CALCULATING THE INHOMOGENEOUS REIONIZATION OF THE UNIVERSE

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Abstract

A numerical scheme for the solution of the three-dimensional, frequency- and time-dependent radiative transfer equation with variable optical depth is developed for modelling the reionization of the Universe. Until now, the main difficulty in simulating the inhomogeneous reionization has been the treatment of cosmological radiative transfer. The proposed approach is drastically different from previous studies, which either resorted to a very simplified, parametric treatment of radiative transfer, or relied on one-dimensional models. The algorithm presented here is based on explicit multidimensional advection of wavefronts at the speed of light, combined with the implicit solution of the local chemical rate equations separately at each point. I implement the ray-tracing version of this algorithm on a desktop workstation and check its performance on a wide variety of test problems, showing that explicit advection at the speed of light is an attractive choice for simulation of astrophysical ionization fronts, particularly when one is interested in covering a wide range of optical depths within a 3D clumpy medium.

This scheme is then applied to the calculation of time-dependent, multi-frequency radiative transfer during the epoch of first object formation in the Universe. In a series of models, the 2.5 Mpc (comoving) simulation volume is evolved between the redshifts of $z = 15$ and $z = 10$ for different scenarios of star formation and quasar activity. The highest numerical resolution employed is $64^3$ (spatial) $\times 10^2$ (angular) $\times 3$ (frequency), and at each point in space I calculate various stages of hydrogen and helium ionization accounting for nine chemical species altogether.

It is shown that at higher numerical resolution these models of inhomogeneous reionization can be used to predict the observational signatures of the earliest astrophysical objects in the Universe. At present, the calculations are accurate enough to resolve primordial objects to the scale typical of globular clusters, $10^6 M_\odot$. 

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Chapter 1

Introduction to Cosmological Radiative Transfer

One of the most fundamental problems in astronomy is the nature of the very first generation of astrophysical objects at high redshifts, which formed when the Universe was only 5 – 10% of its present age. Two facets — the dynamics of dark matter and the thermal properties of the high-redshift gas — shaped the physical evolution at those early epochs. Over the last 15 years the theory of large-scale structure formation has benefited significantly from numerical N-body and gas-dynamical simulations, which successfully describe the emergence of hierarchical structures out of primordial density fluctuations, as well as the collapse of individual objects. These techniques work quite well when properties of the gas are not coupled strongly to the spatial gradients in the radiation field; e.g., in the small optical depth regime one can approximate the energy balance between matter and radiation via a combination of photoheating by a uniform background flux and a parametric cooling function associated with this radiation (Efstathiou 1992, Miralda-Escudé & Rees 1994, Katz et al. 1996b, Quinn et al. 1996, Navarro & Steinmetz 1997, Haehnelt & Steinmetz 1998, Bryan et al. 1999), or even derive an effective equation of state of the intergalactic medium (IGM) in the presence of a uniform ionizing background (Hui & Gnedin 1997, Schaye et al. 1999, Ricotti et al. 1999). This approximation is sufficient in the low-density, completely ionized IGM which is exposed to the bath of ultraviolet (UV) photons at lower redshifts, but it breaks down in the cores of collapsed halos or in the neutral, high-redshift IGM which is still opaque to ionizing photons. At present, the majority of cosmological gas-dynamical simulations lacks a proper description of radiative transfer (RT) making these models inapplicable to more realistic states of opaque and inhomogeneous IGM.
Chapter 1. Introduction to Cosmological Radiative Transfer

An approach traditionally popular in cosmology is to solve the radiative transfer equation (RTE) in a space-averaged way (Miralda-Escudé & Ostriker 1990, 1992, Giroux & Shapiro 1996) assuming that the matter distribution is homogeneous, the radiation field is uniform and isotropic, and neglecting RT effects within individual clouds. The mean effect of clumps is usually smoothed over a uniformly distributed ambient gas. These techniques can describe the overall RT in the IGM reasonably well if the effective optical depth of the Universe is smaller than unity; however, even then, they fail woefully inside dense structures.

The simplest approximation which takes into account the effects of RT with spatially variable optical depth is probably that of an infinite slab (Haiman et al. 1996, Haardt & Madau 1996) or a spherically symmetric cloud (Kepner et al. 1997, Tajiri & Umemura 1998, Abel & Haehnelt 1999, Loeb & Rybicki 1999, Haiman et al. 1999) irradiated by a uniform background field. This model can be a good approximation to a virialized halo immersed into a UV background after the epoch of reionization (Kepner et al. 1997, Tajiri & Umemura 1998), or to a small \((10^{4-5} M_\odot)\) cloud illuminated by low-energy (below 13.6 eV) photons before reionization (Haiman et al. 1999), but it does not account accurately for the clumpiness of the IGM and for the spatial distribution of sources.

As we shall see, there are reasons to believe that the radiation field has an important effect on the thermal state of interstellar and intergalactic medium, which can be accounted for only with a detailed model for cosmological RT. Within currently popular cosmological scenarios, the Universe recombined around redshift \(z \sim 1000\), as it was expanding and cooling down after the primordial hot phase. At some stage, after decoupling from radiation at a redshift of few hundred, the gas began to collapse slowly under its own gravity forming the very first bound objects (Peebles 1993, p. 176). It is believed that the light from these objects later reionized most of the gaseous component of the Universe (Fig. 1.1). Observations of the cosmic microwave background (CMB) fluctuations on the sky, on the one hand, and of absorption features in the spectra of high-redshift quasars, on the other hand, place the epoch of reionization somewhere
in the redshift interval $6 \lesssim z \lesssim 40$ (Haiman & Knox 1999).

Figure 1.1: A schematic diagram showing the epoch of reionization.

The best upper limit on the reionization redshift comes from the analysis of CMB anisotropies. The scattering of CMB photons off free electrons appearing in abundance during reionization has several important effects on the CMB (see, e.g., Peebles 1993, p. 581, also Tegmark et al. 1994). Most notably, it changes the paths of the photons, suppressing primary CMB fluctuations on degree and sub-degree scales. Besides that, free electrons Doppler shift CMB photons leading to secondary anisotropies. From a compilation of all existing data of CMB anisotropies, Griffiths et al. (1998) recently derived a model-dependent upper value of the redshift of reionization, with the best fit around $z_{\text{reion}} \sim 35 - 40$.

On the other hand, the optical depth of the neutral IGM to Ly$\alpha$ absorption (Haiman & Knox 1999)

$$\tau_{\text{Ly}\alpha} \sim 10^5 \times \frac{\Omega_b h}{0.03} \left(\frac{1 + z}{6}\right)^{3/2}$$

is very high, destroying radiation from all sources beyond the redshift $z$ at observed wavelengths shorter than $\lambda_{\text{Ly}\alpha}(1 + z)$. The absence of strong absorption blueward of the Ly$\alpha$ line in the spectra of high-redshift objects suggests that hydrogen is almost completely ionized by $z = 5$ (Gunn & Peterson 1965). Individual Ly$\alpha$ forest clouds reveal themselves in absorption at distinct redshifts. However, the optical depth of the IGM is $\tau_{\text{Ly}\alpha} \lesssim 1$, yielding the average neutral hydrogen fraction $\lesssim 10^{-5}$. Recent discoveries of Ly$\alpha$ emitting galaxies at even higher
redshifts ($z = 6.68$, Chen et al. 1999; $z = 5.74$, Hu et al. 1999; $z = 5.60$, Weymann et al. 1998) move the lower limit for the epoch of reionization even further back in time.

Patchy reheating and reionization are interesting for a number of reasons. It is likely that observational data on the earliest luminous objects in the Universe will first come from the study of the thermal state and the distribution of the inhomogeneous IGM around these objects (e.g., see Tables C.1 – C.2 in Appendix C for a list of observational programs). A number of fundamental questions could be addressed in a comparison between the predicted and observable features of this high-redshift gas:

- What is the nature of the sources of reionization? Was the Universe ionized by stars or quasars, or both?
- How were the first luminous objects distributed in space? When did they form? What were their spectra and luminosities?
- How long did reionization last?
- What is the connection between reheating and reionization?
- Was reheating efficient in providing the negative feedback on subsequent quasar activity or star formation?
- How does clumping of the IGM affect the timescale of reionization? What is the resulting cooling function?
- How large were inhomogeneities at the time of the first structure formation?

It is important to understand how many photons are actually needed to reionize the Universe. The most probable source of ionizing radiation is the population of stars and quasars formed during the gravitational collapse of the earliest structures. It has been claimed (Shapiro & Giroux 1987, Miralda-Escudé & Ostriker 1990, Shapiro et al. 1994, Madau et al. 1999) that
since the observed population of quasars in both optical and radio wavelengths declines steadily beyond $z \sim 3$ (Warren et al. 1994, Pei 1995, Schmidt et al. 1995), the UV radiation from quasars alone is not sufficient for reionization. However, in the past few years, there has been a growing interest in models which predict many more low-luminosity quasars at ultra-high redshifts ($z \sim 10 - 15$), based on a suggested correlation between the masses of host dark matter halos and central black holes (Haiman & Loeb 1998, Haehnelt et al. 1998). On the observational front, recently, some bright quasars were detected to as far as $z \sim 5$ (Fan et al. 1999, and references therein), with a dozen or so objects known at $z \gtrsim 4.5$. The recently begun Sloan Digital Sky Survey (SDSS) has the potential to increase this number to a few hundred over the next five years, possibly, with the detection of bright objects in the redshift interval $5.5 \lesssim z \lesssim 7$.

In addition, there might be some evidence for a large population of low-luminosity quasars at high redshifts from recent X-ray data (Miyaji et al. 1998) which do not show any decline in the quasar number density at $z > 2.7$ (Haiman & Loeb 1999). On the other hand, if reionization is caused by a generation of stars not long before $z = 5$, the rate of star formation must be similar to or bigger than that inferred from galaxy observations at $z = 3$ (Madau et al. 1999).

Additional constraints on the efficiency of star formation at higher redshifts come from studies of metal enrichment of the IGM. The detection of heavy elements in Ly$\alpha$ absorption systems shows a clear correlation between metallicities and the degree of collapse of these objects. Damped Ly$\alpha$ systems (those with neutral hydrogen column densities $N$(H$\text{I}$) $\gtrsim 10^{20}$ cm$^{-2}$) demonstrate metal abundances in the range $3 \times 10^{-3} < Z/Z_{\odot} < 10^{-1}$ (Lu et al. 1996) indicating that these are young galaxies with strong local star formation. Low column density clouds ($N$(H$\text{I}$) $\sim 3 \times 10^{14}$ cm$^{-2}$) which can be associated with the diffuse IGM and which exhibit metallicities of order $Z/Z_{\odot} \sim 10^{-2}$ (Cowie et al. 1995), might have been enriched by Population III stars formed in virialized objects with masses $10^5 - 10^7$ M$_{\odot}$ at much higher redshifts ($30 \lesssim z \lesssim 15$, Haiman et al. 1996a). However, recent observations of very low column-density clouds (those with $3 \times 10^{13} N$(H$\text{I}$) $\lesssim 10^{14}$ cm$^{-2}$, Lu et al. 1998) seem to have ruled out the
possibility that Population III stars could have polluted the entire Universe to a uniform metallicity level of $Z/Z_\odot \sim 10^{-2}$ — instead, the inferred value is closer to $Z/Z_\odot < 10^{-3}$. Note that the amount of heavy elements which one would expect to detect if these elements were produced by the same early generation of stars that reionized the Universe and were later ejected into the low-density IGM is of order $Z/Z_\odot \sim 3 \times 10^{-5}$ (or lower, depending on the clumpiness of the gas and star formation efficiency, Gnedin & Ostriker 1997), hence, the observed metallicities are more or less consistent with our theoretical insight on Population III objects (Lu et al. 1998, Ciardi et al. 1999).

Energetically, it would be sufficient to convert only a small ($\lesssim 10^{-5} - 10^{-3}$, Haiman & Loeb 1997) fraction of baryons into quasars and stars to reionize the IGM. However, photoionization is balanced by recombinations, the efficiency of which is a sensitive function of the local matter density, thus depending on the redshift and on the clumpiness of the gas. In a homogeneous universe the ratio of recombination time to the Hubble time is (Haiman & Knox 1999)

$$\frac{\tau_{\text{rec}}}{\tau_{\text{Hub}}} \sim \left(\frac{1 + z}{11}\right)^{-3/2},$$

that is, recombinations are much more important at higher redshifts ($z \gtrsim 10$). Similarly, the efficiency of recombinations rises sharply in high-density clouds.

There is no reason to think that reionization was an instantaneous, phase-like transition. To the contrary, the gaseous component must have been clumpy enough to allow for the collapse of individual objects. Therefore, one should expect that the ionizing radiation will first stream into the low-density voids, where absorption by neutral hydrogen is the lowest. One complication arises though. Sources which caused reionization most likely reside inside virialized dark matter halos within highly overdense spherical knots at the intersection of large-scale filaments (Abel et al. 1998b). A question is then whether low-density voids or high-density regions get ionized first (Haiman & Knox 1999). The answer is not trivial since it depends on the details of RT in a highly inhomogeneous IGM. Gnedin & Ostriker (1997) calculated reionization numerically
concluding that clumping of the gas increases the global recombination rate, making it harder to reionize the Universe. In this scenario, at the beginning, a large fraction of the ionizing photons does not travel far from sources, since these are located inside dense structures. It is in these clumps that the ionization proceeds first, and at some stage it is followed by an almost instantaneous decrease in the neutral hydrogen fraction in low-density regions. In this case, the Universe becomes transparent to the ionizing continuum on a very short timescale, since most of the neutral hydrogen inside dense filaments must have been ionized by then.

However, in a more detailed model (albeit with an approximate treatment of the RT) Gnedin (1998) concluded that reionization proceeds in the reverse direction: first, ionization fronts (I-fronts) propagate into voids and quickly ionize the low-density IGM. In the second stage the ionizing radiation eats into high-density filamentary structures until they get ionized and the universe as a whole becomes transparent. Similarly, Miralda-Escudé et al. (1998) argue that — despite the clumpiness of the gas — recombinations are not very important globally since the high-density filamentary gas is not ionized until a later time. In this scenario, ionizing photons escape sources within dense structures through a small solid angle, without causing complete local ionization. In fact, the ionization occurs “outside-in”, starting in voids and gradually eating into overdense regions. For this reason, the complete overlap of H II regions occurs at much later times after reionization. Until then the Universe stays globally opaque to ionizing photons.

The reionization of the gas has three dramatic consequences for the subsequent evolution of the Universe. First of all, the photoionized gas is much warmer, and is therefore is far less likely to collapse into bound structures. In other words, reionization raises the overall Jeans mass. Second, the cooling of a neutral hydrogen/helium medium with primordial abundance in the absence of any ionizing flux is dominated by line cooling. If the same medium is submerged in the bath of photoionizing radiation, line cooling is far less efficient (the gas is ionized), and cooling is dominated by recombinations (Efstathiou 1992). On the other hand, objects
which reionize the Universe will also enrich it with heavy elements, enhancing cooling in the
temperature range $10^4 - 10^7$ K. Finally, the ionized gas is virtually transparent to high-frequency
photons streaming from nearby quasars or star forming regions — unlike the neutral medium
which blocks all radiation with frequencies above the Ly$\alpha$ line.

Unfortunately, the evolution of I-fronts in a general 3D medium is an unsolved problem. It
now seems clear that the full solution requires a detailed treatment of the effects of RT. To com­
licate matters, by the time of the first star formation, the small-scale density inhomogeneities
have entered the non-linear regime, and the medium was filled with clumpy structures (Gnedin
& Ostriker 1997). In recent years, hydrodynamical simulations of structure formation in a
universe dominated by cold dark matter (CDM) and often including an ionizing background,
have been very successful in quantifying the density distribution and the ionization state of the
IGM (e.g., Cen et al. 1993, Hernquist et al. 1996, Katz et al. 1996, Zhang et al. 1998). The
degree of sophistication of these simulations suggests that the next step will be to include the
effects of global energy exchange by radiation. Indeed, there is a need for time-dependent 3D
RT models as numerical tools for understanding the effect of inhomogeneities on the dynamical
evolution of the interstellar/intergalactic medium. For instance, the ability of gas to cool down
and form structures depends crucially on the ionizational state of a whole array of different
chemical elements, which in turn directly depends on the local energy density and spectrum of
the radiation field.

Most of the previous studies which included some elements of radiative transfer into cosmo­
logical simulations had to rely on a number of very simplifying assumptions, such as a unique
dependence of the radiation field at each point on the local matter density and the local density
gradient (the so called ‘local optical depth approximation’, Gnedin & Ostriker 1997), or adopt
an optically thin Universe with cooling rates depending on the strength and spectrum of a
uniform UV background field with complete self-shielding of gas from the external radiation
field beyond some critical density (Efstathiou 1992, Chiba & Nath 1994, Navarro & Steinmetz
1997, Weinberg et al. 1997). It was only during the last couple of years that it has become possible to numerically model some aspects of the full 3D RT problem.

Challenges seem to abound, not least of all, the fact that the intensity of radiation in general is a function of seven independent variables (three spatial coordinates, two angles, frequency and time). While for many applications it has been possible to reduce the dimensionality (e.g., in classical stellar atmosphere models), the clumpy state of the interstellar or intergalactic medium does not provide any spatial symmetries. Moreover, coupled equations of radiation hydrodynamics (RHD) have very complicated structure, and are often of mixed advection-diffusion type which makes it very difficult to solve them numerically. Besides that, the radiation field in optically thin regions usually evolves at the speed of light, yielding an enormous gap of many orders of magnitude between the characteristic time-scales for a system. One way to avoid the latter problem is to solve all equations on the fluid-flow time-scale. While there are arguments which seem to preserve causality in such an approach (Mihalas & Mihalas 1984, p. 342), even then the numerical solution is an incredibly difficult challenge (Stone et al. 1992).

Since any two points can affect each other via the radiation field, even for a monochromatic problem, we must describe the propagation of the radiation field anisotropies in the full five-dimensional space. Standard steady-state RT solvers, which have been widely used in stellar atmosphere models, are not efficient in this case. Non-local thermodynamic equilibrium (NLTE) steady-state radiative transport relies on obtaining the numerical solution via an iterative process for the whole computational region at once, and is usually effective only for very simplified geometries. Any refinement of the discretization grid and/or increase in the number of atomic rate equations to compute NLTE effects will necessarily result in an exponential increase in the number of iterations required to achieve the same accuracy. On the other hand, the 3D solution of the steady-state transfer equation in the absence of any spatial symmetries can often be obtained with Monte Carlo methods (Park & Hong 1998). However, these methods demonstrate very slow convergence at higher resolutions and are hardly applicable if one is interested in
Chapter 1. Introduction to Cosmological Radiative Transfer

Recently, the problem of simulating 3D inhomogeneous reionization with realistic radiative transfer has attracted considerable interest in the scientific community. Umemura et al. (1998) calculated reionization from $z = 9$ to $z = 4$, solving the 3D steady-state RT equation along with the time-dependent ionization rate equations for hydrogen and helium. The radiation field was integrated along spatial dimensions using the method of short characteristics (discussed in Sec. 2.5.2). The steady-state solution implies the assumption that the radiation field adjusts instantaneously to any changes in the ionization profile. One draw-back of this approach, however, is in low-density voids where there are probably enough Lyman continuum photons to ionize every hydrogen atom, so that the velocity of I-fronts is simply equal to the speed of light. Then the rate equations still have to be solved on the radiation propagation timescale. Besides, implicit techniques in the presence of inhomogeneities will become exponentially complicated, if we want to solve time-dependent rate equations for multiple chemical species.

Norman et al. (1998) and Abel et al. (1998a) present a scheme for solving the cosmological radiative transfer problem by decomposing the total radiation field into two parts: highly anisotropic direct ionizing radiation from point sources such as quasars and stellar clusters; and the diffuse component from recombinations in the photoionized gas. In their method the direct ionizing radiation is being attenuated along a small number of rays, each of which is set up to pass through one of the few point sources within the simulation volume. The diffuse part of the radiation field is found with a separate technique which might benefit from a nearly isotropic form of this component, for instance, through the use of the diffusion approximation. Both solutions are obtained neglecting the time dependent term in the radiative transfer equation, with the default time-step dictated by the speed of the atomic processes.

If reionization by quasars alone is ruled out (Madau 1998, however see Haiman & Loeb 1998), then I-fronts are most likely to be driven by ionizing photons from low-luminosity stellar sources at high redshifts. In this case, the pressure gradient across the ionization zone is more
likely to become important before the front is slowed down by the finite recombination time. In this thesis I ignore hydrodynamical effects, concentrating on an efficient method to track supersonic I-fronts. My approach is to solve the time-dependent RT coupled with an implicit local solver for the rate equations. This method gives the correct speed of front propagation, and it also quickly converges to a steady-state solution for equilibrium systems. However, I should note that until a detailed comparison is made between explicit advection (at the speed of light) and the implicit reconstruction (through an elliptic solver), it is difficult to judge which approach works best in simulating inhomogeneous reionization in detail.

Aside from their relevance to numerical cosmology, high-resolution multi-dimensional conservation techniques and numerical RT in particular represent a formidable computational problem, the solution of which will be useful in many areas of computational astrophysics. The main question I want to address in this thesis is: can we numerically solve the problem of global energy transfer in a general 3D highly inhomogeneous medium via the radiation field? The present work describes one of the first attempts to attack this problem.

This thesis is organized as follows. In Chapter 2, I review techniques for solution of the time-dependent RTE. In Chapter 3, a method for accurate advection of radiation intensity in 3D for monochromatic problems is developed. In Chapter 4, this scheme is extended to include frequency dependency of the radiation field, and I also introduce the detailed primordial chemistry equations into the model. In Chapter 5, I compute a number of models for different scenarios of cosmic reionization, and quantify some of the observational predictions of the epoch of reionization. Finally, I present concluding remarks in Chapter 6.
Chapter 2

Numerical Radiative Transfer in an Inhomogeneous Medium

2.1 Radiative Transfer in Moving Media

For a moving medium the radiative transfer equation (RTE) in the inertial frame is (Mihalas & Mihalas 1984)

\[
\frac{1}{c} \frac{\partial I(\mathbf{n}, \nu)}{\partial t} + \mathbf{n} \cdot \nabla I(\mathbf{n}, \nu) = \epsilon(\mathbf{n}, \nu) - \kappa(\mathbf{n}, \nu)I(\mathbf{n}, \nu),
\]

(2.1)

where \( \mathbf{n} \) is the direction of photon propagation, \( I \) the intensity of radiation (per unit frequency per unit time per unit square area per unit solid angle), \( \epsilon \) the emissivity and \( \kappa \equiv \kappa_{\text{th}} + \kappa_{\text{sc}} \) the total (absorption and scattering) extinction coefficient. For simplicity, we have omitted the variable denoting the dependence on spatial coordinates. Since the background material through which the light propagates is moving, \( \epsilon \) and \( \kappa \) are anisotropic in general. For numerical simulations it is convenient to rewrite eq. (2.1) in the form where all matter properties are isotropic. Historically, the comoving RTE was first derived by Castor (1972), using a full general relativity formalism in application to spherically symmetric flows. Mihalas (1980) was the first to derive the comoving RTE exactly to all orders in \( \nu/c \) within special relativity, again in spherical symmetry. Through conservation of the number of photons one can show (Castor 1972) that the specific intensity, emissivity and opacity can be written in the frame comoving with the fluid using the following invariants:
\[ I(n, \nu) = \left( \frac{\nu}{\nu_0} \right)^3 I_0(n_0, \nu_0), \]
\[ \epsilon(n, \nu) = \left( \frac{\nu}{\nu_0} \right)^2 \epsilon_0(\nu_0), \]
\[ \kappa(n, \nu) = \left( \frac{\nu}{\nu_0} \right) \kappa_0(\nu_0), \]

(2.2)

where the emissivity \( \epsilon_0 \) and the absorption \( \kappa_0 \) are isotropic in the material’s frame, and the Doppler shift and the angle of aberration are obtained with the Lorentz transformations

\[ \nu_0 = \gamma \nu \left( 1 - \frac{n \cdot v}{c} \right), \]
\[ n_0 = \left( \frac{\nu}{\nu_0} \right) \left\{ n - \gamma \left( \frac{v}{c} \right) \left[ 1 - \frac{\gamma n \cdot v}{(\gamma + 1)c} \right] \right\}. \]

(2.3)

After some algebraic work eq. (2.1) can be written to order \( O(\nu/c) \) in the comoving frame (Buchler 1979):

\[
\frac{1}{c} \frac{\partial}{\partial t_0} \left[ \left( 1 + \frac{n_0 \cdot v}{c} \right) \frac{I_{\nu_0}}{\nu_0} \right] + \nabla_0 \cdot \left[ \left( n_0 + \frac{v}{c} \right) \nabla I_{\nu_0} \right] + \frac{\partial}{\partial \nu_0} \left[ -\frac{(n_0 \cdot \nabla_0)(v \cdot n_0)}{c} I_{\nu_0} \right] + \frac{\partial}{\partial n_0} \left[ -n_\perp \cdot \frac{(n_0 \cdot \nabla_0) v I_{\nu_0}}{c} \frac{1}{\nu_0} \right] = \frac{\epsilon_{\nu_0}}{\nu_0} - \frac{\kappa_{\nu_0}}{\nu_0} I_{\nu_0}. \]

(2.4)

Here \( n_\perp \) is a unit vector along the projection of the fluid velocity onto the plane perpendicular to \( n_0 \) (in the comoving frame). In writing this equation we have already neglected the acceleration term, assuming that the fluid frame is inertial. Eq. (2.4) is not considerably easier to solve numerically than eq. (2.1): all matter properties are isotropic — but now we have to solve the equation in the comoving frame, which means that the discretization grid has to move with the fluid (the Lagrangian grid). Eq. (2.1) or eq. (2.4) coupled with the equations of hydrodynamics
mass conservation (continuity): \[ \frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} = 0, \]
momentum conservation: \[ \rho \frac{D\mathbf{v}}{Dt} = -\nabla p - \rho \nabla \Phi + \frac{1}{c^2} \chi_F \mathbf{F}, \]
matter energy conservation: \[ \rho \frac{D(e/\rho)}{Dt} = -p \nabla \cdot \mathbf{v} - 4\pi k_S S + c k_E E, \]
equation of state: \[ p = p(\rho, T_e), \]

(written in the Lagrangian frame) constitute a general problem of radiation hydrodynamics (RHD). Here \( \rho, p, e \) and \( \mathbf{v} \) are the fluid density, pressure, energy density and velocity, respectively; \( \Phi \) the external (gravitational) potential; \( E \) the energy density of the radiation field; \( \mathbf{F} \) the radiative flux; \( T_e \) the electron temperature; \( S \) the radiation source function; \( c \) the speed of light; \( \chi_F, k_S, k_E \) various opacities (see eq. (2.9)-(2.11) for exact definitions); and \( D/Dt \) denotes the Lagrangian derivative. The numerical solution of a coupled RHD problem is, perhaps, the most fundamental challenge of computational astrophysics.

The topic of this thesis is radiative transfer in static media. In what follows, we will neglect Doppler shifts within the volume (unless indicated otherwise), the effects of aberration, and radiation pressure. Each of these elements can be included explicitly into the method we are developing here, since we will solve the problem on the smallest of all advection times — the light crossing timescale. The goal of this study is develop a fast and accurate scheme for energy transfer via radiation in general 3D inhomogeneous media.

