp \left[ -\chi_v(x_t - x_0) \right] .
\]  

(6)

In the next section we describe an efficient implementation for solving equation (5) on rays emanating from point sources within a uniform Cartesian grid. Several methods of solving equation (5) are discussed in Norman et al. (1998). More arguments justifying the physical basis of our approach are also given in the next section.

3. IMPLEMENTATION

Figure 1 gives the flowchart of the simple algorithm. Details of the individual computational steps are given in the sections following. For each point source in our volume, a set of radial rays quasi-uniformly distributed in solid angle are constructed. Enough rays are used such that every cell at large distances from the source is crossed by at least one ray on average. We are able to use fewer angles than one would naively assume by Monte Carlo sampling of angles within a radiation-matter coupling timescale. Each ray is discretized, “cast” into ray segments according to how it intersects the cell boundaries. On each ray segment the intensity is attenuated according to equation (5) using an absorption coefficient appropriate to that cell. The number of absorptions in the frequency interval \((v, v + dv)\) in each ray segment inside a cell is simply related to the decrease in \( I_v^{\text{ps}} \) along that segment. The total number of photoionizations in the cell is the sum over all ray segments crossing the cell.

3.1. Choosing Angles

To properly describe the I-front, one needs at least \( N_a = f_a (2\pi r/\Delta x) \) rays, so that at least one ray is cast to each cell of side length \( \Delta x \) at the equator of a sphere with radius \( r \). We introduce the factor \( f_a \) to allow us to control the number of rays. To adopt the minimum number of rays needed, we store the maximum radius, \( r_{\text{max}} \) needed to capture the farthest point of the I-front.

We use spherical coordinates \((r, \phi, \theta)\),

\[
x = r \cos \phi \cos \theta , \quad 0 \leq \phi \leq 2\pi ,
\]

\[
y = r \sin \phi \cos \theta , \quad -\frac{\pi}{2} \leq \theta \leq \frac{\pi}{2} ,
\]

\[
z = r \sin \theta ,
\]  

(7)

and divide the sphere into segments of similar size such that all rays will have similar fluxes (see Fig. 2). We can now find the angles that define the rays that pierce through segments of roughly equal area. The discrete values for \( \theta \) are given by

\[
\theta_j = \left( j - \frac{1}{2} \right) \frac{2\pi}{N_a} - \frac{\pi}{2} , \quad 1 \leq j \leq N_a / 2 .
\]  

(8)

Closer to the poles fewer azimuthal angles are required:

\[
N_\phi = \max \left( N_a \cos \theta, 1 \right) .
\]  

(9)

The azimuthal angles are now chosen to be

\[
\phi_i = \left( i - \frac{1}{2} \right) \frac{2\pi}{N_\phi} , \quad 1 \leq i \leq N_\phi .
\]  

(10)

One also needs to know the area of the sphere segment, \( A(i, j) \), described by each ray. In units of the surface of the
spherical (4πr²), this is

\[ A(i, j) = \frac{\left| \sin \theta_2 - \sin \theta_1 \right|}{2N^2_\phi}, \]

\[ \theta_1 = (j - 1) \frac{2\pi}{N_s} - \pi, \quad \theta_2 = j \frac{2\pi}{N_s} - \pi. \]  

(11)

A random rotation of the coordinate system is then introduced for each snapshot solution of I_r to avoid any possible pole artifacts and reduce the number of angles required.

3.2. Casting Rays

Ray casting is the next step. This means to compute, for a given ray (θ, ϕ), the indices i(l), j(l), and k(l) of the grid cells it traverses, as well as the lengths of the ray segments ∆S(l) within each cell. Here i, j, and k are the indices of grid cells in a Cartesian lattice x(i), y(j), and z(k), and l is the index of the ray segment. For simplicity, we restrict our discussion to uniform, isotropic grids such that x(i) = iΔx, y(j) = jΔy, and z(k) = kΔz, where Δ is the cell size and 0 ≤ i ≤ N_x, similarly for j and k. Ray casting is a problem in computational geometry, with efficient methods discussed in books on computer graphics. For a uniform Cartesian grid the problem is straightforward. Here we write down a direct algorithm (i.e., requiring no costly sorts). Consider a point source at coordinate (x_s, y_s, z_s) in cell (i_s, j_s, k_s). We have simply i(1) = i_s, j(1) = j_s, and k(1) = k_s. We cast a ray in direction (θ, ϕ) and ask which cell boundary it intersects first. If it intersects an x boundary first, i(2) = i(1) + sign(cos ϕ), j(2) = j(1), k(2) = k(1), and analogously if the y or z boundaries are crossed first. To determine which cell face is crossed first, we compute the distances (radii) from the source to the next x, y, or z crossings. Call these distances r_x, r_y, and r_z. The minimum of these three distances determines which cell boundary is crossed first.

