Heating the Early Universe
Numerical Methods and Their Analysis

Kai Yan Lee
Cover image: Once upon a time, a Pharaoh watched the beautiful night sky (Carina Nebula, credit to NASA, ESA, and the Hubble SM4 ERO Team). Inspired, he conceived the idea of pyramidal grid. I thank Vincent Fu for this creative artwork.


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Abstract

During the epoch when the first collapsed structures formed \((6 < z < 50)\) our Universe went through an extended period of changes. Some of the radiation from the first stars and accreting black holes in those structures escaped and changed the state of the Intergalactic Medium (IGM). The era of this global phase change in which the state of the IGM was transformed from cold and neutral to warm and ionized, is called the Epoch of Reionization.

In this thesis we focus on numerical methods to calculate the effects of this escaping radiation. We start by considering the performance of the cosmological radiative transfer code \(C^2\)-RAY. We find that although this code efficiently and accurately solves for the changes in the ionized fractions, it can yield inaccurate results for the temperature changes. We introduce two new elements to improve the code. The first element, an adaptive time step algorithm, quickly determines an optimal time step by only considering the computational cells relevant for this determination. The second element, asynchronous evolution, allows different cells to evolve with different time steps.

An important constituent of methods to calculate the effects of ionizing radiation is the transport of photons through the computational domain or “ray-tracing”. We devise a novel ray tracing method called PYRAMID which uses a new geometry - the pyramidal geometry. This geometry shares properties with both the standard Cartesian and spherical geometries. This makes it on the one hand easy to use in conjunction with a Cartesian grid and on the other hand ideally suited to trace radiation from a radially emitting source.

A time-dependent photoionization calculation not only requires tracing the path of photons but also solving the coupled set of photoionization and thermal equations. Several different solvers for these equations are in use in cosmological radiative transfer codes. We conduct a detailed and quantitative comparison of four different standard solvers in which we evaluate how their accuracy depends on the choice of the time step. This comparison shows that their performance can be characterized by two simple parameters and that the \(C^2\)-RAY generally performs best.
This thesis is dedicated to my parents
List of Papers

The following papers, referred to in the text by their Roman numerals, are included in this thesis.

**PAPER I:** *Efficient photoheating algorithms in time-dependent photoionization simulations*
DOI: 10.1093/mnras/stv2556

**PAPER II:** *PYRAMID - a novel ray-tracing method*

**PAPER III:** *Mathematical Analysis of the Coupled Ionization and Thermal Equations*
Lee, K. Y., Mellema, G., (2016), submitted to *CompAC*

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Author’s contribution

I briefly summarize my contribution to the three papers included in the thesis.

- **Paper I:** The project was proposed by my supervisor. His primary suggestion was to force the ionization front to proceed slowly such that all the nonphysical oscillations in the temperature solution for long time-steps would disappear. I followed the general idea and developed the adaptive time-step algorithm. I introduced the $f$ parameter and developed the ray-tracing algorithm which works on the pyramidal components. The idea of asynchronous evolution was proposed by me. My supervisor and I had thorough discussions on its actual implementation in the simulation. The code work of asynchronous evolution was done by me and the paper was written by me with contributions from the co-authors.

- **Paper II:** I observed the geometrical incompatibility between a Cartesian grid (Cartesian geometry) and a bundle of rays casted from a source in all directions (spherical geometry). I devised a new geometrical system (pyramidal geometry) to bridge the difference between these two different geometries. I coded the PYRAMID and the co-authors provided suggestions and recommendations to improve the project. The paper was mainly written by me and corrected by the co-authors.

- **Paper III:** The fundamental problem in the thermal evolution described in Paper I is due to a wrong estimate of photoheating rate. Instead of qualitatively explaining the reasons for this flaw, I suggested a project in which we quantitatively study this fundamental problem. In this project, I devised an analytical model which compares the performance of the forward Euler method and the $C^2$-RAY method. My supervisor suggested the inclusion of the backward Euler and the mid-point methods so the whole project covers more of the existing methods. The analytical work and code work were performed by me. The paper was mainly written by me with assistance from my supervisor.

Part of the material covered in this thesis was also printed in my Licentiate thesis (2015).
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1. Introduction To Cosmic Reionization

1.1 The Epoch of Reionization

Approximately 50 million years after the Big Bang, the first stars formed in structures of gas and dark matter which had collapsed gravitationally out of the initial density fluctuations present in the Universe. The radiation from these stars illuminated the early Universe which at that time was still in its infancy and filled with cold and neutral gas. These bright objects emitted large amounts of high energy photons which gradually ionized and heated the cold and neutral hydrogen medium around them. Subsequent star and galaxy formation further ionized and heated a larger fraction of the cold neutral gas in their surroundings. As over the next hundreds of millions of years more and more structures formed and the already existing ones grew in size, these warm ionized regions continuously grew in size and started to overlap with each other. Eventually, at an age of approximately 1 billion years, the entire Universe had become ionized and warm, marking the end of this global process. The period when this important large scale phase transition of the entire Universe occurred is called the Epoch of Reionization (EoR).