### 2.2 The Equation of Radiative Transfer in Stationary Material

The RTE (without cosmological terms) in the static medium is (Chandrasekhar 1950)

\[
\frac{1}{c} \frac{\partial I_\nu}{\partial t} + \mathbf{n} \cdot \nabla I_\nu = \epsilon_\nu - \kappa_\nu I_\nu, \tag{2.6}
\]

where \( I_\nu \) is the intensity of radiation in direction \( \mathbf{n} \) and \( \epsilon_\nu \) and \( \kappa_\nu \) are the local emissivity and opacity. Eq. (2.6) is a 7-dimensional partial differential equation, since the intensity \( I_\nu \)
is a function of three spatial coordinates \( \mathbf{r} \), two angles in the direction of photon propagation \( \mathbf{n} \), frequency \( \nu \) and time. To get a numerical solution to eq. (2.6), we have to discretize the intensity on a grid in the six-dimensional (without time) phase space which immediately results in large amounts of data and the corresponding need for the computational power to deal with these data. A grid of say 64 points along each of the six independent variables would yield 512 GB of data to store just one time snapshot of the intensity in double precision. Needless to say, these memory requirements are well beyond the capabilities of modern computers.

A number of different techniques have been suggested to reduce the dimensionality of this problem. Historically, the radiative transfer problem was of crucial importance for modelling stellar atmospheres. In the plane parallel geometry or in spherical symmetry all differential equations were usually written as functions of two variables: the radius (or the mass within that radius) and the frequency. The angle dependence was taken care of using various approximations, such as, historically, the Schwarzschild-Schuster approximation (Schuster 1905), or the Eddington approximation, commonly used even today.

### 2.3 The Eddington Approximation

The approach leading to the Eddington approximation consists of rewriting eq. (2.6) as a system of angle-averaged moment equations (Krook 1955, Unno & Spiegel 1966). In a static medium integration over all directions and frequencies inside some range \( \nu_1 \leq \nu \leq \nu_2 \), with corresponding angular weights, yields an infinite number of moment equations, the first two of which are

\[
\frac{\partial E}{\partial t} = -\nabla \cdot \mathbf{F} + 4\pi \kappa S - c\kappa E \quad \text{(radiation energy density conservation),} \tag{2.7}
\]

and

\[
\frac{1}{c^2} \frac{\partial \mathbf{F}}{\partial t} = -\nabla \cdot \mathbf{P} - \frac{1}{c} \chi \mathbf{F} \quad \text{(flux conservation).} \tag{2.8}
\]
Here we have introduced the frequency-averaged opacities

\[ \chi F \equiv \frac{F}{F^2} \int_{\nu_1}^{\nu_2} \kappa_\nu F(\nu) d\nu; \tag{2.9} \]

\[ \kappa_S \equiv \frac{1}{S} \int_{\nu_1}^{\nu_2} \kappa_\nu S(\nu) d\nu; \tag{2.10} \]

\[ \kappa_E \equiv \frac{1}{E} \int_{\nu_1}^{\nu_2} \kappa_\nu E(\nu) d\nu. \tag{2.11} \]

The energy density \( E \), the flux \( F \) and the radiation pressure tensor \( P_{\alpha\beta} \) are the first three moments (zero, first and second rank tensors, respectively) of the specific intensity \( I_\nu \) defined as angle-averaged integrals of the specific intensity (Unno & Spiegel 1966)

\[ E \equiv \frac{1}{c} \int_{4\pi} I d\Omega, \tag{2.12} \]

\[ F \equiv \int_{4\pi} I \nu d\Omega, \tag{2.13} \]

\[ P_{\alpha\beta} \equiv \frac{1}{c} \int_{4\pi} I n_\alpha n_\beta d\Omega. \tag{2.14} \]

Krook (1955) studied the hierarchy of moment equations (2.7) – (2.8) and the validity of different approximations for one-dimensional problems (stellar atmospheres). Unno & Spiegel (1966) were the first to investigate the accuracy of moment equations for a general 3D inhomogeneous medium. Clearly, one can form an infinite hierarchy of moment equations. Unfortunately, like with any system of differential moment equations, there is always one more unknown compared to the number of equations, thus requiring an additional equation of state to close this system. Over the years a number of different closure schemes have been suggested. The most common approach is to stop at the second moment equation and add an approximate relation between \( E \)
and $P_{\alpha\beta}$; often it is written in the form of the so-called dimensionless tensor Eddington factor (Auer & Mihalas 1970)

$$f_{\alpha\beta} \equiv \frac{P_{\alpha\beta}}{E} \quad (2.15)$$

Originally, Eddington derived a relation between $E$ and $P_{\alpha\beta}$ assuming a particular form for $I(\theta, \phi)$. Since a number of different dependencies $I(\theta, \phi)$ can give the same value of $f_{\alpha\beta}$, it is the final form of the Eddington tensor that is usually referred to as the Eddington approximation. The factors $f_{\alpha\beta}$ essentially determine the degree of anisotropy of the radiation field but, unfortunately, can be calculated exactly only for the two extreme cases:

1. For free streaming (optical depth $\tau \ll 1$, i.e., the mean free path of a photon $\lambda_p$ is much larger than the typical length $L$ of the system) for a beam propagating in the direction $n$ the flux $F = cE n$ and the Eddington factor is highly anisotropic

$$f_{\alpha\beta} = n_\alpha n_\beta; \quad (2.16)$$

2. In the diffusion limit ($\tau \gg 1$) the flux $|F| = cE \cdot O(\lambda_p/l) \approx 0$ and the Eddington factor is isotropic

$$f_{\alpha\beta} = \frac{1}{3} \delta_{\alpha\beta}, \quad (2.17)$$

where $\delta_{\alpha\beta}$ is the Kronecker delta symbol. As for its value in between, the degree of anisotropy has to be computed numerically. Clearly, it has to be done accurately; e.g., applying the diffusion limit value of $f_{\alpha\beta}$ in the near free-streaming regime would result in overestimating the flux of radiation, effectively giving the wrong speed of energy propagation. Very often in numerical calculations the Eddington factors are evaluated using the flux-limited diffusion approximation, a modification of the diffusion theory which gives the right flux of radiation in the optically thin
regime as well (see, e.g., Alme & Wilson 1974 or Levermore & Pomraning 1981). While this method gives the correct values in both limits (optically thin and optically thick media), it effectively results in dropping the time-derivative in the radiation momentum equation (eq. (2.8), see Mihalas & Mihalas 1984), which can lead to serious errors for intermediate optical depths.

The best existing solution to recover the Eddington tensor is to resort to formal closure, reconstructing the angle-dependent intensity via a separate technique (Mihalas & Mihalas 1984, Stone et al. 1992). This is usually done by integrating intensities over all sources within the computational volume, taking into account boundary conditions and the opacity inside the volume.

2.4 Time-Dependent vs. Steady-State Techniques

Another complication in obtaining a meaningful numerical solution of eq. (2.6) arises from the fact that radiation at least in optically thin regions propagates at the speed of light, requiring one to take very small time steps to avoid propagation of unphysical oscillations. At the same time all fluid flows evolve on much slower, hydrodynamical timescales $t_f$.

An extreme example of such a situation would be formation of winds at the base of stellar atmospheres. Consider a low-mass main sequence (MS) star in a low-mass X-ray binary which is being irradiated by a hard flux of X-rays from a companion accreting neutron star. To compute the reaction of the MS star to this irradiation, one would have to build a self-consistent dynamical model of the system evolving at the smallest of the characteristic timescales: the light crossing timescale $t_R$ through one pressure scale-height is of order $10^{-4} - 10^{-3}$ s; the dynamical timescale for wind acceleration is typically a few seconds; the timescale of energy transport via horizontal surface motions is of order a few days; while the global convection (mixing) timescale approaches one month. Thus the range of timescales, each of which is of crucial interest for the behaviour of the irradiated star, covers more then ten orders of magnitude, making it hopeless
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Methods to solve the RTE numerically

**quasi-static solvers**
(multigrid techniques might be the best; all equations are solved implicitly)
- solution of the first two moment equations (energy & flux conservation) + some closure scheme (Eddington approximation)

**explicit advection**
(combined with an implicit chemistry solver)
- solution of as many moment equations as possible, with some "symmetric" closure scheme, e.g.
- time-dependent ray tracing (discrete ordinates)
- Monte Carlo methods (very low resolution)
- solve the photon Boltzmann equation directly in 5D (or 6D with frequency) phase space using modern, high-order multidimensional conservation schemes

- diffusion approximation
- flux-limited diffusion
- formal closure
- isotropic radiation pressure tensor
- isotropic higher-order moments (n>30)
- diffusion
- good approximation to free streaming

- long characteristics
- short characteristics

Figure 2.1: Methods to solve the RTE numerically.
to talk about any numerical model at first glance.

A common approach widely used in the literature (Mihalas & Mihalas 1984, Stone et al. 1992, Abel et al. 1998a) is to assume that the radiation field adjusts instantaneously to any changes in the matter density distribution, and the RTE can be solved implicitly on much longer timescales, e.g., on the fluid flow timescale $t_f$. The arguments supporting this approach were originally put forward by D. Mihalas (Mihalas & Mihalas 1984, p. 342) and are based on an order-of-magnitude analysis of different terms in the equations of RHD (see also Stone et al. 1992). For example, in optically thin regions, the ratio of the light crossing timescale $t_R$ to $t_f$ is $O(v/c)$, which is a small number in most astrophysical situations, typically in the range $10^{-4}$ — $10^{-2}$. Therefore, in most cases one can safely ignore all terms in the RHD equations which are $O(v/c)$ and smaller, unless one is dealing with relativistic flows. For processes occurring with timescales larger than $t_R$, one can simply neglect the explicit variation of the radiation field with time, assuming that it is always frozen to the current density distribution. This radiation field is often referred to as quasi-static. The terms describing the interaction of radiation with matter (emissivity and opacity) depend on the current microphysical state which is in turn governed by atomic and molecular rate equations. These can have very steep time dependence evolving on timescales sometimes even faster than $t_R$. Accordingly, all microphysical population rate equations must be solved implicitly as well. Hence, all computations can be followed on the timescale of typical changes in material properties inside the computational volume.

While this approach is very powerful, the major uncertainty here is the accuracy at which the matter-radiation interaction is treated. Also, since the great majority of equations is solved implicitly, the numerical implementation of quasi-static techniques usually involves the solution of a large system of coupled non-linear elliptic equations. The computer requirements for such calculations are known to grow steeply with higher numerical resolution and the introduction of more complicated physics.
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Mathematically, it is possible that the usage of fast multigrid techniques might actually give algorithms which scale linearly with the amount of data processed at each time step. However, at the time of writing of this thesis multigrid techniques have been successfully applied only to those systems of conservation laws which demonstrate a 'fair' degree of ellipticity, e.g., to the steady state Navier-Stokes equations (Sidilkover 1989).

On the other hand, several astrophysical problems allow one to follow the system of interest on a radiation propagation time-scale, without imposing a prohibitively large number of time steps. In the context of cosmological RT, we would like to resolve the characteristic distance between the sources of reionization. Cold dark matter (CDM) cosmologies predict the collapse of the first baryonic objects as early as \( z = 30 - 50 \), with the typical Jeans mass of order \( 10^5 \, M_\odot \) (see Haiman & Loeb 1997, and references therein). The corresponding comoving scale of fragmenting clouds is \( \sim 7 \, \text{kpc} \). If stellar sources reside in primordial globular clusters of this mass, then for \( \Omega_b = 0.05 \) the average separation between these objects is \( \Delta x \sim 20 \, \text{kpc} \) (comoving). For explicit schemes the Courant condition imposes a time-step

\[
\Delta t \leq t_R = \frac{\Delta x}{c(1 + z)} \sim \frac{10^5}{1 + z} \, h^{-1} \text{yrs.}
\] (2.18)

Thus evolution from \( z = 20 \) to \( z = 3 \) takes \( \sim 7.5 \times 10^8 \, h^{-1} \text{yrs} \) (assuming the density parameter \( \Omega_0 = 1 \), and defining the Hubble constant to be \( H_0 = 100 \, h \, \text{km s}^{-1} \, \text{Mpc}^{-1} \)). Substituting \( z = 3 \) and \( z = 20 \) into eq. (2.18) yields the total number of time-steps in the range \( 20,000 - 150,000 \) over the entire course of evolution. In other words, to resolve reionization by \( 10^5 \, M_\odot \) stellar clusters, we need to compute \( \sim \text{few tens of thousands} \) of time-steps on average, and for \( 10^8 \, M_\odot \) clusters the number of steps required will be even ten times smaller. A \( 100^3 \) grid with the required resolution will result in computational boxes of several Mpc on a side. A full cosmological radiative transfer simulation with boxes at least this big and for all the required timesteps has not been feasible in the past.
The rest of this chapter is devoted to the methods for solution of the time-dependent equation (2.6) on the light-crossing timescale \( t_R \). These are the main requirements for such a method:

- fast advection in 5D or 6D;
- high spatial resolution of 3D fronts (little dispersion);
- correct front speed in 3D;
- reasonable angular resolution for a given spatial mesh.

There now exist a large variety of different techniques for the explicit solution of the time-dependent RTE in 3D on the light propagation timescale. The major ones are listed in Fig. 2.1. Because of the inherent complexity of multi-dimensional advection, there is no single method which is best suited for cosmological RT. In sections 2.6 – 2.8 we will go in more detail through some of the techniques we have tried to implement numerically. It seems likely that each of the methods covered — (1) an explicit 3D moment solver, (2) a combination of a large number \((n \leq 30)\) of moment equations with a ‘symmetric’ closure scheme, or (3) a high-resolution conservation scheme for the multi-dimensional photon Boltzmann equation — could be developed to be equally efficient in studies of inhomogeneous I-fronts. Each of these techniques relies on explicit advection of wavefronts across the computational volume at the speed of light, hence, the timesteps are always limited by the Courant condition. We have optimized a further method, (4) time-dependent ray tracing to the degree that it can be used for modelling reionization at spatial resolution of \(64^3\), and describe it separately in Chapter 3.

### 2.5 Formal Solution of the Transfer Equation

The first step in computing a numerical solution to the RTE is to build a grid on which it can be discretized. Since the intensity of radiation depends both on the spatial coordinates and on
the direction of photon propagation, one has to discretize simultaneously in 3D space and in two angles. Ideally, we would like to put enough angular data points $N_{\theta}N_{\phi}$ to resolve all 3D grid points along the boundary of the computational volume. Therefore, if $N$ is the number of spatial grid points in each direction, the number of angles would scale roughly as $N_{\theta}N_{\phi} \sim N^2$ ensuring that even small clumps within the volume are taken into account. Clearly, if the average absorption inside the volume is large, the information about the precise location of the sources will be lost on a diffusion timescale, making it unnecessary to draw a lot of rays. In this case even the diffusion approximation will do the job. However, generally one has to worry about the precise geometry of the field inside or close to optically thin regions. If the opacity is known beforehand (which is not usually the case in the study of steep I-fronts), a simple rule is that the resolved number of angles should be a monotonically increasing function of $\lambda_p/L$, the ratio of the mean free path of a photon to the size of the volume.

Fig. 2.2 demonstrates a typical situation arising with poor angular resolution. The wavefronts are transported along a finite number of rays going through the source in the centre. At large distances from the source the separation between the rays in the adjacent directions is several times larger than the 3D mesh size. In general, the business of interpolation between rays to get non-zero intensities is a tricky one, since it can easily lead to the wrong I-front speed in 3D. Smoothing of the source improves the situation slightly but clearly loses in resolution (Fig. 2.3).

Once the discretization of angular variables is done, one has to devise an efficient way of transporting the angle-dependent intensity. For both quasi-static and explicit advection schemes two methods have been traditionally employed (Stone et al. 1992, Nakamoto & Umemura 1998).

2.5.1 Long Characteristics

Since in a flat spacetime the paths of photons are straight lines, one can difference the RTE along multiple lines in 3D. The idea of long characteristics is to draw, at each point on a 3D mesh, a set
Figure 2.2: The effect of poor angular resolution around a point source of radiation. This figure shows a particular isosurface of equal ionization for a front expanding from a point source of radiation into a homogeneous, pure hydrogen medium. The true solution is an expanding H\textsubscript{II} spherical bubble.

of rays covering all directions (Fig. 2.4). Reconstruction of the energy and radiation moments at each point then involves a simple integration at that point over all directions. Although it is possible to match the discretization in angle and space in such a way that individual rays will pass exactly through more than one point, in general one has to draw the same set of rays individually through each point. Hence, the memory requirements for this method scale as $O(N^4N_\theta N_\phi)$, since one has of order $N_\theta N_\phi$ rays for each cell and $N$ points along each ray. Clearly, this method is the easiest to implement numerically, but it is also by far the most inefficient in CPU time and memory usage.

A modification of this method relies on evaluation of the formal solution of eq. (2.6) only along the main axes and principal diagonals of the 3D mesh (NEWS, see Norman et al. 1998 for details). However, its angular resolution is only $\pi/4$, placing its accuracy next to the diffusion
2.5.2 Short Characteristics

The goal of any formal closure scheme is to minimize the number of data points preserving the numerical accuracy in a multi-dimensional phase space. The idea of short characteristics (see, e.g., Stone et al. 1992) is to calculate the intensity along short ray segments bounded by the edges of a 3D cell (Fig. 2.5). The values of the intensity at the ends of each ray segment are interpolated along principal spatial axes from the closest 3D grid points. Then one has to store only the angle-dependent intensity on the 3D grid, with the overall memory requirements of order $O(N^3 N_\theta N_\phi)$. However, since the very nature of this method is based on iterations in the plane not coinciding with the direction of photon propagation, consecutively at each 3D mesh layer along the beam, it leads to large angular dispersion (see the numerical domain of approximation.

Figure 2.3: A model similar to the one in Fig. 2.2 except that here we show the projected (integrated column) energy density with no smoothing and with smoothing of the source, respectively. The colour gradient represents the energy density in relative units.
Figure 2.4: In the method of long characteristics rays are drawn to cover the entire sphere independently at each point. The intensity at point A in a given direction depends on the intensity advected from point B (and earlier from C) in that direction, corrected for emissivity and absorption along the ray segment BA (based on the diagram from Nakamoto & Umemura 1998).

dependence in Fig. 2.5, based on Nakamoto & Umemura 1998; this effect was also demonstrated in the searchlight beam test in Stone et al. 1992).

2.6 Time-dependent 3D Moment Solver

Assume that we can estimate Eddington factors via a stand-alone fast closure scheme, be it an accurate formal solution or a variant of the flux-limited diffusion approximation. The Eddington factors set the direction and speed of photon propagation. However, they do not give an explicit update to radiation variables — we still have to solve moment equations

\[
\frac{\partial E}{\partial t} = -\nabla \cdot F,
\]
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\[ \frac{\partial F}{\partial t} = -c^2 \nabla \cdot (f_{\alpha\beta}E). \]  

(2.19)

In an attempt to perform fast explicit advection of radiation variables in 3D on the light-crossing timescale, we have developed an unsplit multidimensional solver of the truncated moment equations (2.19). The details of this method are described in Appendix B. We have carried out a number of tests concluding that this solver gives a very accurate description for an isotropic radiation field (e.g., in the diffusion limit). On the other hand, for free streaming it tends to quickly lead to negative radiative energy densities \( E \), since it does not have a built-in positivity requirement. In practice, negative values of \( E \) appear in those regions where there are large spatial gradients in the Eddington factors \( f_{\alpha\beta} \).

How can we construct a scheme the advection part of which always gives positive energy densities? It seems likely that such a requirement has to be tied to the one-dimensional Riemann...
solver (eq. (B.7)). However, the full development of this technique is beyond the scope of this thesis.

### 2.7 Truncating the System of Moment Equations at a Higher Order

The main limitation of the Eddington approximation is that it requires a separate, often very computationally intensive closure scheme. Another — perhaps more mathematically elegant — idea which has been developed primarily for relativistic RT is to extend the system of moment equations to higher orders. Anderson & Spiegel (1972) showed that, in a medium with relativistic differential motions, the Eddington approximation does not necessarily work even for optically thick cases. They develop a next-order approximation with an arbitrary number of moments of the type

\[
M_{\mu_1, \mu_2, ..., \mu_n} = \frac{1}{4\pi} \int I(\Omega) l_{\mu_1} l_{\mu_2} \cdots l_{\mu_n} d\Omega, \tag{2.20}
\]

— where \( l \) is a 3D unit vector, and \( l_{\mu_\alpha} \) is its projection on the \( \mu_\alpha \)-axis — and suggest the use of a 'symmetric' closure scheme which assumes that the highest order non-zero moment is isotropic. To illustrate the idea, let us expand the angle-dependent intensity in terms of moments defined in eq. (2.20). The expansion polynomials are generalized spherical functions (Anderson & Spiegel 1972)

\[
Y_{\mu_1, \mu_2, ..., \mu_n} = \frac{(-1)^n}{n!} \frac{\partial^n}{\partial l_{\mu_1} \partial l_{\mu_2} \cdots \partial l_{\mu_n}} \frac{1}{l}, \tag{2.21}
\]

which are orthogonal,

\[
\int Y_{\mu_1, \mu_2, ..., \mu_n} Y_{\mu_1, \mu_2, ..., \mu_m} d\Omega = 0 \quad \text{for } n \neq m, \tag{2.22}
\]

and traceless, with the first ones being
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The intensity can then be written as

\[ I(\Omega) = \sum_{n=0}^{\infty} A_{\mu_1 \mu_2 \ldots \mu_n} Y_{\mu_1 \mu_2 \ldots \mu_n}, \tag{2.24} \]

where the coefficients \( A_{\mu_1 \mu_2 \ldots \mu_n} \) are expressed through the moments:

\[ Y = 1, \tag{2.23} \]
\[ Y_\alpha = n_\alpha, \]
\[ Y_{\alpha \beta} = n_\alpha n_\beta - \frac{1}{3} \delta_{\alpha \beta}, \]
\[ Y_{\alpha \beta \gamma} = n_\alpha n_\beta n_\gamma - \frac{1}{3} (\delta_{\alpha \beta} n_\gamma + \delta_{\gamma \alpha} n_\beta + \delta_{\beta \gamma} n_\alpha), \]

\[ \vdots \]

The intensity can then be written as

\[ I(\Omega) = \sum_{n=0}^{\infty} A_{\mu_1 \mu_2 \ldots \mu_n} Y_{\mu_1 \mu_2 \ldots \mu_n}, \tag{2.24} \]

where the coefficients \( A_{\mu_1 \mu_2 \ldots \mu_n} \) are expressed through the moments:

\[ A = M, \tag{2.25} \]
\[ A_\alpha = -3M_\alpha, \]
\[ A_{\alpha \beta} = \frac{15}{2} \left( M_{\alpha \beta} - \frac{1}{3} M \delta_{\alpha \beta} \right), \]

\[ \vdots \]

The proposed closure scheme simply states

\[ A_{\mu_1 \mu_2 \ldots \mu_n} \equiv 0 \quad \text{for } n > n_{\text{max}}. \tag{2.26} \]

Choosing \( n_{\text{max}} = 1 \) gives the classical diffusion approximation with an isotropic radiation field. Taking \( n_{\text{max}} = 2 \) gives the next-order approximation.

This formalism was further developed by Thorne (1981) and Struchtrup (1997), both in the covariant form in the context of relativistic RT. In this theory, individual moment equations are
coupled by matrices of mean absorption and scattering coefficients, which reduce to the well-known Rosseland mean values for local thermodynamic equilibrium (LTE). It is interesting to note that Struchtrup (1997) derived a closure scheme from maximization of entropy in the rest frame of the fluid. More recently, Struchtrup (1998) applied this formalism to the case of homogeneous matter at rest, showing that the number of moments $n_{\text{max}}$ needed to represent a particular geometry of the radiation field varies with the optical depth. In fact, $n_{\text{max}} = 30$ is a good approximation for free streaming. For a system of moment equations, the speed of propagation in a particular direction (the characteristic speed) is given by the eigenvalue of the transport matrix in the corresponding direction (see eq. (B.3) in Appendix B). It is easy to check that the highest characteristic speed (given by the largest eigenvalue) approaches the speed of light asymptotically as $n_{\text{max}} \to \infty$. E.g., in the diffusion approximation ($n_{\text{max}} = 1$), the advection speed is always $c/\sqrt{3}$, whereas at $n_{\text{max}} = 30$ it is within 1% of the speed of light.

Here, we suggest that it might be possible to use this property of moment equations to develop an automatic closure scheme which will adjust itself to the current optical depth. The moment of truncation $n_{\text{max}}$ can be given a simple functional dependence on the local absorption coefficient, whereas the numerical solution of the moment equations up to $n_{\text{max}}$ will set the preferential direction of photon propagation at the corresponding characteristic speed. Initial attempts proved to be computationally time-consuming. However, full development of this approach is beyond the scope of this thesis, but future work could incorporate this idea into a numerical method and compare its performance to other closure schemes.

### 2.8 Solution of the Multi-dimensional Photon Boltzmann Equation

Instead of solving the truncated system of moment equations, an alternative possibility is to employ a multi-dimensional, high-resolution conservation scheme to solve the photon Boltzmann equation directly in the five- (without frequency) or six-dimensional (with frequency) phase
space. The advantage of this technique is that one uses a single grid for all calculations, with high-order corrections reducing numerical dissipation, and it can, in principle, be implemented in curved spacetimes and/or non-inertial frames.

For simplicity, to illustrate the basic idea of the method, let us consider monochromatic transfer in flat spacetime. The photon Boltzmann equation

\[ M^\alpha \frac{\partial f_R}{\partial x^\alpha} + \tilde{M}^\alpha \frac{\partial f_R}{\partial \tilde{M}^\alpha} = \eta - \chi f_R, \tag{2.27} \]

is the conservation law for \( f_R \), the photon distribution function, defined as the number of photons per unit volume per unit momentum \( p = n \hbar \nu / c \), and related to the intensity of radiation via

\[ I(r, n, \nu, t) = \frac{\hbar^4 \nu^3}{c^2} f_R(r, n, \nu, t). \tag{2.28} \]

Above we also introduced the photon four-momentum

\[ M^\alpha = \frac{\hbar \nu}{c} (1, n). \tag{2.29} \]

For flat spacetimes — in which photon paths are straight lines (\( \tilde{M}^\alpha = 0 \) — eq. (2.27) can be easily reduced to the standard RTE (eq. (2.6)). In 3D Cartesian coordinates the monochromatic version of eq. (2.6) can be written as a 5D scalar advection problem with coefficients constant in the first three variables:

\[ I_t + A(\theta, \phi) I_x + B(\theta, \phi) I_y + C(\theta, \phi) I_z = c(\epsilon - \kappa I), \tag{2.30} \]

where the intensity is a function of six independent variables \( I = I(r, n, t) \), the speed of advection along the principal axes is \( (A, B, C) \equiv c \cdot (\cos \theta \cos \phi, \cos \theta \sin \phi, \sin \theta) \), and indices are short-hand notation for time and coordinate derivatives.
A high-resolution, multi-dimensional wave-propagation algorithm for general time-dependent hyperbolic systems of conservation laws was developed by R. LeVeque and collaborators (LeVeque 1997, 1998, Langseth & LeVeque 1997). Although this technique is not based on the solution of the multi-dimensional Riemann problem (evolution of the discontinuity at the interface between adjacent cells) but rather combines the first-order solution of 1D Riemann problems (in the directions normal to the interfaces between adjacent cells on a rectangular spatial grid) with special second-order multidimensional corrections, it achieves a big step forward in both stability and accuracy of the calculation.