This can be expressed as follows: define

\[ \mu = \cos \theta, \quad s_\mu = \text{sign}(\mu), \]

\[ \gamma = \sin \theta, \quad s_\gamma = \text{sign}(\gamma), \]

\[ \zeta = \text{sign} \theta, \quad s_\zeta = \text{sign}(\zeta). \]  

(12)

then for all l ≥ 2 we have

\[ r_x(l) = \frac{|\Delta x(l) + (s_\mu + 1)/2| - x_s}{\max(e, |\mu \cos \theta|)}, \]

\[ r_y(l) = \frac{|\Delta y(l) + (s_\gamma + 1)/2| - y_s}{\max(e, |\gamma \cos \theta|)}, \]

\[ r_z(l) = \frac{|\Delta z(l) + (s_\zeta + 1)/2| - z_s}{\max(e, |\mu \zeta|)}. \]  

(13)

if [r_x(l) ≤ min (r_x(l), r_y(l))], then

\[ S(l) = r_x(l), \quad i(l) = i(l - 1) + s_\mu; \]

if [r_y(l) ≤ min (r_x(l), r_y(l))], then

\[ S(l) = r_y(l), \quad j(l) = j(l - 1) + s_\gamma; \]

if [r_z(l) ≤ min (r_x(l), r_y(l))], then

\[ S(l) = r_z(l), \quad k(l) = k(l - 1) + s_\zeta. \]  

(14)

Here ε is a small number to avoid dividing by zero.

3.3. Computing Rates

Although the above technique can be applied to any absorption process, we here discuss the specific case of hydrogen photoionization and compute the photoionization rate coefficient and the associated heating term. Additional species can be treated in an analogous way. Given the path length ∆S(l) = S(l) - S(l - 1) and the absorption coefficient in cell [i(l), j(l), k(l)], the optical depth for photoionization along this path is given by \( \tau^i = \frac{\Delta S(l)}{\Delta S(l)} \). Furthermore, from the solution of the static transfer equation (6), one sees that \( \delta \bar{N}_e(l - 1)(1 - e^{-\tau^i}) \) photons are absorbed in the time interval \( \delta t \). Hence, the rate of change of the neutral hydrogen density, \( n_H \), due to photoionization is simply given by

\[ \dot{n}_H = \frac{\bar{N}_e(l - 1)(1 - e^{-\tau^i})}{V_{cell}}. \]  

(15)

where \( \bar{N}_e \) is the monochromatic number of photons emitted by the source per unit time, and \( V_{cell} \) denotes the volume of the cell. The heating rate is then

\[ \dot{e}_H = \frac{(h\nu - 1 \text{ ryd})\bar{N}_e(l - 1)(1 - e^{-\tau^i})}{V_{cell}}. \]  

(16)

6 Details of the primordial gas chemistry are summarized in Abel et al. (1997).
Both of the above rates are summed over the contributions of all rays. Employing the analytical solution for each ray segment insures that I-fronts move at the correct speed independent of spatial resolution.

3.4. Faster-than-Light I-Fronts

In deriving equation (3) we have neglected the time-dependent term of the transfer equation (1). The assumption that the light crossing time is shorter than the ionization timescale breaks down close to the source. As a consequence, the I-front expands at a speed exceeding the speed of light. This can also be seen from the simple jump condition in a static universe,

$$4\pi \frac{n_H}{n_I} \frac{dr}{dt} = N - 4\pi \alpha_B \int_0^{r_I} n_e n_p r^2 \, dr,$$

where $\alpha_B$ is the recombination coefficient to the excited states of hydrogen. In this expression, $dr/dt$ exceeds the speed of light for radii less than $r_c = (N/4\pi n_H) 10^{-5} \approx 5.3$ kpc (for $n_H = 50$ cm$^{-3}$). To avoid this unphysical effect, we simply do not compute rates at distances farther than $r_I = c(t - t_0)$. The radius $r_I$ is also used in the computation of the optical depths in equations (16) and (15). In addition, to speed up the calculation for radii $r < r_c$, we evolve the equations on $1/10$ of the light travel time across one cell. As a consequence, the time evolution of the ionized fraction close to the source will not be computed correctly. However, we do not consider this a severe limitation, since the neutral fraction becomes practically zero in regions within a light travel time from the radiation source.

4. A TEST AND AN APPLICATION

In this section we first provide a test case that demonstrates the accuracy of the method and then, as first application, compute the ionized region surrounding a “mini-quasar” in a cosmological density field at $z = 7$. Mini-quasars could be common at early epochs if black holes can form in the first $10^8 M_\odot$ cold dark matter (CDM) condensations (Haiman & Loeb 1998b).

4.1. Spherical I-Front Test

To test our algorithm we set up a point source in a uniform medium and neglect the effect of radiative recombinations. The radius of the spherically expanding I-front can be derived analytically by balancing the number of emitted photons with the hydrogen atoms that are present in the ionized volume,

$$R_I(\Delta t) = \left( \frac{3 N}{4 \pi n_H} \Delta t \right)^{1/3}.$$  \hspace{1cm} (18)

Figure 3 compares this analytical solution with the results of our algorithm on a 64$^3$ grid. The radius and the spherical geometry are perfectly recovered within the accuracy of the spatial resolution. The specific parameters used in this test were $N = 10^{51}$ s$^{-1}$, $n_H = 10^{-2}$ cm$^{-3}$, and $\Delta x = 1$ kpc. The algorithm has also been tested to accurately reproduce the size of a classical Strömgren sphere in calculations that include radiative recombinations.