When and how the reionization took place is currently not well known. We need to explore different ways to observe this era and to interpret these observations in order to resolve this mystery. We also need a robust theoretical understanding of how the first stars were formed and other relevant physical processes during the EoR. Many of these theoretical works require the use of sophisticated numerical algorithms. Besides ionization of hydrogen during the EoR, the heating induced by the photoionization process (hereafter photoheating process) was also important because it caused a global thermal state change of the Universe. The temperature structure of the ionized medium is determined both by the photoheating from the sources and by the radiative and adiabatic cooling of the gas. The dominant radiative cooling process is collisional excitation cooling which becomes important when the ionized fraction and the temperature of the gas increases. After the typical cooling time, the photoheating and radiative cooling attain a balance and a thermal equilibrium state is established. However, the low density and negligible amount of met-
als found in the IGM during the EoR imply that the cooling time-scale was relatively long. Consequently these cooling processes only changed the temperature structure negligibly and an equilibrium state was never reached. The temperature distribution therefore contained imprints of the photoheating effect by the sources and thus stored a wealth of important information about reionization.

The two major IGM heating mechanisms during the EoR are categorized into a global and a local one. The global IGM heating (effective on scales larger than 100 comoving Mpc) is expected to be driven by the very hard photons produced by for example X-ray binaries, supernovae and gamma ray bursts in the first galaxies. These photons have relatively large mean free paths in the IGM which makes them a diffusive heating source. The patchy IGM heating (at scales of the order of 10 comoving Mpc) is associated with the softer UV photons released by the first galaxies and accreting supermassive black holes which were located in the high density regions of the IGM. These photons may have effectively ionized and heated the gas close to the sources, establishing a patchy ionization and temperature structure in the IGM.

Besides hydrogen, helium in the IGM plays an important role in the photoheating process. Neutral and singly ionized helium gas are more likely to capture hard UV photons than neutral hydrogen atoms do, given that hard UV photons have larger mean free paths than soft UV photons. Though the number density of helium is one order of magnitude lower than the number density of hydrogen, the effect of its presence is not negligible. The evolution of both hydrogen and helium ionization by these hard photons can only be investigated through numerical simulations.

In this chapter, we give a brief review cosmology related to reionization and the IGM. Section 1.2 outlines the evolution of the early Universe according to the Big Bang model and the structure formation model associated with the first stars and galaxies. A numerical model for reionization requires robust input parameters in order to correctly predict the IGM evolution. Most of the time the input parameters can be derived only from observation. In Section 1.3 we provide an overview of the key observational constraints on the EoR. They include observations of the spectra of high redshift quasars, the cosmic microwave background (CMB) radiation, the star forming galaxies and the 21-cm signal.

1.2 Theoretical understanding

To understand reionization we need to knowing the time and manner in which the first stars and galaxies formed. To solve this we need to trace the evolution of our Universe and follow how structures formed in the matter distribution.
1.2.1 Big Bang Model

The Big Bang model is nowadays the commonly accepted standard cosmological paradigm. It describes how our Universe started from a singularity and expanded continuously. Recent estimates of the Universe’s age by the Planck mission data of CMB radiation is $13.798 \pm 0.037$ billion years (Planck Collaboration et al. 2014a). An important ingredient of the Big Bang model is cosmic inflation. Cosmic inflation occurred around $10^{-36}$ to $10^{-33}$ seconds after the Big Bang. During this short period of time our Universe expanded exponentially. Cosmic inflation smoothed out any large scale inhomogeneities and anisotropies in the matter distribution. This explains why our Universe appears to be homogeneous and isotropic at large scales, as observed in galaxy redshift surveys and the distribution of the CMB radiation. Nevertheless, on small scales some significant inhomogeneities remained originating from tiny quantum fluctuations made macroscopic by inflation. These inhomogeneities were the seeds of the subsequent structure formation.

1.2.2 Lambda Cold Dark Matter model

In order to understand the matter evolution which leads to the formation of the first structures, we need to know the composition of matter in our Universe and their properties. Our Universe is composed of ordinary (baryonic) matter and the dark matter. These constitute $\sim 17\%$ and $\sim 83\%$ of the total matter by mass respectively. The Lambda Cold Dark Matter ($\Lambda$CDM) model assumes that dark matter is cold and only interacts with itself and ordinary matter through gravity. The $\Lambda$CDM model also include a cosmological constant $\Lambda$ which is often associated with dark energy. Unfortunately the properties of dark energy are poorly known. It should correspond to a negative pressure which implies an anti-gravity effect: When our Universe expands, the amount of dark energy increases leading to accelerated expansion. Similarly, during any contraction, the amount of dark energy would decrease leading to accelerated contraction.