2.8.1 Normal Flux Update

We start by writing the first-order Godunov’s scheme (LeVeque 1997) for fluxes normal to the cell interfaces. For example, an update along the x-axis involves the solution of the scalar linear wave equation

\[ I_t + A(\theta, \phi) I_x = 0. \]  

(2.31)

The corresponding Godunov’s (1959) flux update is

\[ I_i^{n+1} = I_i^n - \frac{k}{h} \left[ A^+ \Delta I_{i-1/2} + A^- \Delta I_{i+1/2} \right], \]  

(2.32)

where \( i \) labels cells, \( n \) labels timesteps, and \( A^+ \) and \( A^- \) are the positive and negative values of the wave speed \( A \) and \( \Delta I_{i-1/2} \equiv I_i - I_{i-1} \). Here \( h \) is the mesh size and \( k \) is the time step. The term \( A^+ \Delta I_{i-1/2} \equiv A^+ I_i - A^- I_{i-1} \) is the difference of two waves travelling to the right from points \( x_i \) and \( x_{i-1} \), respectively. Alternatively,

\[ A^+ \Delta I_{i-1/2} + A^- \Delta I_{i+1/2} \equiv (A^+ I_i + A^- I_{i+1}) - (A^+ I_{i-1} + A^- I_i) \]

can be interpreted as the difference of net waves travelling to the right and to the left from
xi. In comparison, expressions for $A^\pm$ for systems of equations or non-linear equations are considerably more complicated (see Appendix A).

The full normal first-order update in 3D is a combination of updates along all three principal axes:

$$I^{n+1}_{ijklm} = I^n_{ijklm} - \frac{k}{h} \left[ A^+_{lm} \Delta I_{i-1/2,jklm} + A^-_{lm} \Delta I_{i+1/2,jklm} \right]$$

$$- \frac{k}{h} \left[ B^+_{lm} \Delta I_{i,j-1/2,klm} + B^-_{lm} \Delta I_{i,j+1/2,klm} \right]$$

$$- \frac{k}{h} \left[ C^+_{lm} \Delta I_{i,jk-1/2,lm} + C^-_{lm} \Delta I_{i,jk+1/2,lm} \right],$$

(2.33)

where the subscripts denote discretization of the intensity on the numerical grid:

$$I(r_{ijk}, n_{lm}, t_n) = I^n_{ijklm}.$$ 

The stability condition of this scheme is given by the sum of the 1D Courant conditions, that is the timestep $k$ in eq. (2.33) cannot exceed the time it takes a wave travelling at the sum of the maximum advection speeds along individual axes [$\max(A) + \max(B) + \max(C)$] to cross one computational grid zone.

2.8.2 First-order Transverse Fluxes in 3D

In flat spacetimes with no scattering the trajectories of photons are straight lines, therefore, in the 5D phase space $(r_{ijk}, n_{lm})$ information can only propagate to cells adjacent in the first three indices $(i, j, k)$. The normal flux update (eq. (2.33)) takes care of waves moving normal to cell interfaces. If the speed of advection in the $y$-direction (given by the operator $B$ in eq. (2.30)) is not identically zero, some part of the wave moving from the cell $(i-1, j, k, l, m)$ to $(i, j, k, l, m)$ will be advected to the cell $(i, j+1, k, l, m)$ during the same time step (Fig. 2.6). To take this transverse flux into account, we have to include spatial cross-derivative terms like $L_{xy}$ (LeVeque 1997). Later on these terms will be important for extending the method to second-order accuracy. Also, the transverse terms will improve the stability of the multi-dimensional
numerical scheme to the full Courant number of 1, in units of the maximum advection speed in any given direction (Langseth & LeVeque 1997).

Consider the advection terms in eq. (2.30):
\[ I_t = -(AI_x + BI_y + CI_z). \] (2.34)

A simple Taylor series expansion of the solution at time \( t + \Delta t \) around the already known solution at time \( t \) yields:
\[
I(r, n, t + \Delta t) = I(r, n, t) + I_t(r, n, t)\Delta t + \frac{1}{2} I_{tt}(r, n, t)\Delta t^2 + \frac{1}{6} I_{ttt}(r, n, t)\Delta t^3 + O(\Delta t^4), \tag{2.35}
\]
where the third and fourth RHS terms can be obtained by differentiating eq. (2.34):
\[
I_{tt} = A(AI_{xx} + BI_{yx} + CI_{zx}) + B(AI_{xy} + BI_{yy} + CI_{zy}) + C(AI_{xz} + BI_{yz} + CI_{zz}), \tag{2.36}
\]
\[-I_{ttt} = A^2(AI_{xxx} + BI_{yxx} + CI_{zxx}) + AB(AI_{xyx} + BI_{yxy} + CI_{zyx}) + AC(AI_{xzx} + BI_{yxz} + CI_{zxy}) + BA(AI_{xxy} + BI_{yxy} + CI_{zxy}) + BC(AI_{xzy} + BI_{yyz} + CI_{zyz}) + C^2(AI_{xxx} + BI_{yxx} + CI_{zxx}).\]

The first-order normal flux update outlined in the previous section takes into account only the first two terms on the RHS of eq. (2.35). Part of the normal wave transported in the \( x \)-direction will almost always (since \( B \neq 0 \) in general, see Fig. 2.6) be advected along the \( y \)- and \( z \)-axes during the same time step into neighbouring cells. The \( O(\Delta t^2) \) term in eq. (2.35) corresponds to the transverse propagation yielding an update to eq. (2.33) which can be written schematically in terms of contributions to transverse fluxes:
In this notation, the superscript $b$ on the RHS labels the transverse wave update to the normal flux along the $y$-axis. Since eq. (2.30) is a single PDE, all wave spectra are scalars, and wave strengths are given by the positive and negative parts of advection matrices $A$, $B$ and $C$. Other $O(\Delta t^2)$ spatial cross-derivative terms ($A^\pm B^\pm$, $A^\pm C^\pm$, $B^\pm C^\pm$, $C^\pm A^\pm$, and $C^\pm B^\pm$, contributing to $\Phi^a$, $\Phi^b$ and $\Phi^c$) are formed similarly to eq. (2.37). The resulting transverse flux update is then
\[ I_{ijkm}^{n+1} \leftarrow I_{ijkm}^{n+1} - \frac{k}{h} \left( \Phi_{i+1/2,jkml}^{e} - \Phi_{i-1/2,jkml}^{e} \right) - \frac{k}{h} \left( \Phi_{ij+1/2,kml}^{b} - \Phi_{ij-1/2,kml}^{b} \right) - \frac{k}{h} \left( \Phi_{ijk+1/2,lm}^{c} - \Phi_{ijk-1/2,lm}^{c} \right). \] (2.38)

### 2.8.3 First-order Corner Fluxes in 3D

Accordingly, in three spatial dimensions, part of the transverse flux will transported into the corner cell, all during the same time step (Fig. 2.7). The corresponding update accounts for cross-derivative \( \mathcal{O}(\Delta t^3) \) terms in eq. (2.35):

\[ -\frac{1}{6} \left( ABCI_{xyz} + ACBI_{yzz} + BACI_{zxy} + BCAI_{zzy} + CABI_{yxz} + CBAl_{xyz} \right) \Delta t^3. \] (2.39)

![Figure 2.7: Propagation of transverse and corner fluxes in 3D (based on LeVeque 1997).](image)

Since eq. (2.30) is scalar, the first-order corner update consists simply of first-order upwind terms along each of the coordinate axis. The corner update corresponding to the first term in
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eq. (2.39) is

\[
\frac{1}{6} \left( \frac{k}{\Delta} \right)^2 A_{lm}^+ B_{lm}^- C_{lm}^+ \Delta I_{ijk-1/2,lm} \quad \rightarrow \quad \Phi^a_{i+1/2,jklm},
\]

\[
\frac{1}{6} \left( \frac{k}{\Delta} \right)^2 A_{lm}^- B_{lm}^+ C_{lm}^- \Delta I_{ijk-1/2,lm} \quad \rightarrow \quad \Phi^a_{i-1/2,jklm},
\]

\[
\frac{1}{6} \left( \frac{k}{\Delta} \right)^2 A_{lm}^+ B_{lm}^- C_{lm}^- \Delta I_{ijk-1/2,lm} \quad \rightarrow \quad \Phi^a_{i+1/2,jklm},
\]

\[
\frac{1}{6} \left( \frac{k}{\Delta} \right)^2 A_{lm}^- B_{lm}^+ C_{lm}^+ \Delta I_{ijk-1/2,lm} \quad \rightarrow \quad \Phi^a_{i-1/2,jklm},
\]

\[
\frac{1}{6} \left( \frac{k}{\Delta} \right)^2 A_{lm}^+ B_{lm}^- C_{lm}^- \Delta I_{ijk+1/2,lm} \quad \rightarrow \quad \Phi^a_{i+1/2,jklm},
\]

\[
\frac{1}{6} \left( \frac{k}{\Delta} \right)^2 A_{lm}^- B_{lm}^+ C_{lm}^+ \Delta I_{ijk+1/2,lm} \quad \rightarrow \quad \Phi^a_{i-1/2,jklm},
\]

\[
\frac{1}{6} \left( \frac{k}{\Delta} \right)^2 A_{lm}^+ B_{lm}^- C_{lm}^- \Delta I_{ijk+1/2,lm} \quad \rightarrow \quad \Phi^a_{i+1/2,jklm},
\]

\[
\frac{1}{6} \left( \frac{k}{\Delta} \right)^2 A_{lm}^- B_{lm}^+ C_{lm}^+ \Delta I_{ijk+1/2,lm} \quad \rightarrow \quad \Phi^a_{i-1/2,jklm}.
\]

(2.40)

Other terms contribute similar updates to the transverse fluxes $\Phi^a$, $\Phi^b$ and $\Phi^c$ in eq. (2.38).

2.8.4 Second-order Updates

Second-order corrections can be performed separately for each of the normal, transverse and corner fluxes. Note that the transverse advection of normal waves in eq. (2.38) already accounts for $O(\Delta t^2)$ cross-derivative terms in the Taylor expansion (eq. (2.35)). The full second-order accurate update formally has to include the terms $A^2 I_{xx}$, $B^2 I_{yy}$ and $C^2 I_{zz}$ which is carried out by propagating the second-order correction wave for the normal update (eq. (2.33)) using techniques described in Appendix A. However, as pointed out by LeVeque (1997) and Langseth & LeVeque (1997), to keep good stability properties, it is also useful to perform a transverse propagation of the correction wave. The implementation details can be found in Langseth & LeVeque (1997).
2.8.5 Summary

There are several clear advantages of the numerical solution of the photon Boltzmann's equation over the formal closure along a large number of rays. First of all, the direct Boltzmann solver uses a single 5D grid for all calculations, eliminating the need for interpolation between the 3D mesh and the rays. It can also naturally deal with multiple point sources within the volume. Since the wavefronts streaming from these sources are tracked explicitly, at the speed of light, there is no need to calculate the optical depth along the line connecting every single grid cell and the point source, as we do for direct ionizing photons (eq. (3.1)). However, a finite angular resolution in the direct Boltzman solver will still result in a numerical diffusion similar to the one shown in Fig. 2.2, implying that the number of angles resolved should roughly match the 3D spatial resolution. Note that normal, transverse and corner propagation of both the first-order and the second-order correction waves have to be performed at each time step.

We have numerically implemented the first-order monochromatic Boltzmann solver in three spatial dimensions. Since the Boltzmann's eq. (2.30) is a scalar PDE with coefficients constant in spatial variables, and since the intensity is discretized on a single grid in the 5D phase space, without the need to draw rays, its numerical implementation does not present much of a challenge on the programming side. Preliminary tests have demonstrated large dissipation across the wavefront, indicating that second-order updates are essential. On the other hand, experience has shown that the explicit ray tracing method described in the next chapter can get similar results for the diffuse part of the radiation field — although with some tradeoffs — at a fraction of the computational cost. In the rest of the thesis we shall concentrate on the ray-tracing algorithm.
Chapter 3

Time-Dependent Ray Tracing

3.1 Description of the Method

The basic idea of our technique is to solve eq. (2.6) directly for the angle-dependent intensity $I(r, n, \nu, t)$ at each point. The total radiation field at each point is divided into the direct (from ionizing sources) and diffuse (due to recombinations in the gas) components:

$$E_{\nu,i,j,k} = E^\text{src}_{\nu,i,j,k} + E^\text{diff}_{\nu,i,j,k},$$

where $i, j, k$ are the three indices in a rectangular grid. The energy density $E^\text{src}_{\nu,i,j,k}$ due to direct photons coming from point sources of ionization can be easily calculated on the 3D grid via summation over all sources (assuming that there are not too many of them within the volume):

$$E^\text{src}_{\nu,i,j,k} = \sum_s \frac{h\nu N_{ph}}{4\pi c r_{i,j,k,s}^2} e^{-\tau_{\nu,i,j,k,s}} \times \begin{cases} 1 & \text{if } r_{i,j,k,s} \leq c t_s \\ 0 & \text{if } r_{i,j,k,s} > c t_s, \end{cases}$$

where $\tau_{\nu,i,j,k,s} = \int_{r_s}^{r_{i,j,k,s}} d\tau_\nu$ is the optical depth, $r_{i,j,k,s}$ is the physical distance between the current point and the source, and $t_s$ is the age of the source. Note that the rate of emission of photons $N_{ph}$ can be modified to allow for variability of sources on short timescales. Clearly, this calculation is very computer intensive since for each cell where we want to reconstruct the intensity we have to integrate the opacity along the line connecting this cell and the source, and the summation over all sources will result in $\mathcal{O}(N^4 N_{\text{src}})$ operations. Fortunately, this update has to be done either on the
timescale of typical changes in the opacity in the volume, or the variability timescale of sources. This is achievable only for a small number of sources.

For the diffuse component we use an upwind monotonic scheme to propagate 1D wavefronts $I(r, n, \nu, t)$ along a large number of rays in 3D at the speed of light. Following Stone & Mihalas (1992), we apply an operator split explicit-implicit scheme, in which advection of radiation variables is treated explicitly and the atomic and molecular rate equations are solved implicitly and separately at each point. Unlike Abel et al. (1998a), we use rays to track the diffuse component of the radiation field and the direct ionizing background radiation (streaming into the computational volume). Since we need to draw rays essentially through every grid point in the 3D volume, at first glance this approach appears to have very large memory requirements. However, efficient placing of the rays can significantly reduce the computational effort.

3.1.1 A Uniform and Isotropic Grid of Rays

At each time-step we are interested in getting a solution for the mean radiation energy density and material properties on a 3D $N^3$ rectangular grid. Instead of shooting rays through each grid node in 3D, we choose to cover the whole computational volume with a separate grid of rays which is uniform both in space and in angular directions. Assuming that the computational volume corresponds to the range $0 \leq x, y, z \leq 1$, we first construct a 2D rectangular base grid containing $N^2$ nodes (where $N$ can be the same as the number of data points on each side of the computational volume) with coordinates with the origin at the centre of the cube

$$x_{ij} = \sqrt{3} \left( \frac{i - 1/2}{N} - \frac{1}{2} \right) + \frac{1}{2},$$
$$y_{ij} = \sqrt{3} \left( \frac{j - 1/2}{N} - \frac{1}{2} \right) + \frac{1}{2},$$
$$z_{ij} = \frac{1}{2}, \quad \text{with } i, j = 1, \ldots, N,$$  

(3.3)

where the $\sqrt{3}$ factor ensures that the entire volume is covered with rays, and we shoot rays normal to the base grid through all of its grid points. Note that the separation between 2D
nodes is allowed to be larger than $1/N$. To cover the whole volume with rays, we then rotate the base grid by an angle $\theta_i - \pi/2$ around the $y$-axis and by $\phi_{lm}$ around the $z$-axis, where the rotation angles are discretized to mimic an isotropic distribution of rays (with fewer azimuthal angles close to the poles)

$$\theta_i = \pi \left( \frac{l - 1}{N_\theta - 1} - \frac{1}{2} \right), \quad 1 \leq l \leq N_\theta,$$

$$\phi_{lm} = \frac{2\pi m}{N_\phi}, \quad 1 \leq m \leq N_\phi, \quad N_\phi = 2N_\theta \cos \theta_i.$$

Figure 3.1: Rays shooting through the base grid in the direction $(\theta, \phi)$.

Only those rays which pass through the volume (and not all of them do!) are stored in memory. Let the total number of all possible orientations of the base grid be
Chapter 3. Time-Dependent Ray Tracing

\[ N_{\text{angles}} \sim \frac{4}{\pi} N_\theta (N_\theta - 1). \]  

(3.5)

The total number of rays scales as \( O(N^2 N_{\text{angles}}) \), which for large \( N \) is significantly smaller than \( N^3 \times N_{\text{angles}} \) (long characteristics, Sec. 2.5.1). In fact, with \( N = 64 \) and \( N_{\text{angles}} = 110 \) \((N_\theta = 10)\), we only require 218,242 rays. Since there are \( \sim 2/3 \times N \) points along each ray on average, the total memory requirements of the method are of order \( O(N^3 N_\theta N_\phi) \), the same scaling as for the method of short characteristics (Sec. 2.5.2). However, time-dependent ray tracing does not have the angular dispersion which is typical of short characteristics.

Now, that we have the grid of rays and the 3D rectangular mesh, we have to specify the rules of interpolation between them. This task is complicated, since we have to ensure that 3D wavefronts will be reasonably sharp (the ideal situation is to preserve 2nd- or 3rd-order accuracy from 1D rays after interpolation to three spatial dimensions), as well the correct speed of I-fronts in 3D. Among a large variety of possible schemes we tried, here we present the two mostly used in the tests.

Since our primary goal is to minimize the number of rays (and thus greatly reduce the computer memory requirements), using more than one ray to reconstruct the intensity at the point \((i, j, k)\) in the direction \((\theta_i, \phi_{lm})\) implies that 1D data points on the rays might fall outside the cell \((i, j, k)\). Therefore, we need to use some smoothing which, however, will preserve the correct front speed. An alternative is to use a one-to-one correspondence between the 1D data points along the rays and 3D mesh points. This later method guarantees the right shock velocity (given that it is correct in 1D) but requires several times more rays.

**A: Smooth Interpolation**

Before we start our simulations, for each 3D grid point \((i, j, k)\) we also store an array of the closest four rays going through its neighbourhood in the direction \((\theta_i, \phi_{lm})\). Since the rays do not pass exactly through 3D grid points, we use the values of the intensity on the four closest
rays in that direction to compute the angular-dependent intensity. Assume that for the point \((i,j,k)\) the distances to the four closest rays going in the direction \((\theta_l, \phi_{lm})\) are \(d_1, d_2, d_3\) and \(d_4\), respectively. We project the point \((i,j,k)\) onto these rays and read the values of the intensities, which we write as \(I_1, I_2, I_3\) and \(I_4\). We then calculate the intensity at \((i,j,k)\) in the direction \((\theta_l, \phi_{lm})\) according to

\[
I_{i,j,k,l,m} = \sum_{q=1}^{4} \frac{d_1 d_2 d_3 d_4}{d_q} w_q I_q / \sum_{q=1}^{4} \frac{d_1 d_2 d_3 d_4}{d_q} w_q, \tag{3.6}
\]
where the weights \( w_q \) for \( q > q_0 \) are set to zero if \( q_0 < 4 \) rays were found in the immediate
neighbourhood of \((i,j,k)\). This might be the case close to the edges of the computational
volume; we shall comment more on this while discussing the boundary conditions. The form of
eq (3.6) was chosen specifically because: (1) if a ray labeled \( q \) happens to pass exactly through
the point \((i,j,k)\), then \( I_{i,j,k,l,m} = I_q \); (2) if all four rays encompass the point, \( \min(I_q) \leq I_{i,j,k,l,m} \leq \max(I_q) \); and (3) if \((i,j,k)\) happens to be far from all four rays, then the resulting
intensity will just be an average of the four \( I_q \)'s.

B: One-to-One Correspondence

With the interpolation scheme in eq. (3.6) there is always the possibility that the emissivity
and opacity calculated in a 3D cell will be using 1D intensities from rays in adjacent cells.
This – unless the interpolation scheme is specially debugged for a fixed set of grids (spatial and
angular) at a fixed resolution – will cause the wrong speed of advection in 3D, even though we
might be using the correct high-resolution Riemann solver along 1D rays. The cure is simple:
the interpolation between 3D cells and 1D data points on the rays has to be on a one-to-one
correspondence. The energy density reconstructed from intensities from a given set of 1D ray
points has to contribute to the emissivity and opacity of that and only that same set of points.
Therefore, in a given direction \((\theta_l, \phi_{lm})\), the separation between rays should be small enough
to guarantee at least one ray data point within that 3D cell. The consequence is a few times
(3 – 4 in practice) larger number of rays required to cover the entire computational volume.

3.1.2 Angular Reconstruction

At each point on our 3D rectangular mesh we assume a piece-wise linear dependence of the
intensity \( I \) on two angles, \( \theta \) and \( \phi \),

\[
I(\theta, \phi) = (1 - \xi_\theta)(1 - \xi_\phi)I_{l-1,n-1} +
\]
within a spherical rectangular element (or a spherical triangle adjacent to either of the poles) bounded by the angles $\theta_i$, $\theta_{i-1}$ in $\theta$ and $\phi_n$ and $\phi_{n-1}$ in $\phi$, with the rectangular grid defined as

$$\theta_i = \pi \left( \frac{l-1}{N_\theta - 1} - \frac{1}{2} \right), \quad 1 \leq l \leq N_\theta,$$

$$\phi_n = \frac{2\pi n}{N_\phi}, \quad 1 \leq n \leq N_\phi,$$

and

$$\xi_\theta = \frac{\theta_1 - \theta_{i-1}}{\theta_i - \theta_{i-1}}, \quad \xi_\phi = \frac{\phi - \phi_{n-1}}{\phi_n - \phi_{n-1}}.$$ 

We then integrate the intensity over $4\pi$ with appropriate weights to get the scalar radiation energy density at each point $(l, n)$ of the rectangular spherical grid

$$E_{1, j, k}^{\text{diff}} = \frac{1}{c} \int_{4\pi} I_{i, j, k}(\theta, \phi) d\Omega \approx \frac{1}{c} \sum_i \sum_n I_{l-1/2, n-1/2},$$

where the quadrature terms

$$I_{l-1/2, n-1/2} \equiv \int_{\phi_{n-1} \leq \phi \leq \phi_n} \int_{\theta_{i-1} \leq \theta \leq \theta_i} I_{i, j, k}(\theta, \phi) d\Omega$$

after integration inside each spherical rectangle or triangle (Fig. 3.2) can be written as

$$I_{l-1/2, n-1/2} = \frac{\Delta \phi_{n-1/2}}{\Delta \theta_{i-1/2}} \times \begin{cases} (I_{l-n} + I_{l-n-1})(\Delta \theta_{l-1/2} \sin \theta_1 + \Delta \cos \theta_{n-1/2}) - \\ - (I_{l-1,n} + I_{l-1,n-1})(\Delta \theta_{l-1/2} \sin \theta_{l-1} + \Delta \cos \theta_{l-1/2}) \end{cases} \quad \text{for rectangles},$$

$$I_{l-1/2, n-1/2} = \frac{(I_{l,n} + I_{l,n-1})(\Delta \theta_{l-1/2} \sin \theta_1 + \Delta \cos \theta_{n-1/2})}{2} -$$

$$- (I_{l-1,n} + I_{l-1,n-1})(\Delta \theta_{l-1/2} \sin \theta_{l-1} + \Delta \cos \theta_{l-1/2}) \frac{1}{2} \quad \text{for triangles}.$$ 

The RHS of this expression is then multiplied by appropriate coefficients to allow for the non-orthogonal angular grid (eq. 3.4), to yield the final weights.
Since the advection part on the left-hand side of eq. (2.6) is strictly linear, the simplest way to propagate intensities is just to shift wavefronts by one grid zone at each time-step, accounting for sources and sinks of radiation. Assuming that all discretization points along each ray are strictly equidistant, the intensity at a point \( j \) is updated simply as

\[
I_{j}^{n+1} = I_{j-1}^{n}e^{-\kappa_j c \Delta t} + \epsilon_j c \Delta t.
\] (3.11)

Alternatively, one could take special care of the length of each ray segment contained within a particular 3D grid cell, and use a scheme similar to the third-order-accurate piecewise parabolic advection method (PPA) of Stone & Mihalas (1992). In either case we can track sharp discontinuities in 1D with very little numerical diffusion, and, therefore, our approach is well suited to the calculation of I-fronts.

Note that our placing of rays is functionally similar to the method of of accelerated ray tracing employed by Nakamoto & Umemura (1998) for the quasi-static reconstruction (formal solution) of the angle-dependent intensity. However, here we are solving the advection problem explicitly, propagating wavefronts in the multidimensional phase space at the speed of light, in a sense making radiative transfer a local problem.

### 3.1.3 The Algorithm

We start calculations by specifying the initial conditions (temperature, degree of ionization, and in the simplest cases no radiation field inside the volume) and boundary conditions (the intensity of radiation entering the volume – all outward flux at the edges can freely escape the computational box). The inward flux at the boundaries is isotropic within \( 2\pi \) and is simply

\[
I^+ = \frac{c}{4\pi} E_b,
\]

where \( E_b \) is the average background radiation energy density. Since each ray within the volume starts and ends at the sides of the volume, we automatically have boundary conditions for each
of the 1D advection problems. The density field is kept static for all tests in this study, but since the radiation field is being evolved explicitly at the speed of light, one could easily evolve the underlying density distribution on a much slower fluid flow timescale if desired.

The course of the algorithm at each time step can be divided into the following steps:

- project the emissivity $\varepsilon_\nu$ and opacity $\kappa_\nu$ from 3D grid to rays,
- evolve wavefronts along individual rays by $\Delta t$,
- project intensities from rays to 3D to reconstruct $I_\nu$ as a function of five variables $I_\nu(\mathbf{r}, \theta, \phi)$,
- calculate the radiation energy density $E(\mathbf{r})$,
- solve all chemical equations via an implicit iterative technique to get new state variables, separately at each point, and
- compute new $\varepsilon_\nu$ and $\kappa_\nu$.

At the beginning of each time-step we advect 1D intensities according to eq. (3.11) along each ray. The numerical resolution along each ray is simply set to the resolution $1/N$ of the 3D rectangular mesh, so that along the ray $i$ the point $j$ has a coordinate

$$\lambda_j = \frac{j - 1/2}{N}, \quad j = 1, \ldots, N_i, \quad N_i = l_i N,$$

where $l_i$ is the length of the ray segment inside the cube. Note that one can have much coarser 1D grids along rays, speeding up the advection but sacrificing both spatial and angular resolution. The advected intensities $I_j^{n+1}$ are then projected onto a 3D grid to reconstruct the mean energy density at each point using eq. (3.6 - 3.9). This operation is one of the most demanding from the computational point of view, since at each of our $N^3$ points we have to deal with the angular dependence of the radiation field. When this update is done, we solve
the matter-radiation interaction equations implicitly to compute the local level populations (eq. (3.20)). This gives us the 3D distributions of emissivity and opacity (eq. (3.14 - 3.17)) which are then mapped back to the rays and used in the advection scheme at the next time-step.