4.2. Cosmological Density Field

Our first interesting application is the evolution of the ionization zone surrounding a mini-quasar that turns on at $z = 7$ in the inhomogeneous density field derived from cosmological simulations. The evolutionary timescale of the ionization front within our volume is $\approx 1$ Myr. During this time no noticeable change in the density distribution will take place on the scale of the smallest resolution element ($\approx 3$ kpc), because of the small peculiar velocities ($< 300$ km s$^{-1}$). For simplicity, we do not solve the energy equation and include hydrogen radiative recombinations by assuming a constant case B recombination rate of $\alpha_B = 3.4 \times 10^{-13}$ cm$^{-3}$ s$^{-1}$ everywhere on the grid. This corresponds to a temperature of $\approx 7000$ K, chosen to be rather low to enhance the effect of recombinations. For a more detailed discussion of the temperature distribution in cosmological H II regions, see Abel & Haehnelt (1999).

For the background medium we use the H I distribution computed in a standard cold dark matter cosmology (with $\Omega_b = 0.06$ and $h = 0.5$) at $z = 6.941$ from Bryan et al. (1999). The 2.4 Mpc box length corresponds to 300 proper kpc. At the densest cell, which is found in a virialized halo of total mass $\approx 1.3 \times 10^{11} M_\odot$, we introduce a quasar-type source with an ionizing photon emission rate of $N = 5 \times 10^{53}$ s$^{-1}$. The gas clumping factor is $(\langle n_H^2 \rangle/\langle n_H \rangle)^2 = 59.2$, and is larger than the ionized hydrogen clumping factor, $C = (\langle n_{H^+}^2 \rangle/\langle n_{H^+} \rangle)^2$, since clumps that are dense and thick enough to be self-shielded from UV radiation remain neutral and do not contribute to the recombination rate.

Figure 4 illustrates the evolution of the I-front during the first 0.6 Myr. The initial spherical expansion (at the speed of light, since the number of available photons exceeds by far the number of neutral hydrogen atoms and recombinations) is quickly broken as the front expands first into the voids (increasing their thermal pressure by many orders of magnitude by photoheating), then more slowly into the denser filaments.

In a highly inhomogeneous universe, the volume-averaged gas recombination timescale,

$$t_{rec} = (n_e \alpha_B C)^{-1} = 0.1 \text{ Gyr} \left( \frac{1 + z}{8} \right)^{-3} C^{-1} Z_{20}^{-1}$$  \hspace{1cm} (19)

(for $\Omega_b h^2 = 0.015$), is much shorter than the Hubble time. At later epochs, when the size of the H II region is large
compared to the scale of the clumping, the front will fill its
time-varying Strömgren volume, $V_s$, in a few recombination
times, just like in the static case (Madau et al. 1999),

$$V_s = \frac{N_{\text{rec}}}{n_H} = 0.63 \text{ Mpc}^3 \left( \frac{1 + z}{8} \right)^6 C_{20}^{-1}.$$  (20)

This is 20 times larger than our simulation box.

5. SUMMARY

Not only for theoretical reasons, but also in light of
upcoming space missions such as the Microwave Anisotropy
Probe (MAP), Planck, and the Next-Generation Space
Telescope (NGST), a detailed understanding of the thermal
history of the IGM and reionization is highly desirable. In
this paper we have described a photon-conserving algo-

rithm that allows us to simulate inhomogenous reionization
self-consistently within a cosmological hydrodynamical
simulation. The method employs an on-the-spot approx-
imation to treat the effects of the diffuse emission of ionizing
photons. For scenarios in which stellar sources are
responsible for the reionization of hydrogen, the on-the-
spot approach is expected to give reliable results. However,

for calculations in which the diffuse radiation due to helium
reionizations is expected to be important, a separate
solver must be used. In addition, if the exact topology of
the ionization front needs to be captured to high accuracy, one
needs to solve for the diffuse radiation separately in order
to not to overestimate the effect of shadowing (Norman et al.
1999). In applications where radiative recombinations can
be neglected, the number of rays used can be reduced sig-
ificantly because of the variable choice of coordinate
system for the selection of rays. Recently, a different algo-

rithm for three-dimensional radiative transfer in cosmo-
ological situation has been presented by Razoumov & Scott
(1998). Their explicit advection scheme (at the speed of light)
seems well suited for situations in which the I-fronts move
faster than any hydrodynamical flow. Only temporary two-
dimensional arrays are used in the method presented here,
requiring negligible small additional memory for three-
dimensional cosmological hydrodynamics simulations.

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