This simple scheme which we will refer to as *time-dependent ray tracing* can be used as a stand-alone solver, or as a closure scheme for the system of moment equations through the use of variable Eddington factors (as in Stone *et al.* 1992). In the absence of any sinks and sources of radiation, the intensity is conserved exactly along each ray. Since the number of rays does not vary with time, the advection part of our algorithm – in other words, the proper solution of the 1D RT equation (2.1) with the zero right-hand side – can guarantee exact conservation of the total number of photons in the volume, once these photons have been mapped to the rays at time \( t = 0 \). On the other hand, since emissivities and opacities entering the transfer equation as sources and sinks on the right-hand side are interpolated quantities, the total energy stored in the radiation field at any given moment is subject to the interpolation error, which is a function of the spatial and angular resolution.

One advantage of the use of angle-averaged moments of radiation is that the advection mechanism is essentially reduced to 3D, and it is relatively straightforward to implement the multi-dimensional conservation scheme for the linear advection part of the moment equations. Then one could use a much denser spatial grid for the solution of the moment equations, and a relatively course grid for the angular reconstruction of the intensity of radiation via ray tracing. In practice, however, we have found that the mismatch between the spatial resolutions of the moment solver and of the ray tracing usually leads to numerical instabilities. In what follows, we consider ray tracing only as a stand-alone solver.

Another – perhaps, a better – way of coupling angular and spatial variations of the intensity may be an extension of the Spherical Harmonics Discrete Ordinate Method (Evans 1998). For steady-state transfer problems, instead of storing the radiation field, this method keeps track of the source function as a spherical harmonic series at each point. Although the direct
implementation of this technique for time-dependent problems is probably not realistic, due to the lookback time (i.e. the finite speed of light propagation), the spherical harmonic representation of the radiation field might require less storage and might result in smoother angular dependence as compared with a pure ray tracing approach.

3.1.4 Adaptive Time Stepping

Note that if I-fronts do not propagate fast compared to the speed of light, for instance, in the cosmological context where the evolution on the light-crossing timescale will normally require many thousand time steps, it is possible to update the radiation energy density $E(r)$ once every few tens or few hundred time steps, while still evolving the intensities and solving all rate equations properly at the speed of light. We found that in practice this shortcut leads to an increase in speed by a factor of 10 or even higher without any loss of accuracy. However, it is important to compute the energy density properly along the edges of I-fronts to guarantee the correct rate of growth of ionized regions.

To further accelerate this computation, we use adaptive time stepping to put lower time resolution on the 3D cells far from I-fronts. Since wavefronts cannot propagate further than one grid zone during one time step, only those cells which just experienced large change in $E(r)$ and their immediate adjacent neighbours need a proper update of $E(r)$. Depending on the width of I-fronts, typically only a few percent of all 3D cells require the new, exact value of $E(r)$.

3.2 Tests

3.2.1 Local Chemistry Equations

Since in our calculation all advection of radiation variables is performed explicitly, we can solve NLTE rate equations separately at each point. This makes it relatively easy to implement an implicit solver for all atomic and molecular processes.
Chapter 3. Time-Dependent Ray Tracing

To demonstrate the capabilities of explicit advection, instead of solving the proper chemistry equations for multiple species with primordial chemical composition, we have here adopted a simple toy model with just photoionization and radiative recombination in a pure hydrogen medium. The implicit solution of possibly stiff rate equations described below can be implemented in a similar manner for more realistic chemistry models. One of these models is later developed in Chapter 4.

Let us assume that the change in the degree of ionization $dx_e/dt$ due to photoionizations is simply proportional to the energy density of the monochromatic radiation field $E$ of frequency $\nu_1$, with the proportionality factor $(1 - x_e) * g_{HI}$, where the photoionization coefficient $g_{HI}$ has the dimensionality $\text{cm}^3 \text{erg}^{-1} \text{s}^{-1}$. The total change in fractional ionization is

$$\frac{dx_e}{dt} = g_{HI} E (1 - x_e) - x_e^2 n_H \alpha, \quad (3.12)$$

where $\alpha$ is the recombination coefficient. For an arbitrary optical depth, the finite difference approximation to eq. (3.12) can be written in the conservation form,

$$\frac{x_e(t + \Delta t) - x_e(t)}{\Delta t} = \frac{E}{h \nu_1} \left( 1 - e^{-\kappa \Delta t} \right) - x_e^2 n_H \alpha, \quad (3.13)$$

with opacity

$$\kappa = (1 - x_e) n_H h \nu_1 g_{HI}/c. \quad (3.14)$$

Instead of computing the true emissivity of the hydrogen medium (which depends on recombination rates to different atomic energy levels and a Maxwellian velocity distribution of recombining electrons), we obtain the total emissivity $\epsilon$ of the gas by considering conservation of the thermal energy density $E_{\text{th}}$ for matter,

$$\Delta E_{\text{th}} = E \left( 1 - e^{-\kappa \Delta t} \right) - 4\pi \epsilon \Delta t = h \nu_1 n_H \Delta x_e, \quad (3.15)$$
where all $\Delta$ symbols represent the change of variables during one time step. The full recombination coefficient

$$\alpha = \alpha_1 + \alpha_B \quad (3.16)$$

is the sum of recombination coefficients to the ground state ($\alpha_1$) and to all levels above the ground state ($\alpha_B$, the 'case B' recombination coefficient), $\nu_1$ is the frequency just above the Lyman limit, and we assume that recombinations in Lyman lines occur on a short timescale compared to $(x_e n_H \alpha_B)^{-1}$. Similarly, the full emissivity (or gas energy loss through recombinations) is

$$\epsilon = \epsilon_1 + \epsilon_B, \quad (3.17)$$

where $\epsilon_1/\epsilon = \alpha_1/\alpha$. This simple notation ensures radiation energy conservation in eq. (2.6) for pure scattering of Lyman continuum photons (i.e., when $\alpha_B = 0$). Eq. (3.13) does not account properly for the number of photons entering the volume, so that a large photoionization coefficient $g_{HI}$ might lead to overproduction of ions. To compensate for this, the number of photoionizations inside a 3D grid cell per unit time is not allowed to be larger than the number of photons actually absorbed inside this cell, i.e.

$$\frac{dx_e}{dt} \leq \frac{E}{h \nu_1} \frac{1 - e^{-\epsilon \Delta t}}{n_H \Delta t}. \quad (3.18)$$

Eq. (3.13,3.18) are solved separately at each point, given the local radiation energy density $E$. Discretization of eq. (3.13) in time yields

$$\frac{x_e^{n+1} - x_e^n}{\Delta t} = (1 - \theta) f_1(x_e^n) + \theta f_1(x_e^{n+1}), \quad (3.19)$$

where $f_1(x_e)$ is just the right-hand side of eq. (3.13) and $1/2 < \theta \leq 1$ for stability. Such equations can almost always be solved via Newton’s method for small enough $\Delta t$. Linearizing
eq. (3.19), we get the \( (i + 1) \)-th approximation to the value of \( x_e \) at time \( t^{n+1} \):

\[
x_e^{n+1,i+1} = x_e^{n+1,i} + \left[ \frac{\partial f_1(x_e^{n+1,i})}{\partial x_e^{n+1,i}} - \frac{1}{\theta \Delta t} \right]^{-1} \times \\
\left[ \frac{1 - \theta}{\theta} f_1(x_e^n) + f_1(x_e^{n+1,i}) - \frac{x_e^{n+1,i} - x_e^n}{\theta \Delta t} \right],
\]

(3.20)

which can then be iterated.

### 3.2.2 Test Parameters and Resolution

For all of our test runs, except the study of the shadow behind a neutral clump in Sec. 3.2.6, we set up a numerical grid with dimensions \( 64^3 \times 10^2 \). We have experimented with different angular resolutions finding that \( N_{\text{angles}}^2 \sim 10^2 \) produces reasonably accurate results for the amount of gas clumping typically found in cosmological simulations. Much higher resolutions \( (N_{\text{angles}}^2 \gg 10^2) \) do not provide any significant gain, since, even at \( 10^2 \), rays which are adjacent in angles resolve all 3D grid cells within the mean free path of a photon. It is interesting to point out that \( N_{\text{angles}}^2 \sim 10^2 \) also matches the equivalent resolution of \( 64^5 \) data points for 5D advection. There are \( N_{\text{angles}}^2 \) rays passing in the immediate neighbourhood \( (1/64^3\text{th of the total computational volume}) \) of each 3D grid cell, each ray containing \( N_p \approx 2/3 \times 64 \) grid nodes. Thus, in 5D we obtain the equivalent resolution of \( N_p \times 64^3 \times N_{\text{angles}}^2 \sim 1.1 \times 10^9 \sim 64^5 \) data points.

Lower angular resolutions \( (N_{\text{angles}}^2 < 10^2) \) would probably suffice for those problems where the radiation field is nearly isotropic (that is, the mean free path of a photon is comparable to or smaller than the grid resolution), or where the angular variation is dominated by the lower frequency harmonics.

For all test runs we take a 2.5 Mpc (comoving) cosmological volume, with the physical scale corresponding to \( z = 10 \). All densities (from low-density optically thin ambient gas to dense clumps) fall in the range \( \Omega_{\text{gas}} = 0.001 - 0.05 \) (in units of the critical density of the
Universe), assuming a Hubble constant of 50 km s\(^{-1}\) Mpc\(^{-1}\). This low density contrast is chosen to cover the typical range encountered in cosmological hydrodynamics, and is ideally suited to demonstrate transient features during patchy ionization. The absorption coefficients are taken to mimic complete self-shielding (assumed to be \(\tau \gtrsim 10\)) at neutral hydrogen column densities higher than 10\(^{18}\) cm\(^{-2}\) (for which the optical depth at the Lyman limit exceeds unity, see, e.g., Zhang et al. 1997), except where we probe different regimes, specifically in Sec. 3.2.5 where \(\tau = 10\) corresponds to 10\(^{17}\) cm\(^{-2}\), and Sec. 3.2.6 where \(\tau = 10\) corresponds to 10\(^{21}\) cm\(^{-2}\).

### 3.2.3 An Isolated Spherical Expanding I-front

A simple problem that would test the ability of the method to track I-fronts properly is that of a single, isolated Strömgren sphere expanding around a source of ionizing radiation (see, e.g., Abel et al. 1998a). One difficulty of the current approach is that rays are drawn in a way to cover the whole computational volume uniformly and isotropically. For a single point source of radiation this would mean that only a small number of rays pass through its neighbourhood. Hence, although intensities along individual rays are strictly conserved, there is no guarantee that the energy density has the right value far from a source of a specified luminosity. Instead, in the first two tests (Sec. 3.2.3 and 3.2.4), the propagation of ionizing photons is computed on the 3D grid, according to eq. (3.2).

At time \(t = 0\) we turn on a point source, which starts to blow an expanding H\(\text{II}\) bubble around it. The speed of the I-front can be obtained analytically by equating the number of direct ionizing photons to the flux of neutral atoms crossing the front. In the absence of radiative recombinations (\(\alpha = 0\)), the H\(\text{II}\) bubble grows indefinitely (Spitzer 1968):

\[
R_{\text{I}}(t) = \begin{cases} 
  ct & \text{if } t \leq t_c \\
  \left[3\dot{N}_{\text{ph}}(t - \frac{2R_c}{3c})/4\pi n_{\text{H}}\right]^{1/3} & \text{if } t > t_c,
\end{cases}
\]

where \(t_c = \left(\dot{N}_{\text{ph}}/4\pi c^3 n_{\text{H}}\right)^{1/2}\). Parameters used for this calculation are the diffuse neutral gas density \(\Omega_0 = 0.01\) (at \(z = 10\)) and the central source luminosity \(\dot{N}_{\text{ph}} = 3 \times 10^{53}\) s\(^{-1}\) (all emitted...
in photons above the hydrogen Lyman limit). The comparison between the numerical speed of the I-front and the exact solution from eq. (3.2.3) is plotted in Fig. 3.3. The difference between the two always stays within one grid zone.

![Graph showing the analytical radius of the spherical H II bubble (solid line) compared to the numerical results (filled data points). The error bars indicate the resolution of the grid (\(\pm \Delta x\)), while the dotted lines give the radius at which the speed of the I-front drops below the speed of light. The horizontal dashed line at the top shows the radius at which the I-front reaches the boundary of the computational volume.](image)

Figure 3.3: The analytical radius of the spherical H II bubble (solid line) compared to the numerical results (filled data points). The error bars indicate the resolution of the grid (\(\pm \Delta x\)), while the dotted lines give the radius at which the speed of the I-front drops below the speed of light. The horizontal dashed line at the top shows the radius at which the I-front reaches the boundary of the computational volume.

### 3.2.4 An Isolated Strömgren Sphere in the Presence of a Density Gradient

Consider a point source of radiation put into a density gradient along one of the principal axes of the cube. In the absence of diffuse radiation from H II regions (\(\alpha_1 = 0\)) the only ionizing photons come directly from the source in the centre, in which case the shape of the ionized bubble would be a simple superposition of Strömgren spheres with radii \(R_S(\phi)\) varying with the azimuthal angle \(\phi\) and given by the classical solution (Spitzer 1968).
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\[ S_0 = 4\pi \alpha_B \int_0^{R_S(\phi)} r^2 n^2_H(r, \phi) \, dr, \]

(3.21)

where \( S_0 \) is the photon production rate of the central source. For an exponential density gradient along the \( y \)-axis

\[ \log n_H = \log n_{H,1} + \frac{r \cos \phi + y_0}{\Delta y} \log \left( \frac{n_{H,2}}{n_{H,1}} \right) \]

(3.22)

\( n_{H,1} \), \( n_{H,2} \) being the hydrogen densities on the opposite faces of the cube), the equilibrium Strömgren radius \( R_S(\phi) \) is given by a simple equation

\[ S_0 = \frac{4\pi \alpha_B}{b^3} \left[ e^{a+bR_S(\phi)} \left( b^2 R_S^2(\phi) - 2bR_S(\phi) + 2 \right) - 2e^a \right], \]

(3.23)

where

\[ a = 2 \left[ \ln n_{H,1} + \frac{y_0}{\Delta y} \ln \left( \frac{n_{H,2}}{n_{H,1}} \right) \right] \quad \text{and} \]

\[ b = \frac{2 \cos \phi}{\Delta y} \ln \left( \frac{n_{H,2}}{n_{H,1}} \right). \]

We take the physical densities on the opposite faces of the volume to be \( \Omega_{gas,1} = 0.001 \) and \( \Omega_{gas,2} = 0.05 \), and the luminosity to be \( \dot{N}_{ph} = 10^{51} \text{s}^{-1} \). To simplify the calculation by avoiding any realistic atomic rate equations, we take the value of the total hydrogen recombination rate from Hummer (1994) for some fiducial temperature \( (T = 10^4 \text{K}) \). In Fig. 3.4 we plot a time sequence of models, for ionization by a central source, with no scattering of Lyman photons (i.e. \( \alpha_1 = 0 \)). The numerical solution at \( t = 4.1 \text{ Gyrs} \) appears to be very close to the exact one for an equilibrium Strömgren sphere. The sharp transition layer between the ionized and the neutral regions in the high optical depth regime indicates that, indeed, the scheme introduces very little numerical diffusion even when extended to 3D (within the accuracy of interpolation between the 3D mesh and the rays, see Fig. 3.5 for details).
3.2.5 Ionization in the Presence of a UV Background

The uniform coverage of the whole volume with rays implies that extended sources of radiation will be represented statistically much better than point sources. A simple test mimicking the evolution of dense clouds in the presence of ionizing radiation is to enclose the computational region in an isotropic bath of photons. The simplest way to accomplish this is just to set up a uniform, isotropically glowing boundary at the edges of the cube at $t = 0$. An effective demonstration of time-dependent ray tracing would be its ability to deal with any distribution of state variables within the simulation volume. For this test, we set up a density condensation shaped like the acronym for 'radiation hydrodynamics' (RHD), with a density 50 times that of the ambient homogeneous medium. The ambient medium has a constant density of $\Omega_{\text{gas}} = 10^{-3}$, and the energy density of the background radiation is $E = 5 \times 10^{-23} \nu_{\lambda} \text{ erg cm}^{-2} \text{ Hz}^{-1} \text{ sr}^{-1}$.

Fig. 3.6 shows the result of this simulation. Most of the low-density environment is ionized on the radiation propagation timescale. It takes somewhat longer for ionizing photons to penetrate into the dense regions. Whether these regions can be ionized on a timescale of interest, depends on the ratio of the recombination timescale to the flux of background radiation. One can easily see ionization 'eating in' to the neutral zone, e.g. in the disappearance of the serifs on the letters at late times. Note that the width of the ionization fronts does not usually exceed one grid zone (Fig. 3.7).

3.2.6 Diffuse Radiation from H II Regions: I. Shadows behind Neutral Clouds

Part of the ionizing radiation at high redshifts comes in the form of hydrogen Lyman continuum photons from recombinations in diffuse ionized regions. The following test, simulating the formation of shadow regions behind dense clouds at the resolution $32^3 \times 10^2$, was adapted from Canto et al. (1998). A neutral clump of radius $R_c = 1.25 \text{ Mpc}$ (comoving) is being illuminated by a parallel flux $F_\star = 6.34 \times 10^{-16} h_{\text{p}}^{-1} \text{ erg cm}^{-2} \text{ s}^{-1} \text{ Hz}^{-1}$ of stellar ionizing photons (just
above 13.6 eV) from one side; here $h_P$ is Planck’s constant. A shadow behind the clump is being photoionized by secondary recombination photons from the surrounding H II region (Fig. 3.8) of physical density $n_H = 3.7 \times 10^{-2} \text{ cm}^{-3}$. Neglecting hydrodynamical effects, the width $R_l$ of the shadow region can be estimated using a simple two-stream approximation (Canto et al. 1998)

$$\xi^2 = \frac{2}{1 + r_l^2(2 \ln r_l - 1)}, \quad \text{where} \quad r_l \equiv \frac{R_l}{R_c},$$

(3.24)

and the dimensionless parameter $\xi$ is defined as

$$\xi = \frac{4R_c n_H^2 \alpha_{\text{B}}^2}{F_s \alpha_1}.$$  

(3.25)

For $\xi^2 \leq 2$, recombination Lyman continuum photons from the illuminated region will eventually photoionize the shadow completely. For $\xi^2 > 2$, radiative losses through low-energy cascade recombination photons will stop the I-front, forming a neutral cylinder behind the dense clump. Strictly speaking, equations (3.24)–(3.25) are valid only for a shadow completely photoionized by secondary photons, and should be viewed as an approximation to I-fronts driven by scattering.

For this run we modify boundary conditions to include the effect of recombination photons originating outside the box. Each of the rays — starting on any face except the upper side of the volume (which goes through the neutral shadow) — carries the additional intensity of $\langle \varepsilon_1 \rangle / \langle \kappa \rangle$, where the angular brackets denote the average throughout the currently photoionized gas inside the box.

Overall, we find a remarkably good agreement between the results of our models and the analytic solution (Canto et al. 1998), taking into account that ionization of the shadow is due to scattering in the medium. In Fig. 3.9 we plot the radius $R_l$ of the shadow neutral region as a function of $\xi$ in our 3D numerical models. To vary the size of the neutral core, we fix the total recombination coefficient but we change the portion of recombinations into the ground
state (which would produce more Lyman continuum photons capable of ionizing the medium). The width of the I-front driven by secondary photons depends on the assumed opacity (the optical depth of $\tau = 10$ corresponding to the column density of $10^{21} \text{cm}^{-2}$). This low opacity was chosen to reach equilibrium quicker – equilibrium itself does not depend on the opacity – but it cannot be too low, otherwise there will be an unnecessary spread of the transition zone in the I-front over many grid cells.

### 3.2.7 Diffuse Radiation from H II Regions: II. Ionization of a Central Void

To demonstrate the ability of our scheme to handle scattering in more complicated situations, we also set up a model with ionization of a central low-density void by secondary, recombination photons. The void region is surrounded by two nested cubes with opposite faces open (Fig. 3.10). The walls of the cubes are set to be much denser than the rest of the medium, to screen completely the central void from direct ionizing photons, and the ionizing UV flux is introduced at all faces of the computational volume. The total hydrogen recombination coefficient $\alpha_1 + \alpha_B$ is again taken for the temperature $T = 10^4 \text{K}$. Similar to Sec. 4.4, we vary the amount of scattering in the medium by changing the fraction $q$ of atoms recombining into the ground state. In reality at $T = 10^4 \text{K}$ the value $q \approx 0.38$ (Hummer 1994) gives a solution in between our extreme values of $q$.

Similar to the test problem of Section 3.2.5, if $\alpha_B = 0$, then the medium will be ionized completely, since there is a constant flux of primordial ionizing photons. The speed of ionization depends on the values of $\alpha_1$, $\alpha_B$, $g_{HI}$ and $n_H$. Note, however, that if $\alpha_1$ is too high, the I-front will be very slow, since a large portion of the original ionizing photons are scattered back. On the other hand, if $\alpha_1$ is too low, the I-front will propagate much faster in those regions where ionization is driven by primordial photons, but in shadowed regions there will be too few recombination photons. Thus, it seems that the speed of ionization of the central void will be the highest at some intermediate $\alpha_1$. 

In Fig. 3.11 we demonstrate ionization of the void region for models with complete scattering and with no scattering at all. The parameters used for this model are \( E = 5 \times 10^{-20} \nu \text{erg cm}^{-2} \text{ Hz}^{-1} \text{ sr}^{-1} \) and the diffuse neutral gas density \( \Omega_{\text{gas}} = 0.01 \).

As expected, for the no-scattering model \((q = 0)\) the central region remains neutral, since there is no direct path for the ionizing photons. However, for the model which includes scattering \((q = 1)\), at least part of the central region becomes ionized. This demonstrates that our scheme is perfectly capable of dealing with re-scattering of the ionizing photons. Beyond this simple test case, there are many astrophysical situations where progress can be made via numerical radiative transfer. For example, analytic solutions are often used, which are steady-state, and which assume a sharp boundary between the neutral and ionized zones. Using our numerical techniques it should be possible to follow general systems with complex density inhomogeneities as well as regions of partial ionization.
Figure 3.4: The cross-section of the numerical 3D ionization front going through the source of ionization for a model with no scattering, shown for six output times. The density of the gas follows an exponential gradient (eq. 3.22) increasing by a factor of 50 from the upper to the lower side of the cube. The dashed line gives the analytic solution (eq. 3.23) for an equilibrium Strömgren sphere without scattering. The width of the transition layer between the neutral and fully ionized regions is consistent everywhere with the mean free path of ionizing photons. The ionizing source of luminosity $N_{ph} = 10^{51}$ s$^{-1}$ (all emitted in photons just above the hydrogen Lyman limit) is marked by the asterisk. The nine contour levels correspond to ionization fractions of $x_e = 0.1, 0.2, ..., 0.9$. 
Figure 3.5: In order to cover the whole computational volume with rays uniformly and isotropically, we set the number of rays inside a latitudinal angle interval $[\theta, \theta + d\theta]$ proportional to $\cos \theta$. An odd number of rays will necessarily introduce slight left-right asymmetry for interpolation between the 3D rectangular grid and the radial grid for any non-central cross-section through the volume. In this figure we show a 2D schematic representation of the two grids employed in our method. To simplify the plot, the source of radiation is assumed to be sitting in the centre, and only radial rays are drawn here. Due to the finite angular resolution, interpolation between the 3D mesh and the rays is not symmetric with respect to the centre. This shows up in the asymmetry between the upper and the lower sides of the ionization contours in Fig. 3.11.
Figure 3.6: The isosurface of ionization level $x_e = 0.5$ is plotted at six time intervals for the model with an ionizing background coming from outside of the cube. The density contrast between the ambient medium and the high-density acronym ‘RHD’ (radiation hydrodynamics) is 50. This simulation demonstrates 5D advection on the radiation propagation time-scale. The numerical resolution is $64^5$. The effects of shielding are clearly visible during partial ionization.
Figure 3.7: Contour plot of ionization in a cross-section through the data presented in Fig. 3.6. There are 11 contour lines spaced linearly from $x_e = 0$ to $x_e = 1$. Note the sharpness of the ionization boundaries, the shielding, and the fact that the most deeply embedded regions take the longest to ionize.
Figure 3.8: Cross-sections of the dense clump (shaded) and the neutral shadow region behind it, for different fractions $q = \alpha_1/\alpha$ of recombination into ground states. The clump is being illuminated with a parallel flux $F_*$ of direct stellar ionizing photons entering through one side of the box (marked with arrows), and the shadow region behind it is being photoionized by recombination Lyman continuum photons from the surrounding H II gas. Each model has been evolved to an equilibrium state, corresponding to many passages of the wavefront across the computational region. The nine contour levels correspond to ionization fractions of $x_e = 0.1, 0.2, ..., 0.9$. This test is adapted from Canto et al. (1998).
Figure 3.9: The width $R_1$ of the shadow behind a neutral clump of radius $R_c$ as a function of the dimensionless parameter $\xi$ of eq. (3.25). The solid line represents the two-stream analytic solution (Canto et al. 1998), assuming an infinitely sharp boundary. The points show the results of our 3D numerical model, plotted explicitly at $x_e = 0.5$, with the errorbars giving the width of the I-front formed by secondary photons. Since the width of the neutral core in our numerical model depends on multiple scatterings in 3D, we would not expect a detailed match; however, the agreement between the approximate analytic and the numerical solutions is remarkably good.
Figure 3.10: The central void region in the test model in Sec. 3.2.7 is completely screened from direct ionizing photons by two nested cubes with opposite faces open. The only way to ionize the void is to allow for scattering of secondary photons in the side tunnels.
Figure 3.11: Diagram demonstrating ionization of the void region, which consists of two nested cubes with opposite sides open. The central void and the side 'tunnels' have the same density as the surrounding medium, and the density of the walls is set to be much higher to completely block all external ionizing photons. In this figure we plot one of the central cross-sections showing contours of ionization at five different output times for the model with complete scattering \((q = 1)\), and a quasi-equilibrium configuration for the model with no scattering \((q = 0)\) after \(n = 500\) timesteps. The shaded areas represent neutral regions.
4.1 Frequency Dependence: Multigroup Transfer

The numerical approach developed in the previous section describes an efficient method for advection of monochromatic intensity in the 5D phase space of three spatial coordinates and two angles. Exactly the same technique will work for broad frequency intervals if all terms with subscript $\nu$ in eq. (2.6) are replaced with frequency-integrated quantities. However, since cross-sections of photoionization for most chemical species drop approximately as $\nu^{-3}$ above the photoionization threshold (e.g., Tucker 1975, p. 236), higher frequencies have very little power in frequency-integrated values of $E$, $\epsilon$ and $\kappa$. Therefore, a scheme which is devised to be sensitive to photoionization of hydrogen will give only a very crude description for ionization rates of species with higher ionization potentials, as well as emissivities of those elements at higher frequencies. Therefore, we would like to include as many frequency intervals as possible. For the study of cosmic reionization it is sufficient to consider three frequency groups, above the hydrogen Lyman limit (13.6 eV) and the single (24.6 eV) and double (54.4 eV) ionizations of helium, respectively, with all frequency-dependent terms being averaged inside those groups. Besides hydrogen and single and double helium photoionization and recombination, there are several other chemical processes which could be easily included. However, at this stage we feel that introducing more than three frequency groups will result in an unnecessary complexity of the numerical model. We neglect entirely the effects of preheating of the neutral IGM by photons below 13.6 eV — which is a very complex process in itself, acting through absorption in all atomic Lyman lines with $2 < n \lesssim 150$, and via absorption in Lyman and Werner lines of molecular $H_2$ (Haiman
et al. 1999) — and we consider radiative processes only above 13.6 eV. The three frequency groups together with some other radiation thresholds are displayed schematically in Fig. 4.1.

![Schematic representation of the three frequency groups, along with some other radiation thresholds.](image)

Figure 4.1: Schematic representation of the three frequency groups, along with some other radiation thresholds.

We define group-averaged values as

\[
I_g = \int_{\nu_g}^{\nu_{g+1}} I_\nu d\nu, \quad \epsilon_g = \int_{\nu_g}^{\nu_{g+1}} \epsilon_\nu d\nu, \quad \kappa_{lg} = \int_{\nu_g}^{\nu_{g+1}} \frac{I_\nu}{I_g} d\nu, \quad (4.1)
\]

where \( g = 1, 2, 3 \) and \( \nu_4 = \infty \). Integrating eq. (2.6) over frequency inside the interval \([\nu_g, \nu_{g+1}]\) we get

\[
\frac{1}{c} \frac{\partial I_g}{\partial t} + \mathbf{n} \cdot \nabla I_g = \epsilon_g - \kappa_{lg} I_g. \quad (4.2)
\]

Let us assume that we know the cross-section of some photochemical reaction (e.g., photoionization) \( \sigma_*(\nu) \). Its contribution to the \( g \)-group average absorption is simply

\[
\kappa_{lg} \leftarrow \frac{n_H}{I_g} \int_{\nu_g}^{\nu_{g+1}} \sigma_*(\nu) I_\nu d\nu. \quad (4.3)
\]
and the total photoionization rate is

\[ k_* = \int_{4\pi} d\Omega \int_{\nu_1}^{\infty} \sigma_*(\nu) \frac{I_\nu}{h\nu} d\nu. \] (4.4)

To calculate \( \kappa_ig \) and \( k_* \), we are free to chose any spectral shape \( I_\nu(\nu) \) to satisfy the definition of \( I_g \). For a simple power law

\[ I_\nu = I_{0g} \left( \frac{\nu}{\nu_g} \right)^{-\alpha_g}, \] (4.5)

we have

\[ I_1 = \frac{I_{01}}{\alpha_1 - 1} \left[ \nu_1 - \nu_2 \left( \frac{\nu_1}{\nu_2} \right)^{\alpha_1} \right], \quad \alpha_1 \neq 1, \] (4.6)

\[ I_2 = \frac{I_{02}}{\alpha_2 - 1} \left[ \nu_2 - \nu_3 \left( \frac{\nu_2}{\nu_3} \right)^{\alpha_2} \right], \quad \alpha_2 \neq 1, \] (4.7)

\[ I_3 = \frac{I_{03}}{\alpha_3 - 1} \nu_3, \quad \alpha_3 > 1. \] (4.8)

In what follows, we will be solving three scalar eq. (4.2) for \( g = 1, 2, 3 \) using the techniques described in Chapter 3.

### 4.2 Rate Equations

We use the atomic data from Abel et al. (1997), including 28 chemical rate equations for nine species: \( \text{H, H}^+, \text{H}^-, \text{H}_2, \text{H}_2^+, \text{He, He}^+, \text{He}^{++} \) and \( e^- \). It is not entirely clear if elements heavier than helium are present in the intercluster environment during the epoch of reionization. While the absorption spectra of ultra-high redshift (up to \( z \sim 5 \)) quasars seem to indicate at least some presence of heavy elements in intergalactic clouds (e.g., see Cowie et al. 1995), there is a consensus that these elements were ejected into the intergalactic medium after the epoch of the first star formation. If most of cosmic reionization occurs via supersonic, R-type shock waves propagating outward from the point sources which made the first light in the Universe, it seems
safe to assume that it takes some time for heavy elements to fill in the Universe more or less uniformly. Metals, if present at that epoch, would supply extra free electrons, which would change the cooling function of the medium (e.g., facilitating cooling in the temperature range $10^4 - 10^7$ K) and affect some of the observable properties of patchy ionization. However, at this stage we do not include metals into our models assuming uniform primordial composition.

Here we give a brief list of the chemical reactions which we take into account. For details of actual microphysics and numerical values of reaction cross-sections we refer the reader to Abel et al. (1997) and Anninos et al. (1997), as well as to the on-line database of primordial gas chemistry made available by T. Abel (the Primordial Gas Chemistry page, at http://zeus.ncsa.uiuc.edu:8080/~abel/PGas).

Collisional:

1) $\text{H} + e^- \rightarrow \text{H}^+ + 2e^-$  
2) $\text{H}^+ + e^- \rightarrow \text{H} + \gamma$  
3) $\text{He} + e^- \rightarrow \text{He}^+ + 2e^-$  
4) $\text{He}^+ + e^- \rightarrow \text{He} + \gamma$  
5) $\text{He}^+ + e^- \rightarrow \text{He}^{++} + 2e^-$  
6) $\text{He}^{++} + e^- \rightarrow \text{He}^+ + \gamma$  
7) $\text{H} + e^- \rightarrow \text{H}^- + \gamma$  
8) $\text{H}^- + \text{H} \rightarrow \text{H}_2 + e^-$  
9) $\text{H}^+ + \text{H} \rightarrow \text{H}_2^+ + \gamma$  
10) $\text{H}_2^+ + \text{H} \rightarrow \text{H}_2 + \text{H}^+$  
11) $\text{H}_2 + \text{H}^+ \rightarrow \text{H}_2^+ + \text{H}$  
12) $\text{H}_2 + e^- \rightarrow 2\text{H} + e^-$  
13) $\text{H}_2 + \text{H} \rightarrow 3\text{H}$  
14) $\text{H}^- + e^- \rightarrow \text{H} + 2e^-$  
15) $\text{H}^- + \text{H} \rightarrow 2\text{H} + e^-$  
16) $\text{H}^+ + \text{H}^- \rightarrow 2\text{H}$  
17) $\text{H}^+ + \text{H}^- \rightarrow \text{H}_2^+ + e^-$  
18) $\text{H}_2^+ + e^- \rightarrow 2\text{H}$  
19) $\text{H}_2^+ + \text{H}^- \rightarrow \text{H} + \text{H}_2$

Radiative:

20) $\text{H} + \gamma \rightarrow \text{H}^+ + e^-$  
21) $\text{He} + \gamma \rightarrow \text{He}^+ + e^-$  
22) $\text{He}^+ + \gamma \rightarrow \text{He}^{++} + e^-$  
23) $\text{H}^- + \gamma \rightarrow \text{H} + e^-$  
24) $\text{H}_2 + \gamma \rightarrow \text{H}_2^+ + e^-$  
25) $\text{H}_2^+ + \gamma \rightarrow \text{H} + \text{H}^+$  
26) $\text{H}_2^+ + \gamma \rightarrow \text{H}^+ + e^- + \text{H}^+$  
27) $\text{H}_2 + \gamma \rightarrow \text{H}_2^* \rightarrow 2\text{H}$  
28) $\text{H}_2 + \gamma \rightarrow 2\text{H}$

We use the following definitions for chemical abundances:
\[
\psi \equiv \frac{n_{\text{He total}}}{n_{\text{H total}}}.
\]
\[
x_1 = \frac{n_{\text{H}^0}}{n_{\text{H total}}}, \quad x_2 = \frac{n_{\text{H}^+}}{n_{\text{H total}}}, \quad x_3 = \frac{n_{\text{H}^-}}{n_{\text{H total}}},
\]
\[
x_4 = \frac{n_{\text{H}^2}}{n_{\text{H total}}}, \quad x_5 = \frac{n_{\text{H}^+}}{n_{\text{H total}}}, \quad x_6 = \frac{n_{\text{He}}}{\psi n_{\text{H total}}},
\]
\[
x_7 = \frac{n_{\text{He}^+}}{\psi n_{\text{H total}}}, \quad x_8 = \frac{n_{\text{He}^{++}}}{\psi n_{\text{H total}}}, \quad x_9 = \frac{n_e}{n_{\text{H total}}},
\]
(4.11)
where $\psi = 0.075$ is helium abundance, and conservation of hydrogen and helium nuclei and electrons reads
\[
x_1 + x_2 + x_3 + 2x_4 + 2x_5 = 1,
\]
\[
x_6 + x_7 + x_8 = 1,
\]
\[
x_2 - x_3 + x_5 + \psi (x_7 + 2x_8) = x_9.
\]
(4.12)
We write down the chemical rate equations in their most general form
\[
\frac{dx_i}{dt} = \frac{n_H}{\psi_i} \sum_j \sum_k \alpha_{ijk} \psi_j x_j x_k + \frac{1}{\psi_i} \sum_j \beta_{ij} \psi_j x_j + \frac{\gamma_i}{\psi_i n_H}, \quad i = 1, \ldots, 9,
\]
(4.13)
where the coefficients $\alpha_{ijk}$, $\beta_{ij}$ and $\gamma_i$ are functions of reaction rates from Abel et al. (1997) and Anninos et al. (1997), with the first term on the RHS of eq. (4.13) accounting for collisional reactions, the second term representing radiative processes, the last term (which might give an implicit conservation of species) being almost always zero, and
\[
\psi_i \equiv (1, 1, 1, 1, 1, \psi, \psi, \psi, 1)^T.
\]
Equations 4.13 describe evolution on drastically different timescales. Photoionization can proceed on timescales much shorter than the light-crossing (of one grid zone) time $t_R$. On the other hand, many species will quickly acquire equilibrium abundances, and any further change in their number density will progress at the Hubble rate. The timescales entering eq. (4.13) span over ten orders of magnitude. For this reason, the numerical solution of chemical rate equations should be based on implicit techniques. Although the routines for solution of
the systems of stiff ordinary differential equations are generally available (e.g., the popular Livermore Solver, LSODAR, at http://gams.nist.gov; or the routine STIFBS in Numerical Recipes, Press et al. 1992), inside each solver it is necessary to update dynamically a large variety of parameters, such as the chemical reaction rates which depend on the temperature, or the strength and spectrum of the radiation field. For this reason, a numerical solver of rate equations optimized for automatic handling of terms with variable stiffness on the RHS of eq. (4.13) was developed specifically for this task. To simplify calculations, we assume that $\alpha_{ijk}$, $\beta_{ij}$ and $\gamma_i$ do not change much with temperature during one integration time step $\delta t(\{\delta x_j\})$ (which can be much smaller than $\Delta t$; as discussed below), although the implicit solver is still temperature-dependent on the $\Delta t$ timescale. We use linearization to construct an implicit, first-order accurate chemistry solver. If we rewrite eq. (4.13) in the form

$$\frac{dx_i}{dt} = f_i(\{x_j\}),$$

(4.14)

and replace it with a finite difference equation

$$\phi_i \equiv (1 - \theta)f_i(\{x_j^n\}) + \theta f_i(\{x_j^{n+1}\}) - \frac{x_i^{n+1} - x_i^n}{\Delta t},$$

(4.15)

where $\theta > 1/2$ for stability, then linearizing eq. (4.15) we can obtain a system of equations

$$\left\| \frac{\partial \phi_i}{\partial x_i^{n+1}} \right\| \cdot \| \delta x_i \| = \| \phi_i \|,$$

(4.16)

where the Jacobian on the LHS is composed of

$$\frac{\partial \phi_i}{\partial x_i^{n+1}} = 2\theta n_H \left( \sum_{j \neq i} \tilde{\alpha}_{ij} x_j^{n+1} + \tilde{\alpha}_{ii} x_i^{n+1} \right) + \theta \tilde{\beta}_{ii} - \frac{\delta_{ii}}{\Delta t}.$$

(4.17)

Here $\delta_{ii}$ is the Kronecker delta symbol and

$$\tilde{\alpha}_{ijk} = \frac{\psi_j \psi_k}{\psi_i} \alpha_{ijk}, \quad \tilde{\beta}_{ij} = \frac{\psi_j}{\psi_i} \beta_{ij}.$$
Note that $\Delta t$ is the time step for the advection problem. As far as the solution of the chemical reactions is concerned, $\Delta t$ is the total period of time during which these reactions have to be evolved. The time step $\delta t(\{\delta x_j\})$ for integration of the rate reactions can be much smaller.

We obtain the implicit solution to eq. (4.13) using the iterations

$$x_i^{n+1,k+1} = x_i^{n+1,k} + \delta x_i, \quad \text{with} \quad x_i^{n+1,0} = x_i^n. \quad (4.18)$$

Since the full change of variables, $x_i^{n+1} - x_i^n$, during one advection time step $\Delta t$ is of order $O(\Delta t)$, we can always guarantee convergence simply by reducing $\Delta t$. Mathematically, the implicit solution (eq. (4.16)—(4.18)) is always stable; the stability is not degraded by the fact that the function $\phi_i(\{x_j\})$ is not very smooth, since it depends on the temperature and is obtained by interpolation from the tabular values. To guarantee high accuracy of the solution, even in the presence of very stiff photoionization terms, we use automatic integration stepping with the time step $\delta t(\{\delta x_j\})$ determined by the largest Jacobian element in eq. (4.17) for $\Delta t \to \infty$.

### 4.2.1 Number Density of Absorption-Induced Processes

Imagine a case where the photoionization rate in eq. (4.4) is very high. Since our chemistry solver is not completely implicit in the strictest sense — we assume that the kinetic temperature of the gas does not change considerably during an integration time step $\delta t$ (derived from the largest element in the Jacobian matrix in eq. (4.17)), hence, the absorption coefficient is constant within $\delta t$ — we might encounter a situation when the total number density of absorption-induced processes in a 3D cell exceeds the number of photons absorbed within that cell. To prevent this, we have to limit the total number of radiative reactions, similarly to eq. (3.18). But contrary to the toy chemistry model in Sec. (3.2.1), we now include multiple processes, both collisional and radiative, so that the number of photons absorbed due to some photochemical
reaction does not give a correct upper limit for the abundance of a particular species. However, for very steep photochemical reactions, we can subtract already thermalized (absorbed) photons

\[
\langle \text{number density of absorbed photons} \rangle \approx \sum_g \left\langle \frac{E}{h\nu} \right\rangle_g (1 - e^{-\alpha_g \Delta t}),
\]

from the radiation energy density \(E_g\) at that point, within the chemistry solver. In the equation above, the quantity

\[
\left\langle \frac{E}{h\nu} \right\rangle_g = \frac{E_g \nu_g - \nu_g + 1}{\nu_g - \nu_g + 1} \left(\frac{\nu_g}{\nu_{g+1}}\right)^{\alpha_g + 1} \frac{\alpha_g - 1}{\alpha_g}
\]

is the local number density of photons in the frequency group \(g\). Note that for large local absorption, the energy density \(E_g \rightarrow 0\) on a timescale much shorter than \(\Delta t\), and new photons have to be supplied to that cell in the advection part of the algorithm.

### 4.3 Absorption Coefficients

To estimate the corresponding absorption coefficient, we can rewrite eq. (4.3) for a contribution from a given photochemical reaction, concluding that it is a constant within each frequency group:

\[
\kappa_{ig} \leftarrow \frac{n_H}{I_g} \frac{I_{0g}}{I_g} \int_{\nu_g}^{\nu_{g+1}} \sigma_\nu(\nu) \left(\frac{\nu}{\nu_g}\right)^{-\alpha_g} d\nu \equiv \frac{n_H}{I_g} \frac{I_{0g}}{I_g} \langle \sigma_\nu \rangle_g,
\]

where both \(I_{0g}/I_g\) and \(\langle \sigma_\nu \rangle_g\) depend on the spectrum of the radiation field, but not on its intensity. The total absorption coefficient accounting for all photochemical reactions from eq. (4.10) in a given cell in 3D is then

\[
\kappa_{ig} = \frac{I_{0g}}{I_g} \left[ n_H \langle \sigma_\nu \rangle_g + n_{He} \langle \sigma_\nu \rangle_g + n_{He}^+ \langle \sigma_\nu \rangle_g + n_{H}^- \langle \sigma_\nu \rangle_g + n_{H}^- \langle \sigma_\nu \rangle_g + n_{H}^+ \langle \sigma_\nu \rangle_g + n_{H}^+ \langle \sigma_\nu \rangle_g + n_{H}^+ \langle \sigma_\nu \rangle_g \right].
\]
Chapter 4. Including the Physics of Matter-Radiation Interaction

4.4 Photoionization Rates in the Low Optical Depth Regime

Again, consider some photochemical reaction with known cross-section $\sigma_\nu(\nu)$. Taking into account the spectrum of the radiation field in eq. (4.4), we can rewrite eq. (4.5) as

$$ k_\sigma = \int_{4\pi} d\Omega \sum_g I_{0g}(\theta, \phi) \int_{\nu_g}^{\nu_{g+1}} \frac{\sigma_\nu(\nu)}{h\nu} \left( \frac{\nu}{\nu_g} \right)^{-\alpha_g} d\nu = \sum_g G_{\sigma g} E_{0g}, \quad (4.23) $$

where

$$ E_{0g} \equiv \frac{1}{c} \int_{4\pi} I_{0g}(\theta, \phi) d\Omega, \quad G_{\sigma g} \equiv \int_{\nu_g}^{\nu_{g+1}} \frac{\sigma_\nu(\nu)}{h\nu} \left( \frac{\nu}{\nu_g} \right)^{-\alpha_g} d\nu. \quad (4.24) $$

The coefficients $G_{\sigma g}$ do not depend on the strength of the radiation field and can be computed once and for all at the start of the calculation. Once we know $E_g$ from the solution of eq. (4.2), we can find the radiation field strength $E_{0g}$

$$ E_{0g} = E_g \begin{cases} (\alpha_g - 1) \left( \frac{\nu_g - \nu_{g+1}}{\nu_g} \left( \frac{\nu_g}{\nu_g+1} \right)^{\alpha_g} \right), & \alpha_g \neq 1, \quad g = 1 \text{ or } 2, \\ (\alpha_g - 1)/\nu_g, & \alpha_g > 1; \quad g = 3. \end{cases} \quad (4.25) $$

Note that this approximation will work only for small optical depths, that is when the optical depth across a 3D cell is smaller than unity.

4.5 Photoionization Rates: the General Case

If a computational cell on the 3D mesh is opaque to some photochemical reaction (which we denote with "*"), one has to use the general expression for the frequency-dependent photoionization rate

$$ k_{\sigma g} = \frac{E_\nu}{h\nu} \frac{1 - e^{-\kappa_\nu \Delta t}}{n_H \Delta t}, \quad (4.26) $$

where $\kappa_\nu$ is one of the individual absorption coefficients from eq. (4.22). After integration over a specific frequency group we get
which can be written approximately as

\[ k_{*g} = \sum_g k_{*g}, \]

### 4.6 Emissivity Inside Each Frequency Group

The rates of radiative recombinations will give us the total energy loss by gas through radiation. Not all of this energy will be emitted in Lyman continuum photons \((h\nu > 13.6 \text{ eV})\). Some might be scattered away close to the Lya line, and some portion of this energy will be lost in low-energy cascade recombination photons. In other words, knowing the rates for the radiative recombinations is not the same as knowing the emissivity inside each of our frequency groups. To calculate emissivities as defined in eq. (4.1), we have to use models for hydrogenic and helium-like ions to compute the energy loss as a function of frequency of the emitted photons.

#### 4.6.1 Hydrogenic Ions

The energy loss coefficient due to recombination to the \(n\)-th level in a hydrogenic ion is (Hummer 1994)

\[
\phi_n(T_e, Z, \nu) = \frac{c \alpha^3}{\sqrt{\pi}} Z^3 \lambda^{5/2} n^{-2} \epsilon (1 + n^2 \epsilon)^2 e^{-\lambda \epsilon} \cdot \frac{\sigma_n(Z, \epsilon)}{Z^2 \nu_1},
\]  

where

\[
\epsilon = \frac{\nu}{Z^2 \nu_1}, \quad \lambda = \frac{Z^2 h \nu_1}{k_B T_e},
\]
\( \alpha \) is the fine-structure constant, \( \nu_1 \) is the hydrogen Lyman limit, \( Z \) is the atomic number, \( k_B \) is the Boltzmann constant and \( \sigma_n(Z, \epsilon) \) is the cross-section of photoionization for level \( n \). Similarly, the free-free energy loss coefficient

\[
\phi_{ff}(T_e, Z, \nu) = \frac{8}{3\pi^2} \left( \frac{\pi}{3} \right)^{1/2} \alpha^2 \lambda^2_c Z \lambda^{1/2} e^{-u} g_{ff}(u, \lambda) \frac{h}{kT_e}. \tag{4.30}
\]

Here we have introduced the free-free Gaunt factor \( g_{ff}(u, \lambda) \), the Compton wavelength \( \lambda_c \), and \( u = h\nu/k_B T_e \) (Hummer 1994). Then the frequency-dependent total energy loss due to recombinations and free-free emission for hydrogenic ions is

\[
\epsilon_\nu = \frac{k_B T_e}{4\pi} n_H n_0 \epsilon_g \left[ \sum_{n=1}^{\infty} \phi_n(T_e, Z, \nu) + \phi_{ff}(T_e, Z, \nu) \right], \tag{4.31}
\]

where \( n_0 \) is either \( n_{H^+} \) for hydrogen or \( n_{He^{++}} \) for doubly ionized helium. We take the numerical values for the hydrogenic photoionization cross-sections \( \sigma_n(Z, \epsilon) \) from Storey & Hummer (1991) and the free-free Gaunt factor \( g_{ff}(u, \lambda) \) from Hummer (1988), and integrate eq. (4.31) numerically to get

\[
\epsilon_g = \int_{\nu_0}^{\nu_{\epsilon+1}} \epsilon_\nu d\nu
\]

for each frequency group.

### 4.6.2 Helium-Like Ions

In helium atoms, at least at lower principal quantum numbers \( n_1 \) and \( n_2 \), the \( nls \) configuration is dominated by both the electron-nucleus and electron-electron interactions. As a result, the model for emissivity due to recombination of singly ionized helium

\[
\text{He}^+ + e^- \rightarrow \text{He}(nS) + \gamma \tag{4.32}
\]

is somewhat more complicated. We calculate the energy loss coefficient due to recombinations to the \( nS \) state of neutral helium using (Hummer & Storey 1998)
\[ \phi_{nlS}(T_e, \nu) = \frac{c\alpha^3}{\sqrt{\pi}} (2l + 1) \frac{S}{4} \lambda^{5/2} \mu^{-4} \epsilon (1 + \mu^2 \epsilon) e^{-\lambda \epsilon \frac{\sigma_{nlS}(\epsilon)}{\nu_1}}. \] (4.33)

Here, again, \( \epsilon = h\nu/\text{Ryd} = \nu/\nu_1 \) is the free electron energy in Ryd, \( \alpha \) is the fine-structure constant, \( \mu \) is the effective quantum number of state \( nlS \), and

\[ \lambda = \frac{\text{Ryd}}{T_e} = \frac{157,890\text{K}}{T_e}. \]

Then the total recombination and free-free emissivity due to singly ionized helium is

\[ \epsilon_\nu = \frac{k_B T_e}{4\pi} n_\gamma n_\theta \left[ \sum_{n=1}^{\infty} \sum_{l=0}^{n-1} \sum_{\tilde{S}=1}^{\tilde{S}=l} \phi_{nlS}(T_e, \nu) + \phi_{\tilde{g}}(T_e, Z = 1, \nu) \right], \] (4.34)

which, again, is averaged within each frequency group at the beginning of simulations. In our calculations we neglect the emissivity from di-electronic recombinations of helium.

4.6.3 Matter Energy Conservation

Similarly to the energy conservation in eq. (3.15), the change in the matter energy density is determined by all time-dependent heating and cooling processes occurring inside a gas cell during one timestep:

\[ T^{n+1} - T^n = [\Gamma(T) - \Lambda(T)] \Delta t \cdot n_H^{-1} \left[ \frac{3}{2} k_B (x_1 + x_2 + x_3) + \frac{5}{2} k_B (x_4 + x_5) + \frac{3}{2} k_B (x_6 + x_7 + x_8) \psi + \frac{3}{2} k_B x_9 \right]^{-1}, \] (4.35)

where the heating

\[ \Gamma(T) = \sum_{\tilde{g}} E_{\tilde{g}} \frac{1 - e^{-\epsilon_{\tilde{g}} \Delta t}}{\Delta t} \] (4.36)

is given by photoionization heating, and cooling

\[ \Lambda(T) = 4\pi \sum_{\tilde{g}} \epsilon_{\tilde{g}} + \Lambda_{\text{ci}} + \Lambda_{\text{Com}} + \Lambda_{\text{ce}} + \Lambda_{\text{mol}} \] (4.37)
includes cooling due to radiative recombination and bremsstrahlung (combined into the first term, the sum of $\epsilon_\text{g}$), collisional ionization cooling $\Lambda_{\text{ci}}$, Compton cooling $\Lambda_{\text{Com}}$ (or heating — depending on whether the kinetic temperature of the gas is higher or lower than the CMB temperature), collisional excitation cooling $\Lambda_{\text{ce}}$, and cooling $\Lambda_{\text{mol}}$ due to molecular hydrogen. The expressions for the latter four terms are taken from Anninos et al. (1997). Also, since we are solving the RTE for a given, precomputed density field without a hydrodynamical module, we also include adiabatic cooling due to expansion explicitly into our model. However, at the redshifts of interest to us (namely, at $z \gtrsim 5$) Compton cooling is the dominant cooling process (Miralda-Escudé & Rees 1994), whereas adiabatic cooling is more important at lower redshifts.

4.7 Testing the Chemistry Model vs. Cosmic Recombination at $z \sim 1000$

A simple test for the chemistry solver described above is to follow the recombination of the Universe at $z \sim 1000$. We assume that the matter distribution is uniform and the radiation field is both uniform and isotropic. For this test we take the “standard” model of Galli & Palla (1998; GP hereafter) with $H_0 = 67 \text{ km s}^{-1}$, $\Omega_0 = 1$ and $\Omega_0 = 0.0367$. Although we could calculate the energy density of the cosmic radiation field in a self-consistent way via

$$E_n^{m+1} = E_n^m e^{-c_\text{g} \Delta t} + 4\pi \epsilon_\text{g} \Delta t,$$

(4.38)

for this particular test this would be a very bad approximation, since most of thermal radiation with a temperature of hundreds or thousands of Kelvin would be inside or below the first frequency group $g = 1$. Instead, we simply use the blackbody Planck spectrum with

$$T(z) = 2.726(1 + z) \text{K},$$

(4.39)

and the gas temperature is calculated from eq. (4.35). The physics of recombination at $z \sim 1000$
is somewhat more complicated than radiative processes at lower redshifts \((50 \gtrsim z \gtrsim 10)\), primarily due to a much higher temperature and abundance of CMB photons during recombination (Seager et al. 1999, and references therein). Since our chemical model does not include any excited states of neutral hydrogen atoms — just the ground state and the continuum — we would not expect close quantitative agreement with other models (Seager et al. 1999, GP). Particularly, we neglect Lyα resonance photons, which keep most of the neutral hydrogen in the first excited state after the epoch of recombination, either until the expansion of the Universe makes the IGM optically thin to Lyα photons (they get redshifted out of the resonance at 10.2 eV before they get absorbed), or until there are sources of reheating/reionization which would change the ionizational balance altogether. Compared to detailed studies of cosmic recombination, our photochemical model features a greatly reduced set of reactions for hydrogen and helium species (compare to GP), and also we do not include any heavy elements other than helium (e.g., deuterium and lithium). However, even for this crude model, we expect to get approximately the right redshift for the epoch of reionization, as well as roughly the correct abundance of primordial molecular hydrogen.

We start evolving our photochemical model at \(z = 2000\), assuming initial complete ionization of both hydrogen and helium:

\[
x_i = (0, 1, 0, 0, 0, 0, 0, 1, 1 + 2\psi)^T.
\]

The result of this calculation is shown in Fig. 4.2. Overall, we get good agreement with the adopted value of the redshift of recombination. Our residual ionization fraction \(n_{e^-}/n_H \approx 1.9 \times 10^{-3}\) is overabundant by a factor of six compared to GP, or by a factor of three compared to some earlier studies (Stancil et al. 1996). Consequently, we get a similar overabundance of molecular hydrogen, \(n_{H_2}/n_H \approx 2.5 \times 10^{-5}\), which at high redshifts \((10^3 > z \gtrsim 400)\) forms primarily through \(H_2^+\) and at lower redshift \((z \lesssim 110 - 200)\) through negative hydrogen ions \(H^-\) (which are not destroyed by the CMB at these lower redshifts), and thus strongly depends
Figure 4.2: Abundances of four chemical species vs. redshift. The vertical axis is log $x_i$ for $i = 2$ (H$^+$, solid line), $i = 4$ (H$_2$, dashed line), $i = 7$ (He$^+$, dash-dot line) and $i = 8$ (He$^{++}$, dotted line), respectively.
on the amount of free electrons (GP). Another shortcoming in this model is that we have not accounted for the population of excited states of H$_2^+$ with an excitation temperature equal to the temperature of the CMB just after recombination, artificially suppressing the photodissociation of H$_2^+$ at $10^3 > z > 400$ and, therefore, getting an overproduction of H$_2$.

In addition, we do not include any reactions which form molecular combinations with He$^+$ (most importantly, HeH$^+$, and the subsequent formation of He$_3^+$), hence, its relatively high residual abundance $n_{\text{He}^+}/n_H \approx 3.3 \times 10^{-8}$. 
Chapter 5

Modelling Inhomogeneous Reionization

5.1 The Density Distribution

To be able to confront RT during the epoch of reionization, we have to construct a realistic density field and evolve it through redshift. Since the RTE is solved on the light-crossing timescale, it is relatively straightforward to add a much slower evolving density field to the model. One way to do that is to use an N-body code working parallel to the RT solver. However, the subject of this thesis is the numerical solution of the RTE. For the sake of simplicity, here we use a series of precomputed N-body density fields kindly supplied by M. White (see, e.g., Meiksin, White & Peacock 1999). The size of the volume is 2.5 Mpc (in units comoving with the Hubble flow), which at $z = 15$ corresponds to $\sim 1/500$ of the Hubble radius. At the present epoch, 2.5 Mpc is similar to the size of a typical rich cluster of galaxies.

One interesting property of reionization is that it probes the formation of objects in the mass range $10^5 - 10^9 \, M_\odot$ (Haiman et al. 1999), with the boundaries set by the Jeans mass and the free-fall timescale, respectively. CMB-normalized cosmological models, which also give approximately the right number of galaxies at low redshifts, can produce very different power spectra at $z \gtrsim 10$. One way to discriminate between the competing models is to match the predicted patterns of reionization to observed quantities. However, at the moment we do not have enough computer power (both CPU time and memory) to run RT models for different cosmologies. Instead, we focus on a particular cosmological model exploring different scenarios of quasar activity and star formation.
We interpolate the density field from a series of eight output times calculated for a cosmological constant dominated Cold Dark Matter cosmology \((\Omega_0 = 0.3, \Omega_A = 0.7, \Omega_b = 0.04)\), and covering the redshift interval \(30 \geq z \geq 8\). Since for a “no evolution” model the comoving density \(1 + \delta_{ijk}(z) = n_{ijk}(z)/(1 + z)^3\) = constant, to obtain a comoving density for an evolving field we use linear interpolation in redshift of \(1 + \delta_{ijk}(z)\) between adjacent precomputed fields.

### 5.2 Temperature of the IGM before Reheating

Due to the expansion and adiabatic cooling after decoupling of matter and radiation at \(z_{\text{dec}} \sim \text{few } \times 100\), and before reheating at \(z \gtrsim 30 - 50\), the kinetic temperature \(T_k\) of the matter drops well below the temperature \(T_{\text{CMB}}\) of the CMB:

\[
T_{\text{CMB}} = 2.726(1 + z)\text{K} \quad \text{and} \quad T_k = \frac{2.726\text{K}}{1 + z_{\text{dec}}(1 + z)^2}.
\]

If there had been no coupling between gas and radiation after recombination at \(z_{\text{rec}}\), then \(z_{\text{dec}} = z_{\text{rec}}\), and prior to the epoch of reionization at \(z \sim 10 - 30\) the matter temperature \(T_k(z)\) would have dropped down to a fraction of a Kelvin. However, even in the absence of sources of preheating there is some residual ionization, with free electrons exchanging energy with CMB photons (before decoupling at redshift of few hundred). In the expanding Universe the scattering of the CMB off free electrons (Compton heating) will raise the electron temperature \(T_e\) (Peebles 1993, p. 177) by

\[
\frac{dT_e}{dt} = \frac{x_e}{1 + x_e} \frac{8 \sigma_T \alpha_R T_{\text{CMB}}^4}{3 m_e c} (T_{\text{CMB}} - T_e) + \frac{2T_e(z)}{1 + z},
\]

where \(x_e\) is the fractional ionization, and the second term on the RHS represents adiabatic cooling due to expansion. Collisions among electrons and neutral particles drive \(T_k \rightarrow T_e\).

The fractional ionization can be calculated analytically, taking into account recombination to excited states of hydrogen atoms (Peebles 1993, p. 167-173):
\[- \frac{d}{dt} n_e = \left( \frac{\alpha_e n_e^2}{n} - \frac{\beta_e n_{18}}{n} e^{-h\nu_e/kT} \right) \frac{1 + K\Lambda n_{18}}{1 + K(\Lambda + \beta_e)n_{18}}, \]  \hspace{1cm} (5.3)

where \(\alpha_e\) is the recombination coefficient to all excited states, \(\beta_e\) is the coefficient of ionization and \(\Lambda = 8.23 \text{ s}^{-1}\) is the two-photon decay rate from the metastable 2s level to the ground state. Slight modifications to these formulae can be found in Seager et al. (1999), but are unimportant for our purposes. Solution of eq. (5.2) - (5.3) shows that heating by CMB through residual free electrons keeps the kinetic temperature around \(\sim 6.5 \text{ K}\) at \(z = 13\) (as opposed to \(\sim 0.5 \text{ K}\) with no fractional ionization at all). However, the temperature of the clumps within the IGM just prior to reionization is likely to be somewhat higher, since in a non-homogeneous Universe denser structures will not expand at the average rate of the Hubble flow, therefore, maintaining warmer temperatures. In addition, shocks from gradually collapsing objects will contribute to the overall heating of the IGM (Sunyaev & Zeldovich 1972), not to mention radiative preheating by the very first stars and quasars. The calculation of the propagation of I-fronts which are going to heat the medium to many thousands of Kelvin is not likely to be very sensitive to whether the initial gas temperature was a few K or a few tens of K. For the purpose of this study we adopt an initially uniform temperature \(T_{\text{gas}} = 30 \text{ K}\).

We also assume that prior to the UV irradiation all the gas is neutral, and that the \(\text{H}_2\) fraction is \(3 \times 10^{-6}\) (Abel et al. 1998b).

### 5.3 Preheating

Light coming from the first collapsed structures gradually builds up a cosmic radiation background. Low-energy (below 13.6 eV) photons do not contribute to photoionization traveling much further in a neutral gas. The photons in the Lyman and Werner bands of molecular hydrogen (in the range 11.2 – 13.6 eV) can photo-dissociate \(\text{H}_2\) both in the IGM and in other collapsing objects (Haiman et al. 1999, Ciardi et al. 1999). Haiman et al. (1997) showed that
the flux which is required for complete H$_2$ photo-dissociation of the Universe is several orders of magnitude smaller than the flux needed for reionization. Since molecular hydrogen is the main coolant for a gas of primordial composition, the UV background below 13.6 eV can strongly affect subsequent small-scale structure formation. Only halos with masses high enough for efficient hydrogen Ly$\alpha$ line cooling can continue further collapse.

In addition, at lower redshifts ($z < 100$), the density of the CMB is not sufficient to keep the majority of neutral hydrogen atoms above the ground state. The optical depth of the IGM inside atomic hydrogen Lyman lines is extremely high (Haiman \textit{et al.} 1999), and a photon redshifted to the frequency of any hydrogen Lyman line with $2 \leq n \leq 150$ gets immediately absorbed. Ly$\alpha$ photons ($n = 1$) can be neglected, since they get re-emitted at the same frequency, while all high ($n \geq 150$) Lyman lines are not important because they have small optical depths. Prior to reionization, absorption in Lyman lines will completely block all sources beyond some redshift $z_{\text{max}}$ given by

$$\frac{1 + z_{\text{max}}}{1 + z_{\text{obs}}} = \frac{\nu_i}{\nu_{\text{obs}}}$$

(Haiman \textit{et al.} 1999), where $\nu_i$ is the frequency of the Lyman line closest from above to the observation frequency $\nu_{\text{obs}}$ at the redshift $z_{\text{obs}}$.

In this thesis, we do not compute radiative transfer below 13.6 eV, neglecting all low-energy photons. In other words, one can argue that we do not conserve the radiation energy density since we allow low-frequency photons to escape the volume. The details of preheating, which are extremely important for subsequent structure formation, depend on the build-up of the isotropic background below 13.6 eV as a function of redshift. Here, we only give a tool for calculating 3D RT in an inhomogeneous medium, and compute propagation of ionizing photons. RT below 13.6 eV could be performed in a similar way, subdividing the interval 11.2 – 13.6 eV into individual frequency groups.
5.4 Time Stepping with Variable Redshift

We start our simulations at the redshift $z = 15$ when the first ionizing photons appear in the volume. For explicit advection of wavefronts at the speed of light, the time steps are bound by the Courant condition

$$\Delta t^{n+1} - \Delta t^n = \frac{\mu \Delta x(t^n) (1 + z(t^{n+1}))}{c} \frac{1 + z(t^n)}{1 + z(t^{n+1})},$$

where $\mu$ is the dimensionless Courant number, $\Delta x(t^n)$ is the 3D mesh size, and $\mu \leq 1$ for stability. Having adopted a particular cosmological model, i.e. knowing the function $z(t)$, we can easily solve eq. (5.5) numerically to determine $t^{n+1}$.

5.5 Modelling the First Objects

We have performed two runs of patchy reionization by sources residing inside the computational volume, as well as a run with reionization by an external background field. Cold Dark Matter cosmologies predict the collapse of objects with masses $\sim 10^5 - 10^6 M_\odot$ around the redshift $z \sim 30$ (Haiman & Loeb 1998, HL98 hereafter; Tegmark et al. 1997) with more massive structures forming at lower redshifts. It is only this relatively dense gas that is able to cool further and collapse into halos, leading to star formation or to quasar activity. To estimate the fraction of baryons that reside in collapsed halos, the dark matter Jeans mass is often written as (Abel et al. 1998b, HL98, Oh 1999)

$$M_{\text{min}} = 10^8 [(1 + z)/10]^{-3/2} M_\odot,$$

which is simply the critical mass needed to reach the virial temperature of $10^4$K to be dense enough for efficient atomic hydrogen cooling. All halos with masses greater than $M_{\text{min}}$ are assumed to be virialized. Note that this virialization threshold assumes that all molecular
Number of virialized halos vs. redshift

<table>
<thead>
<tr>
<th>redshift</th>
<th>number of mini-quasars</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>1</td>
</tr>
<tr>
<td>13</td>
<td>1</td>
</tr>
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<td>10</td>
<td>2</td>
</tr>
<tr>
<td>8</td>
<td>8</td>
</tr>
</tbody>
</table>

Table 5.1: Number of collapsed halos in a 2.5 Mpc (comoving) volume vs. redshift. The virialization mass $M_{\text{min}}$ is given by eq. (5.6).

hydrogen has been previously destroyed during preheating — otherwise $M_{\text{min}}$ can be several orders of magnitude lower (HL98).

We assume that each halo with $M_{\text{halo}} > M_{\text{min}}$ hosts a mini-quasar, the luminosity of which is uniquely determined by the mass of the halo. In Table 5.1 we give the number of such mini-quasars inside our computational volume as a function of redshift. To estimate the photoionization rate of the IGM by early quasars, it is essential to know their luminosity function (LF). The number of observed quasars in both optical and radio wavelengths declines steadily beyond $z \sim 2.8$ (Warren et al. 1994, Pei 1995), although some bright quasars were recently detected to as far as $z \sim 5$ (Fan et al. 1999, and references therein). Also, it is possible that state-of-the-art X-ray observations will provide better constraints on the high-redshift quasar LF than currently inferred from optical data (Haiman & Loeb 1999).

Several analytical models extrapolating the observed low-redshift LF of quasars to higher redshifts have been proposed in the past (HL98, Pei 1995, and references therein). Fitting the observed quasar LF to semi-analytical models of structure formation introduces a number of uncertainties. The quasar LF is more or less established only at lower redshifts ($z < 2.2 - 2.9$), where most phenomenological models predict a double power law LF (for high and low luminosities, respectively), with a redshift dependence of the form $\propto (1 + z)^{3/2}$ (Boyle, Shanks & Peterson 1988, Pei 1995). At higher redshifts, assuming that each black hole (BH) accretes matter at a rate close to the Eddington limit (the mass infall is limited by radiation pressure),
Chapter 5. Modelling Inhomogeneous Reionization

### REIONIZATION MODELS

<table>
<thead>
<tr>
<th>model</th>
<th>description</th>
<th>( z_{\text{start}} )</th>
<th>( z_{\text{finish}} )</th>
<th>( \alpha_g ) (RT module)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>short-lived mini-quasars</td>
<td>15.0</td>
<td>14.4</td>
<td>1.5 1.5 1.5</td>
</tr>
<tr>
<td>B</td>
<td>a single bright quasar</td>
<td>10.0</td>
<td>9.9</td>
<td>1.8 1.8 1.8</td>
</tr>
<tr>
<td>C</td>
<td>an external UV field</td>
<td>13.0</td>
<td>12.6</td>
<td>1.5 1.5 1.5</td>
</tr>
</tbody>
</table>

Table 5.2: Reionization models.

Small & Blandford (1992) have used a universal quasar LF to infer the birthrate of quasar BHs. Haehnelt & Rees (1993), applying the Press-Schechter theory of halo formation and relating the BH-halo mass dependence to both the BH formation efficiency and the accretion luminosity, fitted the observed quasar LF. HL98 used a similar approach to derive the ultra-high-redshift (\( z > 10 \)) quasar LF in the context of reionization, finding that the early population of mini-quasars reionizes the Universe at \( z = 12 \). We take their quasar luminosity model to explore the effects of inhomogeneous reionization.

Note that, in general, we do not assume the same spectral energy distribution for sources of radiation — these can be point-like quasars, star forming regions within the volume or ionizing photons coming from the outside — and for the specific intensity in eq. (4.5). Instead, we adopt a simple power-law spectrum for the calculation of RT of both direct and diffuse radiation, while sources are allowed to exhibit any spectral dependence. E.g., for the UV background (Sec. 5.5.3) we assume a double power-law spectrum accounting separately for stellar and quasar photons.

In Table 5.2 we list the reionization models we use for our computations. It is worth stressing again that direct ionizing photons from point sources within the volume in models A and B are computed on the 3D grid using eq. (3.1)-(3.2), whereas photons reprocessed in the IGM are followed with ray tracing. Let us now examine these models in more detail.

#### 5.5.1 Model A: Reionization by Short-Lived Mini-Quasars

For this model we adopt the high-redshift quasar luminosity function derived by HL98. Their model is normalized to the observed quasar luminosity function at low redshifts (4.5 > \( z > 2.6 \))
and assumes a constant ratio of the central black hole mass to the host halo mass

\[ \epsilon \equiv \frac{M_{\text{BH}}}{M_{\text{halo}}} = \text{constant}. \]

For halos with masses \( M_{\text{halo}} > M_{\text{min}} \) the luminosity of a quasar with a BH mass \( M_{\text{BH}} \) at a time \( t \) after its formation is

\[ L(t) = \frac{\epsilon M_{\text{halo}}}{M_{\odot}} \times 1.4 \times 10^{38} \ e^{-t/t_0} \frac{\text{erg}}{\text{s}}. \]

The fit to the observed luminosity function produces a model in which quasars have very short lifetimes, of order \( t_0 = 10^{5.8} \) yrs, and the mass ratio is \( \epsilon = 10^{-3.2} \). To obtain the number of photons above 13.6 eV, HL98 use the median spectrum of Elvis et al. (1994), to get

\[ \dot{N}_{\text{ph}} \equiv \dot{N}_{\text{ph}}(>13.6 \text{ eV}) = 6.6 \times 10^{47} \text{ s}^{-1} \times \frac{\epsilon M_{\text{halo}}}{M_{\odot}} e^{-t/t_0}, \quad \text{for } M_{\text{halo}} > M_{\text{min}}. \]

Taking into account the variability of quasars and neglecting the lookback effects for the calculation of the optical depth, for a cell \( \{i,j,k\} \) inside our cosmological volume, the summation over all sources gives the energy density of direct ionizing photons (eq. (3.2))

\[ E_{\nu,ij,k}^{\text{src}}(t) = \sum_s \frac{h \nu \dot{N}_{\nu,\text{ph}}(t - r_{ij,k,s}/c)}{4\pi c^2 r_{ij,k,s}^2} e^{-\tau_{\nu,ij,k,s}}, \quad (5.7) \]

and

\[ \dot{N}_{\text{ph}}(t) = 6.6 \times 10^{47} \text{ s}^{-1} \times \frac{\epsilon M_{\text{halo}}}{M_{\odot}} \times \begin{cases} e^{-t/t_0} & \text{if } t \geq t_s; \\ 0 & \text{if } t < t_s. \end{cases} \quad (5.8) \]

where \( t_s \) is the time when the quasar turns on. Integration of eq. (5.7) within each frequency group gives an approximate expression for

\[ E_{\nu,ij,k}^{\text{src}}(t) \approx \frac{h}{4\pi c} \sum_s \frac{e^{-\tau_{\nu,ij,k,s}}}{\tau_{ij,k,s}^2} \int_{\nu_s}^{\nu_{s+1}} \nu \dot{N}_{\nu,\text{ph}}(t - \tau_{ij,k,s}/c) d\nu. \quad (5.9) \]
For modelling quasar spectra, we adopt the same power law as for the intensity within individual frequency groups (eq. (4.5)). Since the energy density \( \nu \dot{N}_{\nu, \text{ph}} \propto \nu^{\alpha_{\nu}} \) for \( \nu < \nu_{g+1} \), we can write

\[
\dot{N}_{\nu, \text{ph}} = \dot{N}_{0g, \text{ph}} \left( \frac{\nu}{\nu_0} \right)^{-(\alpha_{\nu} + 1)} \quad \text{and} \quad \dot{N}_{g, \text{ph}} = \int_{\nu_0}^{\nu_{g+1}} \dot{N}_{\nu, \text{ph}} d\nu.
\]

From continuity of \( \dot{N}_{\nu, \text{ph}} \) over all frequencies the photon energy production within each group is simply

\[
E_{\text{src},i,j,k}^{\nu}(t) = \frac{h c}{4 \pi \nu^3} \sum_{s} e^{-\tau_{i,j,k,s}} \frac{\zeta_{g}}{\xi_{1} + \xi_{2} + \xi_{3}} \times \dot{N}_{\text{ph}}(t - r_{i,j,k,s}/c),
\]

(5.10)

where \( \zeta_{g} \) and \( \xi_{g} \) are constants defining the adopted spectrum of quasar radiation:

\[
\begin{align*}
\zeta_{1} &= \frac{\nu_{1}}{\nu_{2} - \nu_{3}} \left( \frac{\nu_{2}}{\nu_{3}} \right)^{\alpha_{1} + 1} \\
\zeta_{2} &= \left( \frac{\nu_{1}}{\nu_{2}} \right)^{\alpha_{1} + 1} \left( \frac{\nu_{2}}{\nu_{3}} \right)^{\alpha_{2} + 1} \\
\zeta_{3} &= \left( \frac{\nu_{1}}{\nu_{3}} \right)^{\alpha_{1} + 1} \left( \frac{\nu_{2}}{\nu_{3}} \right)^{\alpha_{2} + 1} \nu_{3}.
\end{align*}
\]

For this model we adopt the power law spectrum with \( \alpha_{g} = 1.5 \) for all frequencies shortward of the hydrogen Lyman limit (Haardt & Madau 1996, Haehnelt & Steinmetz 1998).

The result of this run is presented in Fig. 5.2 - 5.3. In Fig. 5.2 we show time evolution of the 3D hydrogen I-front propagating into the inhomogeneous IGM in a cross-section through the quasar (the bright spot in the upper right corner), at four different redshifts. Nine contour levels of hydrogen ionization are plotted on top of the color map representing the logarithm of the total hydrogen number density. For this simulation we employ the full \( 64^3 \) (spatial) \( \times 10^2 \) (angular) \( \times 3 \) (frequency) resolution. The quasar turns on in the densest cell in the volume at \( z = 15 \), and its luminosity is decaying on the timescale of \( t_0 = 10^{5.8} \) yrs according to eq. (5.8), until it becomes negligible around \( z_{\text{off}} \sim 14.92 \). The initial expansion of the hydrogen I-front is driven entirely by direct ionizing photons from the quasar. Close to the quasar, the diffuse radiation from the HII region builds up slowly, dominating the radiation field near the I-front.
after $z_{\text{off}}$. Around this time the I-front starts to show patchiness, due to percolation of the radiation field through the density inhomogeneities. In a separate run we have verified that this patchiness has nothing to do with the finite angular resolution. The intensity of secondary photons within the $\text{H} \, \text{II}$ volume is not large enough to keep up with the initial fast expansion of the front. As it slows down, its thickness clearly reflects the mean free path of photons, being wider in the low-density regions and dropping below the resolution length ($2.5/64 \text{Mpc}$ comoving) inside the dense filament below the quasar (Fig. 5.2).

Singly ionized helium shows a thin, shell-like structure bounded by neutral helium on the outer side and by doubly ionized helium closer to the quasar (Fig. 5.3). The $\text{He} \, \text{II}$ front has the shape similar to the hydrogen I-front, both emphasizing the underlying density profile. The size of the $\text{He} \, \text{II}$ void is smaller due to the higher ionization potential of helium.

We do not compute directly heating of the neutral IGM by photons with wavelengths greater than the hydrogen Lyman edge, accounting only for $h \nu > 13.6 \text{eV}$ radiation. Thus, the resulting temperature ahead of the hydrogen I-front might be somewhat different from more detailed studies considering RT of $\text{Ly} \alpha$ photons. In Fig. 5.4 we show the temperature in the same cross-section at $z = 14.785$. Note that there is a prominent region where the neutral medium is heated to $10^3 - 10^4 \text{K}$ ahead of the I-front, whereas hydrogen ionization occurs at $(3 - 4) \times 10^4 \text{K}$.

5.5.2 Model B: Reionization by Bright Quasars

The major uncertainty in the previous model is the number, distribution and the luminosity function of quasars at $z > 5$. It is likely that preheating of the IGM by the earliest structures at $z \sim 15$ – either by light (soft X-rays or $\text{Ly} \alpha$) or through hydrodynamical shocks – will raise the Jeans mass throughout the Universe, preventing further collapse in many regions. In this case one might expect the medium to stay neutral until bigger halos form closer to $z \sim 10$. In this section we compute a model for the reionization of a periodic 2.5 Mpc (comoving) volume by a single bright ($N_{\text{ph}} = 10^{54} \text{s}^{-1}$) quasar switching on at $z = 10$. Also, for this calculation
we adopt a steeper spectral index, $\alpha_g = 1.8$, throughout all frequency groups, mimicking soft reprocessed radiation originating in the circumnuclear region of the quasar.

Figure 5.5 illustrates the resulting profile of the time-dependent hydrogen I-front at the beginning of the run. The dense filaments near the host halo are ionized almost on the light-crossing time, due to the high luminosity of the source. Not affected by the quasar finite lifetime, ionization proceeds quickly, and by $z \sim 9.6$ most of the low-density gas in the volume is ionized.

In Fig. 5.8 we show the energy density of the radiation field $E_g$ in three frequency groups ($g = 1, 2, 3$), in a cross-section through Model B at $z = 9.473$.

5.5.3 Model C: Reionization by an External UV Field

Let us now consider a model with direct ionizing photons coming exclusively from outside the volume. The common parameterization of the uniform UV background is a simple, redshift-dependent power-law

$$J_\nu(z) \equiv \frac{1}{4\pi} \int_{4\pi} I_\nu(n, z) d\Omega = J_{-21}(z) \times 10^{-21} \left( \frac{\nu}{\nu_g} \right)^{-\alpha_g(z)} \frac{\text{erg cm}^{-3} \text{ s}^{-1} \text{ Hz}^{-1} \text{ sr}^{-1}}{\nu_g \leq \nu < \nu_{g+1}}. \quad (5.11)$$

For this scenario, we have taken an ionizing background evolving with redshift as proposed by Abel & Haehnelt (1999), except that we shift it towards higher redshift. Our form is

$$J_\nu(z) = \frac{1}{1 + [7/(z-8)]^4} e^{-(z-9)/4} \left( \frac{\nu}{\nu_1} \right)^{-5} + \frac{10}{1 + [7/(z-8)]^4} e^{-(z-9)/2.5} \left( \frac{\nu}{\nu_1} \right)^{-1.8} \times 10^{-21} \text{ erg cm}^{-3} \text{ s}^{-1} \text{ Hz}^{-1} \text{ sr}^{-1}, \quad (5.12)$$

with the first term accounting for stellar reionization (with a soft component, $\alpha_g = 5$) around $z \sim 12-14$, and the second term representing the harder quasar radiation reaching its maximum
closer to $z \sim 11 - 12$. For the processed radiation (eq. (4.5)) we assume the spectral power law $a_g = 1.5 \ (g = 1, \ldots , 3)$.

Figures 5.9 - 5.12 show the results of this run. To speed up the evolution, we start calculations when the background field has been already established, at $z = 13$. In addition, the spatial resolution is reduced to $32^3$. All low density hydrogen gas is ionized within about ten passages of the wavefront across the volume, by $z \sim 12.8$. Denser filaments ($\rho/\bar{\rho} \sim 10 - 50$) survive much longer, at least through $z \sim 12.6$ when we stopped the calculations. Note that this simulation does not have the spatial resolution required to compute the evolution of neutral regions to much lower redshifts.

In Fig. 5.13 we present a cross-section through the hydrogen I-front computed at three different spatial resolutions ($8^3 \times 8^2$, $16^3 \times 8^2$ and $32^3 \times 8^2$, respectively), at the same output time. It can be seen that the position of the I-front converges as we go to higher resolution.

5.5.4 Criteria for Reionization by Population III Stars

In the case of numerous and more uniformly distributed faint stellar sources, with softer spectra than for quasars, one would expect to witness a much more homogeneous, and, perhaps, slower reionization. In this section, we discuss how to set up conditions for numerical reionization by stellar sources inside the computational volume. Because of the inherent complexity of the associated physics, there is still no standard theory of star formation. Inside virialized dark matter halos, the gas is supported by the pressure gradient. Its further collapse and fragmentation into stars is possible only if there is additional cooling which will loosen pressure support. For a gas of primordial composition, the most efficient coolant is molecular hydrogen ($H_2$), through collisional excitation of vibrational and rotational levels and subsequent radiative transitions (Lepp & Shull 1983, 1984; Haiman et al. 1996a; Tegmark et al. 1997). The post-recombination fraction of molecular hydrogen is $\sim 3 \times 10^{-6}$. Inside dense halos, in the absence of the UV background, this fraction can rise to $\sim 10^{-4}$ (Haiman et al. 1996b, Tegmark et al. 1997)
facilitating fast cooling. In fact, Haiman et al. (1996b) concluded that it is possible, contrary to naive expectations, that the increased abundance of free electrons due to a UV irradiation of cold gas clouds can catalyze the formation of molecular hydrogen, accelerating line cooling and triggering the eventual collapse and fragmentaion of these clouds. However, it is more likely that in lower density neutral regions, just prior to the epoch of reionization, UV photons below the ionization threshold coming from the very first collapsed objects will propagate ahead of I-fronts easily dissociating H$_2$ molecules (Haiman et al. 1997). During this preheating the soft UV flux required to completely photo-dissociate the Universe is several orders of magnitude smaller than the flux needed for reionization (Haiman et al. 1997).

Now, it seems firmly established that this preheating of the IGM — often referred to as a "negative feedback" — will suppress molecular hydrogen cooling, effectively halting any star formation in objects with masses below $10^{5-6} M_\odot$. The former will remain neutral, pressure-supported gas clouds which later either get slowly evaporated by the UV background or merge into larger objects (Haiman et al. 1999). Therefore, one could assume that if reionization is caused by the early population of stars, these must reside only in virialized halos with masses of at least $10^{7-8} M_\odot$ (or virial temperatures in excess of $10^4$K, Haiman & Loeb 1997) inside which molecular line cooling is efficient before preheating. On the other hand, recently, Haiman et al. (1999) performed detailed calculation of the build-up of the UV background assuming that the first stellar activity occurs in virialized halos appearing near $z \sim 30$. The corresponding Jeans mass is of order $10^{4-5} M_\odot$ giving a virial temperature of a few hundred Kelvin. Star formation inside small clouds suppresses the H$_2$ abundance in these halos and shuts itself off before reionization. Haiman et al. (1999) conclude that their calculations confirm the existence of the negative feedback, but find that it depends sensitively on the spectrum of the first sources. Ciardi et al. (1998) found that the soft UV background in the Lyman and Werner bands builds up to $\sim 10^{-30} - 10^{-27}$ erg cm$^{-2}$ s$^{-1}$ Hz$^{-1}$ which is not sufficient to provide the negative feedback on structure formation in the redshift interval $30 > z > 20$. 
In view of these uncertainties, it is quite questionable to identify star forming regions with a density criterion alone, without relating them to a threshold molecular hydrogen fraction, above which gas clouds can efficiently cool, fragment and form stars. Tegmark et al. (1997) calculated the evolution of the H$_2$ abundance, solving a system of kinetic rate equations within 1D spherically symmetric models of halo profiles for different halo masses, and concluded that this fraction is close to $5 \times 10^{-4}$ to $10^{-3}$. Abel et al. (1998b) performed fully 3D numerical simulations of the first bound objects, confirming that the gas can cool efficiently inside virialized dark matter halos (which form inside spherical knots at the intersection of filaments) once the H$_2$ fraction reaches $5 \times 10^{-4}$. Unfortunately, the spatial resolution in our RT models does not allow to resolve correctly regions of efficient H$_2$ formation. These regions are barely resolved even in the state-of-the-art, high-resolution hydrodynamical simulations (Abel et al. 1998b).

A variety of techniques has been suggested to implement starbursts in numerical simulations. To bypass rigours of not very well constrained physics of star formation, Haiman & Loeb (1997, HL97 hereafter) simply assume that a constant fraction $f_{\text{star}}$ of the virialized gas is converted into stars, calibrating this value against the inferred carbon abundance in the IGM from observations of the Ly$_\alpha$ forest. The central assumption here is that heavy elements detected in high-redshift Ly$_\alpha$ absorbers are produced by the same generation of stars that reionized the Universe. However, the estimate based on the rate of carbon ejection into the IGM presents a number of uncertainties (HL97), since it is not entirely clear how much carbon gets actually ejected into the surrounding medium, or exactly what fraction of carbon burns into nitrogen at the base of convective envelopes of stars with masses in the range $3 - 8 M_\odot$ ("hot bottom burning"). In addition, carbon is produced mostly by $3 - 6 M_\odot$ stars (HL97), while most ionizing photons come from $10 - 12 M_\odot$ stars — hence, due to different lifetimes of stars with different masses, there must be a time delay between stellar reionization and metal enrichment of the IGM. HL97 take the standard model as $f_{\text{star}} = 4\%$, within a broader possible range $1\% < f_{\text{star}} < 99\%$. More recently, Haiman & Loeb (1998) (and later Oh 1999) adopt a
starburst model which is normalized to the observed metallicity range $10^{-3} < Z/Z_{\odot} < 10^{-2}$ of the IGM at $z \sim 3$, inferred from carbon and silicon abundances, yielding the star formation efficiency $1.7\% < f_{\text{star}} < 17\%$. Note that the observed value of $f_{\text{star}}$ in star forming regions (defined as the fraction of H$_2$ gas converted into stars) falls in the range from $\sim 1$% to 30% (Ciardi et al. 1999).

Ciardi et al. (1999) introduce an additional parameter, $f_b$, which represents the fraction of already virialized baryons which are able to cool and form stars, taking the average value $f_b = 8\%$ (given by the 3D numerical simulations of star forming regions in Abel et al. 1998b). In their models, $f_{\text{star}} = 15\%$, which we assume in our simulation.

Finally, not all UV photons produced in a star forming region can escape it easily. The escape probability $f_{\text{esc}}$ of ionizing photons (HL97) depends on a number of factors: the size and density of the ionized H II region associated with the site of star formation, the clumpiness of the gas within that region, the recombination timescale, and the rate of heating (by both UV and winds from young stars or SNe). HL97 calculated 1D ionization profiles of halos of different masses and redshifts, finding that $f_{\text{esc}}$ is almost uniquely determined by the redshift, and giving an approximate fitting formula

$$
\log f_{\text{esc}} = \begin{cases} 
1.92 \left( e^{-\frac{(z-10)^2}{150^2}} - 1 \right) & \text{for } z > 10, \\
0 & \text{for } z \leq 10, 
\end{cases} \quad (5.13)
$$

which we adopt. Again, the value of $f_{\text{esc}}$ inferred from observations of nearby star forming regions is not very well established, but rather falls into a range from few % to $\sim 20$% (see HL97 and Ciardi et al. 1999 for references).

The total stellar component inside a virialized halo of mass $M_b$ can then be written as (Ciardi et al. 1999)

$$
M_{\text{star}} = M_b f_b f_{\text{star}}. \quad (5.14)
$$
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We have attempted to perform a RT run with star formation inside the volume. We have assumed that once conditions for star formation are met (the virialized cell reaches the threshold \( \text{H}_2 \) fraction), there is an instantaneous starburst with a Salpeter initial mass function. We have approximated the composite stellar spectrum (derived in Ciardi et al. (1999), for a metallicity \( Z/Z_\odot = 10^{-2} \)) with a triple power law, \( \alpha_g = (0.95, 5, 12) \). Immediately after the outburst at \( z = 30 \), the spectrum is nearly flat between the \( \text{H} \text{I} \) and \( \text{He} \text{II} \) ionization edges, becoming much softer on a timescale of \( \sim 10^7 \) yrs. At time \( t = 0 \) the luminosity at the hydrogen Lyman edge can be written explicitly as (Ciardi et al. 1999)

\[
L_\nu(\nu_1) \approx 4.8 \times 10^{23} \left( \frac{M_\text{b}}{10^5 \text{M}_\odot} \right) \left( \frac{f_\text{b}}{0.08} \right) \left( \frac{f_\text{star}}{0.15} \right) \text{erg s}^{-1} \text{ Hz}^{-1}.
\] (5.15)

Of these photons, only \( L_\nu(\nu) f_\text{esc} \) escape into the IGM. We adopt the values \( f_\text{b} = 8\% \), \( f_\text{star} = 15\% \) and \( f_\text{esc} = 2\% \).

Unfortunately, the numerical resolution of our model did not allow us to form any significant fraction of molecular hydrogen above the background value of \( 3 \times 10^{-6} \). Additional complication arises from the fact that the first stars can form within \( \sim 10^5 \text{M}_\odot \) clouds as early as \( z \sim 30 - 50 \). Since stellar spectra are much softer than those for quasars, star formation might be able to easily shut itself off due to photodissociation of \( \text{H}_2 \), without leading to any significant hydrogen ionization. Thus reionization might proceed via sporadic starbursts occurring in different parts of the volume and separated by many redshifts units. We started our model at \( z = 30 \) observing only marginal star formation. We conclude that the present spatial resolution (64\(^3\)) is not sufficient for modelling stellar reionization with sources inside the computational volume via full RT.
5.6 Observational Properties of Reionization

Akin to the density and temperature fluctuations in the IGM at high redshifts (1 < z < 5) responsible for the Lyα absorption forest in the spectra of background quasars, the density, temperature and ionization structure fluctuations at ultra-high redshifts (z > 5) should be visible in absorption (either against more distant objects, e.g., quasars, galaxies or γ-ray burst afterglows, or against the CMB) or emission above the CMB. Below we have listed the major possibly detectable manifestations of the epoch of reionization:


- Lyα emission during patchy reionization (Gould & Weinberg 1996, Miralda-Escudé & Rees 1998, Loeb & Rybicki 1999);

- Hα emission prior to and during reionization (Oh 1999);

- complete blanketing of all flux shortward of λ_{Lyman \text{limit}}(1 + z) in spectra of all quasars beyond some critical redshift, as well as observation of the damping wing of Lyα absorption in the neutral IGM around the same redshift;

- 'radio-lines' of atomic hydrogen;

- damping of primary CMB fluctuations and generation of secondary anisotropies;

- free-free emission from ionized halos in Lyman limit systems (N(H I) ~ 10^{17} \text{ cm}^{-2}) during and after reionization (Loeb 1996, Haiman & Loeb 1997, Oh 1999); and

- the absorption properties of He II clouds
Huge datasets which are going to be available soon (see Tables C.1 – C.2 in Appendix C for the list of currently implemented or planned observational programs) will require comparison to high-resolution quantitative theoretical models. Absorption or emission features from the high-redshift gas represent a convolution of 3D distributions of different quantities, such as the temperature, the fractional ionization, the absorption coefficient at a specific frequency, and so on. In case of the inhomogeneous IGM, cosmological hydrodynamical simulations coupled with 3D RT models present an accurate way of predicting observable skymaps. In the next section, for the example of the 21-cm line radiation from atomic hydrogen, we demonstrate how these skymaps can be generated.

5.7 Atomic Hydrogen 21cm Emission

Very-high-redshift sources \( (z > 5) \) can be detected through emission or absorption of 21-cm radiation by the surrounding neutral IGM. The physics of the 21-cm emission and absorption in a diffuse medium was well established in the 1950s (see, e.g., Wouthuysen 1952, Field 1959). A number of researchers at the time were looking for 21-cm features from the intergalactic gas. Sunyaev & Zeldovich (1972) were the first to suggest that a large fraction of the gravitational energy released during collapse of protoclusters of galaxies in the “pancake” scenario will result in shock heating of the IGM, with the spin temperature \( T_s \) of the gas being driven above the background radiation temperature \( T_{CMB} \), potentially leading to detectable 21-cm radiation from neutral hydrogen. Reheating by shocks and light from the first collapsed objects was further investigated by Sunyaev & Zeldovich 1975, Hogan & Rees 1979, Oort 1984, Scott & Rees 1990, and recently by Madau et al. 1997, Gnedin & Ostriker 1997, Tozzi et al. 1999, Meiksin 1999, Shaver et al. 1999. It has been shown that it is possible to detect sources appearing before reionization, through the reheating of the neutral IGM and subsequent emission or absorption against the CMB spectrum at the rest wavelength of the atomic hydrogen 21 cm line. Due
to inhomogeneities in the gas at high redshift these spectral signatures will result in angular fluctuations across the sky, as well as showing some structure in redshift space (Hogan & Rees 1979, Scott & Rees 1990). This potentially opens up the possibility of reconstructing the 3D distribution of gas during patchy reionization.

5.7.1 21-cm Emission and Absorption

The 21-cm line in atomic hydrogen corresponds to the transition between the singlet and triplet \( n = 1 \) hyperfine states which exist due the electron-proton spin coupling. A triplet atom radiates spontaneously with probability \( A_{10} = 2.85 \times 10^{-15} \text{ s}^{-1} \) (Field 1959). The intensity of the 21-cm radiation depends on the spin temperature defined by the Boltzmann equation simply as the excitation temperature of the hyperfine levels (e.g., Meiksin 1999)

\[
\frac{n_1}{n_0} = 3 \exp \left( \frac{-T_s}{T_\pi} \right), \quad T_\pi \equiv \frac{h\nu_{21\text{cm}}}{k_B} \approx 0.068 \text{K},
\]

where \( n_0 \) and \( n_1 \) are the populations of the upper and lower states, and the numeric coefficient is just the ratio of their statistical weights. The coupling between \( T_\pi \) and the temperature of the background radiation \( T_{\text{CMB}} \) is pretty tight, so that in the absence of any other pumping mechanism \( T_\pi \rightarrow T_{\text{CMB}} \) on a timescale \( T_\pi / (T_{\text{CMB}} A_{10}) \sim 2 \times 10^4 \text{ yrs} \) (Meiksin 1999), and there will be no 21-cm absorption or emission features on top of the CMB. Fortunately, there are at least two mechanisms which can decouple the spin temperature from the CMB (Field 1959; also, see Fig. 5.14). First of all, in dense regions collisions between hydrogen atoms can change the collisional/radiative balance between the two levels, essentially driving the spin temperature \( T_\pi \) towards the gas temperature \( T_k \). Before there are any heating sources at \( z \lesssim 30 - 50 \), the collision-induced decoupling of \( T_\pi \) and \( T_{\text{CMB}} \) will be the only mechanism leading to 21-cm spectral features on top of the CMB (Scott & Rees 1990). However, its efficiency is very small
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and might be important only for the densest regions at $\delta\rho/\rho \gtrsim 30[(1 + z)/10]^{-2}$ (Madau et al. 1997).

A more likely mechanism is the excitation to the triplet atom by absorption of a Ly$\alpha$ photon to the $n = 2$ level, a so-called Wouthuysen-Field effect (Wouthuysen 1952, Field 1959). In this process a singlet hydrogen atom in the $1_0 S_{1/2}$ state (where the notation is $n_F L_J$, with $L$ being the electron orbital angular momentum, $J = S + L$ the total electron angular momentum, and $F = (\text{proton spin}) + J$ the total angular momentum) absorbs a Ly$\alpha$ photon and makes a transition to one of the $n = 2$ states, $2_1 P_{1/2}$ or $2_1 P_{3/2}$, decaying in some cases to the triplet $1_1 S_{1/2}$. The opposite reaction, the de-excitation of the hyperfine triplet state through scattering of a Ly$\alpha$ photon is also possible. Since in the neutral medium the optical depth in the Ly$\alpha$ line is very large, multiple scatterings of a Ly$\alpha$ photon drive the temperature in the line close to the kinetic temperature of the gas $T_k$, and, accordingly, the spin temperature $T_s$ might be partially coupled to $T_k$.

With these two mechanisms, the spin temperature can be written as (Field 1959)

$$T_s = T_{\text{CMB}} + \frac{(y_c + y_\alpha)T_k}{1 + y_c + y_\alpha},$$

(5.17)

where $y_c$ is the collisional coupling parameter (see Scott & Rees 1990 for a fitting formula)

$$y_c = \frac{C T_*}{A_{10} T_k},$$

(5.18)

with $C$ being the collisional rate, and $y_\alpha$ is the Ly$\alpha$ pumping coefficient (Field 1959)

$$y_\alpha = \frac{P_{10} T_*}{A_{10} T_k},$$

(5.19)

with $P_{10}$ being the de-excitation rate of the triplet state via absorption of a Ly$\alpha$ photon to the $n = 2$ level.
5.7.2 High-z Absorption Features

At very high redshifts, before any discrete sources of heating, the deviation of the spin temperature from the background radiation temperature is entirely due to collisions between neutral atoms (Scott & Rees 1990). However, this effect is very small (see Fig. 5.15), with $T_s \approx T_{CMB}$, and one would not expect to detect any absorption features on top of the CMB.

After the first sources of reheating appear, Lyα photons will de-excite the upper hyperfine (triplet) state, lowering the spin temperature closer to the gas temperature. During this short epoch $T_k < T_s \ll T_{CMB}$, yielding stronger absorption features. According to an estimate in Tozzi et al. (1999), the IGM will be visible in the 21-cm absorption over a timescale of $\sim 10^7$ yrs, with brightness temperature variations of order $\Delta T_b \sim 40$ mK over a frequency range of $\sim 5$ MHz.

5.7.3 High-z Emission Features

Very soon ($\sim 1-10$ Myrs) after the IGM becomes visible in absorption, the heat input from the first cosmological objects will raise the gas temperature above that of the CMB. Lyα photons of increasing number density will couple the spin temperature $T_s$ to the kinetic temperature $T_k$, driving the former considerably above the temperature of the background radiation and rendering neutral hydrogen observable in 21-cm emission.

Let us see how the Lyα pumping by photons originating close to H II regions (which in turn are driven by UV and soft X-rays from the first cosmological sources) results in angular and redshift-space structures. We determine the temperature of the gas by computing the RT of photons above the hydrogen Lyman edge. In reality, the thermal state of the IGM ahead of the hydrogen I-front is strongly affected by photons below 13.6 eV. Here, we neglect transfer in Lyα and other lines, effectively, lowering the temperature of the neutral medium. However, we still have significant preheating in our models. The higher energy (above 13.6 eV) UV and soft
X-ray photons propagate further in neutral hydrogen since the opacity drops with frequency as $\propto \nu^{-3}$, and they are able to heat the gas ahead of the I-front very efficiently.

In radioastronomy, the specific intensity $I_\nu$ is often replaced by the frequency-dependent brightness temperature $T_b(\nu)$, which in the Rayleigh-Jeans approximation ($h\nu \ll k_B T$) is proportional to the intensity:

$$I_\nu = \frac{2\nu^2}{c^2} k_B T_b.$$ 

Then the RTE

$$\frac{dI_\nu}{d\tau_\nu} = -I_\nu + B_\nu(T)$$

through a medium with some physical temperature $T$ of emission can be written as

$$\frac{dT_b}{d\tau_\nu} = -T_b + T.$$ 

If $T \equiv$ constant along the line of sight, the solution for the brightness temperature is

$$T_b = T_{b0} e^{-\tau_\nu} + T(1 - e^{-\tau_\nu}).$$ 

For a high-redshift neutral cloud, $T_{b0} \equiv T_{\text{CMB}}$, $T \equiv T_s$ and $\tau_\nu \equiv \tau$ is the total 21-cm line optical depth across the region. The resulting brightness temperature can be lower or higher than that of the CMB, hence, the cloud can be visible either in absorption or emission against the background radiation. The differential temperature between the 21-cm signal and the CMB is

$$\Delta T \equiv T_b - T_{\text{CMB}} = (T_s - T_{\text{CMB}})(1 - e^{-\tau}).$$

We will assume that there are enough Ly$\alpha$ photons to couple the spin temperature $T_s$ to the kinetic temperature of the gas $T_k$ throughout the entire volume, and that $T_s \gg T_s \approx 0.068 \text{ K}$
everywhere. In this case, the ratio of the atomic hydrogen densities in the upper and lower hyperfine states

\[ \frac{n_1}{n_0} = \frac{g_1}{g_0} e^{-T_s/T} \]

is equal to the ratio of their statistical weights, \( g_1/g_0 = 3 \), independently of the spin temperature. Then the fluctuations in the 21-cm radiation will be caused only by the gradient of the local neutral hydrogen density, shaped by the edges of H II regions. The 21-cm absorption coefficient is

\[ \kappa = \frac{c^2 A_{10}}{8\pi^2 \nu^2} \frac{g_1}{\Delta \nu g_0} \left( n_0 - n_1 g_0 \right) \approx \frac{3c^2 A_{10}}{8\pi^2 \nu^2} \frac{1}{\Delta \nu} n_0 \frac{T_s}{T} \]  

(5.24)

(see, e.g., Scott & Rees 1990). In this equation, \( \Delta \nu \) is the effective width of the 21-cm line profile (approximated by a rectangle), and \( A_{10} \) is the spontaneous rate for the 21-cm transition. Since \( n_1/n_0 \rightarrow 3 \), the lower level population is \( n_0 = (1 - x_e)n_H/4 \), where \( n_H \) is the number density of atomic hydrogen, and \( x_e \) is the fractional ionization. The 21-cm line optical depth across the cloud, \( \tau = \kappa \times \text{ (path length)} \), is approximately

\[ \tau \approx 2.59 \times 10^{-19} \text{ cm}^2 \text{ Hz K} \frac{N(\text{H I })}{\Delta \nu T_s}, \]  

(5.25)

where \( N(\text{H I }) \) is the neutral hydrogen column density along the line of sight. For small optical depths (\( \tau \ll 1 \)), the differential temperature becomes

\[ \Delta \approx \frac{T_s - T_{\text{CMB}}}{T_s} N(\text{H I }) \frac{1}{\Delta \nu} \times 2.59 \times 10^{-19} \text{ cm}^2 \text{ Hz K}. \]  

(5.26)

Within a large cloud of geometrical depth \( l \), the effective line width is most strongly affected by the Hubble flow velocity gradient \( \Delta \nu \) across the region, and can be written schematically as

\[ \Delta \nu \approx \nu_{21\text{cm}} \frac{\Delta v}{c}, \quad \text{where } \Delta v = H_0 (1 + z)^{3/2} l, \]
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whereas the column density is

\[ N(\text{H}^1) \approx \frac{n_H(1 - x_e)l^3}{l^2}. \]

The final expression for the differential brightness temperature (its sign indicating absorption or emission against the CMB) takes the form

\[ \Delta T \approx \frac{T_s - T_{\text{CMB}}}{T_s} \frac{n_H(1 - x_e)c}{\nu_{21\text{cm}} H_0(1 + z)^{5/2}} \times 2.59 \times 10^{-19} \text{ cm}^2 \text{ Hz K}, \]

(5.27)

where the additional \( 1/(1 + z) \) factor accounts for the change in the observed brightness temperature due the expansion of the Universe.

Our numerical simulations give the 3D distributions of the fraction of hydrogen ionization and temperature. In order to obtain the observed profile of 21-cm radiation on the sky, we integrate the brightness temperature along multiple lines of sight, solving the transfer equation

\[ dT_b = (T_s - T_b) d\tau, \]

with \( T_{b,\text{in}} = T_{\text{CMB}} \), and obtaining the signal \( (T_{b,\text{out}} - T_{\text{CMB}})/(1 + z) \).

Figures 5.16 - 5.17 show a skymap of 21-cm emission originating from the warm neutral IGM around the bright quasar in Model B. We assume that an efficient pumping mechanism (e.g., Ly\( \alpha \) photons) drives the spin temperature of the neutral gas very close to the kinetic temperature everywhere in the volume. This temperature, as well as the ionizational structure of the IGM are calculated via detailed RT above 13.6 eV. The adopted power law for quasar radiation, with the spectral index \( \alpha_g = 1.8 \) in all frequency groups, results in a relatively flat spectrum, quickly raising the temperature of the neutral IGM. The 21-cm signal on the sky is a convolution of the gas temperature and the density of atomic hydrogen, showing an abrupt cut-off near the edge of the expanding H\( \mathbf{II} \) region.

Note, that other theoretical maps of 21-cm emission from the inhomogeneous medium at a high redshift have been recently published (Meiksin 1999, Tozzi et al. 1999). However, to the best of our knowledge, none of them include detailed numerical RT as yet, but are based on an approximate estimate of the radius of a 1D Strömgren sphere which is superimposed on the
existing 3D density distribution. In this thesis, we have shown that such calculations can be performed with detailed time- and frequency-dependent numerical RT.

5.8 Discussion and Conclusions

The speed of I-fronts depends, among other variables, on the ambient neutral hydrogen density. Thus, the timescale on which the ionizing background 'eats in' to dense clumps and filaments is determined by the typical density contrast in the volume. The latter quantity depends crucially on the spatial resolution. In the simulations presented in Sec. 5.5.1 – 5.5.3, the predominant density contrast is of order $\sim 100$ at $64^3$, and closer to $\sim 50$ at $32^3$. Note that the method developed in this thesis does not treat RT on scales smaller than one cell. Therefore, one has to pay special attention to modelling the photochemical evolution of, say, a single overdense cell submerged in a bath of ionizing photons. In the present study, we simply take out the number of photons absorbed within that cell from the radiation field within the chemistry solver, given that this field will recomputed again at the next time step, after one light-crossing time of the cell. However, imagine a cell harbouring a dense halo. The overall transmission properties of this cell (frequency-dependent opacity and emissivity) will differ from those of the same volume element if the halo is not resolved. Here, we can only speculate that, depending on the astrophysical context, it might be possible to introduce a self-shielding fudge factor accounting for clumping of the gas on sub-resolution scales.

In this Chapter, we have performed several runs of cosmic reionization by both point sources and the background radiation field. We solve self-consistently the coupled equations of radiative transfer and non-equilibrium chemistry. It is shown that in general the 3D distribution of ionized regions follows the gas distribution. In all models low density voids are ionized first, and dense filaments are destroyed much more slowly, on the timescale determined by the ratio of the photoionization to recombination rates at those high densities.
In models with quasars inside the volume, the spectrum of the direct radiation does indeed become harder with time due to the wavelength dependence of the optical depth. We have not included any Doppler shifts into the model. However, having periodic boundary conditions allows direct ionizing photons from quasars to travel over many computational volumes and experience the Doppler shift due to the Hubble flow, given that these photons are not absorbed before they get redshifted. The Hubble speed on the scale of 2.5 Mpc is $250 \, h \, \text{km s}^{-1}$. Even with periodic boundary conditions, the error due to neglect of the Doppler shift is not large compared to other sources of uncertainties. The most advanced simulation is model A, which has been evolved from $z = 15.0$ to $z = 12.3$, with slightly under 4000 timesteps. If we assume that there are some direct high-frequency photons which manage to travel over the entire length of the model without being absorbed, they cross the volume $\sim 60$ times, which corresponds to the Hubble speed of $\sim 15 \times 10^3 \, h \, \text{km s}^{-1}$. The resulting error is most certainly smaller than 5% or 10% at most and does not exceed the error coming from the replacement of frequency-dependent quantities with integrals inside each frequency group. In addition, partially due to the limited frequency resolution above 54.4 eV, the vast majority of direct photons gets absorbed in the neutral medium (which still occupies most of the volume in model A at the end of the simulation). Hence, the error resulting from the neglect of the Doppler shift due to the Hubble flow is much smaller than other uncertainties in the model. In future work, we will increase the frequency resolution to calculate the propagation of high energy (UV and X-ray) photons with much greater care. Since these photons can travel much further in a neutral medium, they might be largely responsible for the preheating of the IGM, as well as for "blurring" I-fronts.

We have made no attempt to put observational constraints on different scenarios of reionization, instead, concentrating on developing tools to accomplish this task in the future. On the example of 21-cm line emission in Sec. 5.7, we have demonstrated that full, RT-enabled simulations of this kind will produce maps which could quantitatively show the observational signatures of reionization.
In future work, we will increase the resolution of these simulations to $128^3$ or $256^3$, with the corresponding update in angular resolution. Time-dependent ray tracing (as well as any explicit RT solver) is well suited to clusters of distributed memory machines, since remote volume elements cannot communicate on timescales shorter than the light-crossing time, and therefore can be followed independently.
Figure 5.1: The isosurfaces of the density distribution in a 2.5 Mpc (comoving) volume used for the RT model in the present work are plotted at the overdensity $\delta = 2$ at eight different redshifts. The density field was kindly supplied by M. White.
Figure 5.2: This figure shows a cross-section through a 3D hydrogen I-front propagating into the neutral IGM from a virialized halo hosting a mini-quasar around $z = 15$, at four different output times. The quasar luminosity is $4.2 \times 10^{53} \text{s}^{-1} M_{\text{halo}}/10^9 M_\odot$, and its lifetime is $10^{5.8} \text{yrs}$ (model A, see text in Sec. 5.5.1 for details). The simulation employs the full 3D radiative transfer in three frequency groups (for both direct ionizing and diffuse photons) combined with the solution of the rate equations for nine chemical species, at the spatial resolution $64^3$. The size of the volume is $2.5 \text{Mpc}$ (comoving). The quasar turns off around $z_{\text{off}} \sim 14.92$, and after that the I-front is driven entirely by secondary (recombination) photons coming from the H II bubble. To compare the I-front speed to the speed of light, it’s worth pointing out that by the time of the lower right corner plot, the wavefront would have crossed the volume four times.
Figure 5.3: Same as Fig. 5.2, but for singly ionized helium. Note that the He\textsc{ii} region is a relatively thin shell bounded by neutral helium in the ambient medium and by doubly ionized helium closer to the quasar.
Figure 5.4: Temperature for a cross-section through the IGM in model A at $z = 14.785$. The quasar is at the upper right corner. The long spikes going outward from the quasar are separated by shadows forming behind denser regions (these spikes have nothing to do with the finite angular resolution displayed in Fig. 2.2). Hydrogen ionization corresponds to the temperature range $(3 - 4) \times 10^4$ K.
Figure 5.5: A cross-section through a 3D hydrogen I-front at the beginning of the simulation for Model B, at four different output times. The quasar (in the upper left part of the plot) turns on at $z = 10$ and emits ionizing photons a constant luminosity $10^{54} \text{s}^{-1}$ throughout the entire run.
Figure 5.6: Same as Fig. 5.5, but for singly ionized helium. The He\textsc{II} region is bounded by the He\textsc{III} bubble on the inside, and by neutral helium further away from the quasar. To better illustrate the structure of the front, the fraction of ionization from the lower right plot is displayed in color in Fig. 5.7.
Figure 5.7: Helium I-front from the last snapshot in Fig. 5.6 shown in color.
Figure 5.8: This figure displays the energy density of the radiation field $E_g$ in three frequency groups ($g = 1, 2, 3$ top to bottom) vs. fractional ionization of hydrogen and helium, in a cross-section through Model B at $z = 9.473$. 
Figure 5.9: This figure illustrates hydrogen reionization by a UV background field (model C, see Sec. 5.5.2 for details) starting at $z = 13$. The spatial resolution is $32^3$, the box size is 2.5 Mpc. The speed of complete ionization is a function of the spatial resolution which affects the maximum density contrast within the volume. At $32^3$, the densest neutral filaments survive at least until $z \sim 12.6$ when we stopped the simulation.
Figure 5.10: Same as Fig. 5.9, but for a different cross-section. Continued on Fig. 5.11.
Figure 5.11: Continued from Fig. 5.10.
Figure 5.12: 3D distribution of neutral (atomic and molecular) hydrogen from the simulation on Fig. 5.9 (ionization by the UV background, model C). Note that this is *not* a plot of the integrated column density but rather a 3D rendering of the actual neutral hydrogen number density. The colorbar on the left of each plot is approximate, since it is affected by shielding in the visualization routine, and is given here only for reference.
Figure 5.13: This figure shows a cross-section through the hydrogen I-front in Model C computed at three different spatial resolutions ($8^3 \times 8^2$, $16^3 \times 8^2$ and $32^3 \times 8^2$, top to bottom), at the same output time. To ease the comparison, the underlying density field is visualized at $32^3$ for all three models.
adiabatic expansion \sim (1+z)

\[ T_{CMB} \]

collisions (important in dense clouds at lower \( z \))

Ly alpha photons

\[ T_s \]

adiabatic expansion: no direct effect

\[ T_K \]

adiabatic expansion \sim (1+z)^2

Figure 5.14: Energy contributors to the spin temperature \( T_s \) in an adiabatically expanding universe. Arrows indicate the direction of energy transfer. In the absence of collisional and Ly\( \alpha \) pumping the spin temperature comes to equilibrium with the CMB temperature on a timescale \( T_s/(T_{CMB}A_{10}) \sim 5 \times 10^4 \) yrs (Meiksin 1999).
Figure 5.15: Emergence of 21-cm emission or absorption features at high redshifts.
Figure 5.16: Temperature of the IGM in a cross-section through Model B (upper panel), at two output times, and the resulting map of 21-cm emission against the CMB (lower panel), in terms of the brightness temperature. The spin temperature of the 21-cm transition is assumed to be the same as the kinetic temperature of the gas throughout the entire volume, which is close to the temperature of the CMB far from the quasar. We do not take into account the effects of RT below 13.6 eV. In addition, the adopted spectrum of the quasar is rather flat, resulting in an artificially high temperature in the neutral IGM ahead of the hydrogen I-front.
Figure 5.17: Continued from Fig. 5.16. The snapshot at $z = 9.967$ (the column on the right) is close to complete overlapping of H II regions.
In this thesis, I have described a method for the numerical solution of the frequency- and
time-dependent radiative transfer equation in a three-dimensional inhomogeneous medium. It
is demonstrated that, with existing desktop hardware, it is possible to model cosmological
inhomogeneous reionization on a light-crossing time $t_R$ in three spatial dimensions. Since the photoionization time-scale in the small optical depth regime ($\tau \leq 1$) is of order of the light-
crossing time $t_R$, explicit advection is an efficient method in covering at least these regions.
Compared to elliptic-type solvers on the fluid-flow time-scale or the time-scale of typical changes
in the density and ionization structure distribution, explicit techniques produce very accurate
results without the need to solve a large system of coupled non-linear elliptic equations. The
computing requirements with explicit advection grow linearly with the inclusion of new atomic
and molecular rate equations, which is certainly not the case for quasi-static solvers (although
it is feasible that the development of multigrid techniques for elliptic equations might actually
approach similar scaling).

Using eq. (2.18) one can see that the entire history of reionization can be modeled with
$\sim 10^4$–$10^5$ time-steps (depending on the required resolution), which makes explicit advection
an attractive choice for these calculations. However, the efficiency of this method has still to
be explored. Future work should include a detailed comparison between explicit advection and
implicit reconstruction (through an elliptic solver), to demonstrate which method works best
for calculating inhomogeneous reionization.

As I have demonstrated here, for certain problems, including the propagation of supersonic
I-fronts, the Courant condition does not seem to impose prohibitively small time-steps. In this case, the biggest challenge is to accurately describe anisotropies in the radiation field, that is, to solve for inhomogeneous advection in the five-dimensional (without frequency) phase space, in the presence of non-uniform sources and sinks of radiation. Strictly speaking, the storage of one variable at, say, $64^5$ data points requires about 9 GB of memory, which stretches the capabilities of top-end desktop workstations. One attractive possibility for future exploration is to directly solve the monochromatic photon Boltzmann equation in 5D. To demonstrate the feasibility of the numerical solution, however, among different methods, I have chosen to concentrate on simple ray tracing at the speed of light. The numerical approach being used is completely conservative and produces very little numerical dissipation.

I have computed a series of reionization models for different strengths and spectra of the background radiation, within a fixed cosmological framework. To be able to distinguish between different scenarios of the first object formation, I will attempt to go to a higher spatial resolution ($128^3$ or $256^3$) in the future work, as well as include explicit radiative transfer below 13.6 eV during preheating.

Our simulations show that, depending on the luminosity of the first objects, expanding H\textsc{ii} regions could overlap very soon after these sources turn on (model B). In models with lower photon production rates (models A and C), the complete overlapping happens later, although the densest clouds in the IGM stay neutral by the time we stop calculations. It is worth pointing out that although H\textsc{ii} regions completely overlap at $z \gtrsim 5$ (the exact epoch depends on the scenario of reionization), there is still a significant fraction of residual neutral hydrogen in dense Ly$\alpha$ clouds and Lyman-limit systems. Madau \textit{et al.} 1999 define the so-called \textit{breakthrough} redshift at $z_{\text{br}} \sim 1.6$ when the Universe becomes optically thin to Lyman-continuum photons. In future work we shall evolve our models to much lower redshifts to study how $z_{\text{br}}$ is affected by the details of reionization at earlier stages.

Time-dependent ray tracing (or another explicit advection technique) could be used to solve
Chapter 6. Concluding Remarks

the problem of RT in an inhomogeneous medium in many other areas of astrophysics, especially, when the Courant condition does not result in prohibitively small time steps. Explicit techniques will work well both for monochromatic (line) radiation and for frequency-integrated quantities. Examples of problems with RT in individual lines include cooling in star forming regions, preheating at high redshifts, and Lyα emissivity of partially neutral clouds submerged in a bath of ionizing photons.

The global exchange of energy via the radiation field at a fixed wavelength is probably one of the easiest problems to solve in numerical RT. In the cosmological context, it seems likely that the progress in computer technology, a few years from now, will allow routine solution of this problem in three spatial dimensions with the sort of resolution obtained in modern, state-of-the-art hydrodynamical simulations \(10^7 - 10^9\) three-dimensional data points. On the other hand, the full solution of the RHD equations, retaining all \(O(v/c)\) terms, is a much more complicated problem. In this case one deals with frequency-dependent RT, and issues such as line transfer, broadening effects and spatial motions within the simulation box become important. Nevertheless, despite the high dimensionality of the problem, with a reasonable expenditure of computational resources (of the type available today), it is possible to numerically model many different aspects of the full 3D radiative transfer problem. The method described in this thesis represents a significant and realizable step towards the goal of full cosmological RHD.

Numerical modelling of cosmological RT will need to continue to develop in the near future, in concert with the rapid observational progress in understanding the end of the “Dark Ages”. In conclusion, in Tables C.1 - C.2 I have listed some of the major observational programs currently being planned or already implemented which could potentially probe the reionization epoch and the formation of the first objects.
Appendix A

High-Resolution Schemes for One-Dimensional Hyperbolic Systems

The goal of this appendix is to describe a high-resolution numerical scheme for the solution of 1D non-linear advection problems. The linear version of this algorithm is used to calculate first-order flux updates and higher-order corrections for normal, transverse and corner waves in the numerical Boltzmann solver in Sec. 2.8. The full non-linear version is applied to the derivation of an unsplit 3D moment solver in Appendix B.

First, consider a linear system

\[ q_t + A q_x = 0, \quad q = (Q_1, Q_2, \ldots, Q_N)^T \]  

(LeVeque 1997) of source-free hyperbolic equations in 1D. By “linear” we mean that the operator \( A \) does not depend on the coordinate \( x \). To find the solution of eq. (A.1), we have to separate variables \( Q_1, \ldots, Q_N \), i.e. to diagonalize the matrix \( A \). We begin by introducing a new variable

\[ q \equiv Pu, \]

so that eq. (A.1) becomes

\[ u_t + P^{-1} A P u_x = 0. \]  

We require that \( P^{-1} A P \equiv \Lambda \) is a diagonal matrix. In other words, \( \Lambda \) is the diagonal matrix composed of eigenvalues \( \lambda_i \) of \( A \), and \( P \) consists of right eigenvectors \( (p_\beta) \) of \( A \). Eq. (A.2) yields

\[ q_t + P \Lambda P^{-1} q_x = 0. \]  

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\[ q_t + P \Lambda P^{-1} q_x = 0. \]  

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We continue by dividing $\Lambda$ into positive and negative parts

$$\Lambda = \Lambda^+ + \Lambda^-, \quad \Lambda^\pm = \text{diag}(\lambda_i^\pm, \ldots, \lambda_N^\pm), \quad \lambda^+ = \max(\lambda, 0) \text{ and } \lambda^- = \min(\lambda, 0). \quad (A.4)$$

Since $A$ is linear, we can also write

$$A^\pm = PA^\pm P^{-1}. \quad (A.5)$$

The quantity

$$A^+ \Delta q_{i-1/2} = A^+(q_i - q_{i-1}) = P\Lambda^+ P^{-1} \Delta q_{i-1/2} = P\Lambda^+ \Delta u_{i-1/2} = P \begin{pmatrix} \lambda_1^+ \Delta u_1 \\ \vdots \\ \lambda_n^+ \Delta u_N \end{pmatrix} = \sum_\beta \lambda_\beta^+ \Delta u_\beta (p_\beta), \quad (A.5)$$

(LeVeque 1997) where $\Delta u_\beta$ is a linear combination of $\Delta Q_{1,i-1/2}, \ldots, \Delta Q_{N,i-1/2}$, can be thought of as the difference between all right-going waves to the left ($i-1 \rightarrow i$) and to the right ($i \rightarrow i+1$) from point $x_i$ (waves are numbered $\beta = 1, \ldots, N$). The eigenvectors $\lambda_\beta^+$ are simply the wave speeds, $\Delta u_\beta$ the wave amplitudes and $p_\beta$ the wave spectra. The full Godunov's update to the numerical solution of eq. (A.1) is then

$$q^{n+1}_i = q^n_i - \frac{k}{h} \left[ A^+ \Delta q_{i-1/2} + A^- \Delta q_{i+1/2} \right]. \quad (A.6)$$

Now, instead of eq. (A.1) consider a non-linear system

$$q_t + A(x)q_x = 0, \quad q = (Q_1, Q_2, \ldots, Q_N)^T. \quad (A.7)$$

The wave speeds and spectra now vary with $x$, and eq. (A.5) is not valid any more. Instead, we can write
\[ A^+ \Delta q_{i-1/2} = \sum_{\beta} \lambda_{\beta i}^+ \alpha_{\beta i-1/2} (p_{\beta i}), \]
\[ A^- \Delta q_{i-1/2} = \sum_{\beta} \lambda_{\beta i-1}^- \alpha_{\beta i-1/2} (p_{\beta i-1}). \]

(A.8)

To get the correct wave amplitudes \( \alpha_{\beta i-1/2} \), we have to use the proper jump conditions for the Riemann problem at the interface between \( x_{i-1} \) and \( x_i \):

\[ q_i - q_{i-1} = \sum_{\beta} \alpha_{\beta i-1/2} \left( \begin{array}{ll}
  \uparrow & \downarrow \cr
  p_{\beta i-1} & p_{\beta i}
\end{array} \right), \quad \text{for } \lambda_{\beta i-1}^+ \text{ or } \lambda_{\beta i}^- \]

(A.9)

i.e., the total jump \( \Delta q_{i-1/2} \) is just the sum of jumps across individual waves. Eq. (A.6, A.8 - A.9) ensure the full conservation for original hyperbolic systems; however, they provide only a first-order solution (LeVeque 1997).
Appendix B

An Unsplit Method for 3D Moment Transfer

In this appendix we develop an explicit (on the light-crossing timescale) solver of the first two radiation moment equations for Sec. 2.6 given a separate closure technique. Let us consider the advection part of the truncated system of 3D moment equations (2.7) – (2.8):

\[ \frac{\partial E}{\partial t} = -\nabla \cdot F, \]
\[ \frac{\partial F}{\partial t} = -c^2 \nabla \cdot (f_\alpha \beta E). \]  

(B.1)

Assume, that the Eddington factor coefficients \( f_\alpha \beta (r) \) are already known from some closure scheme (the formal solution for the angle-dependent intensity). Contrary to the 5D Boltzmann equation with constant coefficients (eq. (2.30)), the system (B.1) can be very non-linear, for instance, at the transition layer between optically thin and optically thick regions. The solution of eq. (B.1) on a 3D rectangular mesh begins with the construction of the first-order accurate scheme. It is useful to write eq. (B.1) in the matrix form

\[ q_t + [A(x, y, z)q]_x + [B(x, y, z)q]_y + [C(x, y, z)q]_z = 0, \]

where

\[ q = \begin{pmatrix} E \\ F_1 \\ F_2 \\ F_3 \end{pmatrix}, \quad A = \begin{pmatrix} 0 & 1 & 0 & 0 \\ c^2 f_{11} & 0 & 0 & 0 \\ c^2 f_{21} & 0 & 0 & 0 \\ c^2 f_{31} & 0 & 0 & 0 \end{pmatrix}. \]
Appendix B. An Unsplit Method for 3D Moment Transfer

\[
B = \begin{pmatrix}
0 & 0 & 1 & 0 \\
c^2f_{12} & 0 & 0 & 0 \\
c^2f_{22} & 0 & 0 & 0 \\
c^2f_{32} & 0 & 0 & 0
\end{pmatrix}, \quad \text{and} \quad C = \begin{pmatrix}
0 & 0 & 0 & 1 \\
c^2f_{13} & 0 & 0 & 0 \\
c^2f_{23} & 0 & 0 & 0 \\
c^2f_{33} & 0 & 0 & 0
\end{pmatrix}
\] (B.2)

The first-order normal update in the x-direction is given by the left- and right-going flux differences from eq. (A.8). The speeds of waves along the x-axis are given by eigenvalues of the matrix \( A \)

\[
\lambda_{1,ijk} = 0, \quad \lambda_{2,ijk} = 0, \quad \lambda_{3,ijk} = c\sqrt{\frac{f_{11,ijk}}{f_{21,ijk}}}, \quad \lambda_{4,ijk} = -c\sqrt{\frac{f_{11,ijk}}{f_{21,ijk}}}
\] (B.3)

The corresponding wave spectra (right eigenvectors of \( A \)) are

\[
p_{1,ijk} = \begin{pmatrix}
0 \\
0 \\
-1 \\
1
\end{pmatrix}, \quad p_{2,ijk} = \begin{pmatrix}
0 \\
0 \\
1 \\
1
\end{pmatrix}
\]

\[
p_{3,ijk} = \begin{pmatrix}
\sqrt{\frac{f_{11,ijk}}{c^2f_{21,ijk}}} \\
f_{11,ijk} \\
f_{21,ijk} \\
1
\end{pmatrix}, \quad p_{4,ijk} = \begin{pmatrix}
-\sqrt{\frac{f_{11,ijk}}{c^2f_{21,ijk}}} \\
f_{11,ijk} \\
f_{21,ijk} \\
1
\end{pmatrix}
\] (B.4)

The jump condition (eq. (A.9)) then takes the form

\[
\Delta q_{i-1/2,jk} = \alpha_{1,i-1/2,jk}^q p_{1,ijk} + \alpha_{2,i-1/2,jk}^q p_{2,ijk} + \alpha_{3,i-1/2,jk}^q p_{3,ijk} + \\
+ \alpha_{4,i-1/2,jk}^q p_{4,i-1/2,jk}
\] (B.5)

yielding the strengths of the waves. Since waves \#1 and \#2 have zero velocities, the only amplitudes we are interested in are
Appendix B. An Unsplit Method for 3D Moment Transfer

\[
\alpha_{3, i-1/2, jk} = \frac{f_{21,ijk} \left( \sqrt{f_{11, i-1, jk}} \Delta q_{2,i-1/2,jk} + c f_{11, i-1, jk} \Delta q_{1,i-1/2,jk} \right)}{\sqrt{f_{11, ijk} f_{11, i-1, jk} + f_{11, ijk} \sqrt{f_{11, i-1, jk}}}},
\]

\[
\alpha_{4, i-1/2, jk} = \frac{f_{21, i-1, jk} \left( \sqrt{f_{11, ijk}} \Delta q_{2,i-1/2,jk} - c f_{11, ijk} \Delta q_{1,i-1/2,jk} \right)}{\sqrt{f_{11, ijk} f_{11, i-1, jk} + f_{11, ijk} \sqrt{f_{11, i-1, jk}}}}. \tag{B.6}
\]

The first-order normal update for advection in the \( x \)-direction is

\[
q_{ijk}^{n+1} = q_{ijk}^n - \frac{k}{h} \left( \sum_{\beta} \lambda^+_{\beta,ijk} \alpha^+_{\beta,i-1/2,jk} P_{\beta,ijk} + \sum_{\beta} \lambda^-_{\beta,ijk} \alpha^-_{\beta,i+1/2,jk} P_{\beta,ijk} \right). \tag{B.7}
\]

Normal updates along the \( y \)- and \( z \)-axes are performed in a similar way.
Appendix C

Observing Programs to Detect the Epoch of Reionization

Probing the epoch of reionization

<table>
<thead>
<tr>
<th>Program</th>
<th>Description</th>
<th>First Light</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sloan Digital Sky Survey (SDSS)</td>
<td>⇒ five-color imaging and spectroscopic survey of one quarter of the sky. Possibility of detecting up to a few hundred bright quasars and galaxies at $z &gt; 5$, with the brightest objects in the redshift interval $5.5 \leq z \leq 7$.</td>
<td>1998, duration ~ 5 years</td>
</tr>
<tr>
<td>Chandra X-ray Observatory (CXO)</td>
<td>⇒ $17' \times 17'$ field of view; sensitivity threshold of $\sim 2 \times 10^{-16}$ erg s$^{-1}$ cm$^{-2}$; might detect order a hundred quasars per field of view in the redshift interval $5 \leq z \leq 8$; IR spectroscopy of X-ray selected quasars with NGST could probe the reionization history up to $z \sim 8$.</td>
<td>1999</td>
</tr>
<tr>
<td>Giant Metrewave Radio Telescope (GMRT)</td>
<td>⇒ an array of 30 fully steerable 45m parabolic dishes spread over the area with a baseline of up to 25 km (with a compact central area enclosed in a larger “Y”-shaped configuration); could detect 21-cm emission or absorption against the CMB from high-redshift neutral hydrogen, if reionization occurred at $6 \leq z \leq 10$.</td>
<td>1996 (?)</td>
</tr>
<tr>
<td>Square Kilometer Array (SKA)</td>
<td>⇒ a project to build a giant radiotelescope with the total collecting area of at least a square kilometer; several different options currently under study; could detect 21-cm emission or absorption against the CMB from high-redshift neutral hydrogen, if reionization occurred at $z \leq 15$.</td>
<td>~ 2010</td>
</tr>
</tbody>
</table>

Table C.1: Current and future observing programs potentially able to probe the epoch of reionization (continued on the next page).
Appendix C. Observing Programs to Detect the Epoch of Reionization

<table>
<thead>
<tr>
<th>Program</th>
<th>Description</th>
<th>First Light</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Next Generation Space Telescope (NGST)</strong></td>
<td>⇒ expected imaging sensitivity in the infrared better than 1 nJy at wavelengths 1 – 3 ( \mu )m</td>
<td>( \sim ) 2008</td>
</tr>
<tr>
<td></td>
<td>possibly, will allow the detection of individual galaxies and mini-quasars directly to ( z \sim 10 ), and perform medium-resolution spectroscopy to ( z \sim 8 ); in the case of gradual reionization might measure the Gunn-Peterson optical depth ( \tau_{\text{GP}} &gt; 1 ); might detect Ly( \alpha ) emission from the reionization epoch</td>
<td></td>
</tr>
<tr>
<td></td>
<td><a href="http://www.ngst.stsci.edu">http://www.ngst.stsci.edu</a></td>
<td></td>
</tr>
<tr>
<td><strong>MAP</strong></td>
<td>⇒ all-sky differential map of CMB fluctuations in five frequency bands from 22 to 90 GHz with an angular resolution of ( \geq 0.21^\circ - 0.93^\circ ); will be launched on a stationary orbit around the Sun-Earth Lagrange ( (L_2) ) point</td>
<td>( \sim ) Fall 2000</td>
</tr>
<tr>
<td><strong>Planck</strong></td>
<td>⇒ high-angular resolution mapping of the CMB over the whole sky, simultaneously over a wide frequency range; designed to provide 10 times the sensitivity and more than 50 times the angular resolution of the COBE satellite</td>
<td>( \sim ) 2007</td>
</tr>
<tr>
<td><a href="http://map.gsfc.nasa.gov">http://map.gsfc.nasa.gov</a></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td><a href="http://astro.estec.esa.nl/SA-general/Projects/Planck">http://astro.estec.esa.nl/SA-general/Projects/Planck</a></td>
<td></td>
</tr>
</tbody>
</table>

Table C.2: Continued from table C.1.
Appendix D

Glossary

BH black hole

CDM cold dark matter

CFL, or the Courant condition Courant-Friedrichs-Levy condition

The stability condition in explicit advection techniques requiring the time step to be less than the time taken for a sound wave (or an advection wave for general hyperbolic equations of non-hydrodynamical nature) to cross one computational grid zone.

CMB cosmic microwave background

DM dark matter

FD finite difference

I-front ionization front

IGM intergalactic medium

LTE local thermodynamic equilibrium

An assumption that a small (local) volume element is in thermodynamic equilibrium – although the whole system need not be in equilibrium and might experience large fluxes of energy transport – and consequently the local atomic
population numbers depend only on the local electron temperature and density via the Saha-Boltzmann equations. LTE is enforced by collisional processes.

**LF** luminosity function

**MS** main sequence

**NLTE** non-LTE (absence of LTE)

In NLTE the local level populations depend not only on the local electron temperature and density but on other parameters as well, e.g., the energy density of the radiation field. Models are usually computed by replacing the equilibrium Saha-Boltzmann equations with time-dependent rate equations. NLTE effects are larger at higher temperatures and lower densities when radiative processes might be dominant over collisions.

**PDE** partial differential equation

**PPA** piecewise parabolic advection

**RHD** radiation hydrodynamics

**RT** radiative transfer

**RTE** radiative transfer equation

**SDSS** Sloan Digital Sky Survey

**UV** ultraviolet
References


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[34] Godunov S.K., 1959, Matematichesky Sbornik, 47, 271

References


References


References