The $\Lambda$CDM model successfully reproduces large-scale structure formation, the formation and abundances of elements during Big Bang nucleosynthesis, the existence and detailed properties of the CMB and the recent accelerating expansion of our Universe.

1.2.3 Expansion of space

The state of our Universe, such as the average matter density, pressure and temperature, gradually changed because of the expansion of space. Structure formation was also affected by these changes. The critical density $\rho_c$, is the density for which the spatial geometry of the Universe is flat. If the combined
density of all constituents of the Universe is higher than $\rho_c$ its spatial geometry would be positively curved and if it is less it would be negatively curved. Measurements of the CMB fluctuations spectrum indicate that the geometry of our Universe is consistent with flat and that the total density is to within 0.5% of the critical value (Planck Collaboration et al., 2015).

The critical density is defined as $\rho_c = \frac{3H^2}{8\pi G}$, where $H$ is the Hubble parameter and $G$ is the gravitational constant. It is usual to express cosmological densities in terms of this critical density using the density parameter $\Omega = \rho/\rho_c$. A flat Universe then corresponds to $\Omega = 1$. Assuming our Universe is homogeneous and isotropic, the expansion of the space can be described by the Friedmann equation which is often expressed in terms of the density parameters,

$$\frac{\dot{a}}{a} = H_0 \left[ \frac{\Omega_R}{a^4} + \frac{\Omega_M}{a^3} + \frac{\Omega_K}{a^2} + \Omega_\Lambda \right]^{1/2},$$

(1.1)

where $a$ is the scale factor, $\dot{a}$ its time derivative, $H_0$ the Hubble parameter at the current time, $\Omega_R$ is the radiation density parameter, $\Omega_M$ is the matter density parameter, $\Omega_K = 1 - \Omega$ is the spatial curvature density parameter and $\Omega_\Lambda$ is the dark energy density parameter. We discuss some of the relevant results of this expansion in the next sections.

1.2.4 Recombination era

The recombination era is the epoch when free electrons and protons combined to form neutral atoms. This became possible when the temperature of the mix of radiation and baryonic matter had dropped to $T \approx 3000$ K due to the expansion of space ($\sim 378,000$ years after Big Bang). When this temperature was reached there were no longer sufficient numbers of ionizing photons in the Universe to keep the protons and electrons from forming neutral atoms. The sudden drop in electron density caused by recombination induced an abrupt decrease of rate of Compton scattering between matter and photons. This is known as the decoupling of matter and radiation. The photons were now free to travel through space. These liberated photons we see today as the CMB.

The decoupling of matter and radiation also meant that the effective sound speed in the baryonic matter dropped from the value of a photon gas ($c/\sqrt{3}$) to its thermal value. This enabled gravity to start increasing the density fluctuations present in the baryons. For dark matter, which does not interact with photons, gravity already started to increase the fluctuations since the expansion of the Universe had become matter-dominated at an age of about 47,000 years. Gravity working on this mix of dark and baryonic matter eventually created the first structures capable of forming stars. To understand how gravity governed
the structure formation and how the first stars and galaxies were formed, we need to know how an initial perturbation in the matter distribution grew and led to the formation of collapsed objects.

1.2.5 Growth of perturbations and Spherical collapse

When matter fluctuations are small, i.e. the absolute difference between the density of a given point and the mean density is negligible compared to the mean density, linear perturbation theory can be applied to predict the evolution of the matter density. The fractional density fluctuations $\delta$ and the peculiar velocity $\mathbf{u}$ follow from the continuity and Euler equations for matter. As gravity is a purely attractive force, density fluctuations grow with time. When $\delta \sim 1$ its evolution enters the non-linear regime beyond which its evolution can only be studied computationally. Figure 1.1 shows an example of a computational simulation of cosmological structure formation. The dark matter density is shown in the color scale (light orange indicates higher densities and dark orange lower densities. The matter distributes itself into dense filaments separated by low density voids. The intersection points among the filaments have even higher densities and this is where at any given point in time the most massive structures are found.

Cold dark matter behaves as a pressureless fluid and can form very small gravitationally bound objects known as dark matter halos. However, baryons also have pressure and therefore can only join the dark matter if the total mass of the object is larger than the Jeans mass. The very first gravitationally bound objects which contained both dark matter and baryons had a mass of $\sim 10^5 \, M_\odot$ and formed when the Universe had an age of about 50 million years. To form stars, the baryonic gas needs to lose energy through radiative cooling so that it sinks deeper into the gravitational potential of the dark matter halo and can attain the higher densities needed. The physics of the heating and cooling processes inside the dark matter halos are important in regulating the star formation inside them. However, we will not go into these here.

As time progressed, more and more low mass dark matter halos with baryonic gas formed and the already existing ones grew through accretion and merging with each other. Once structures of masses above $\sim 10^8 \, M_\odot$ formed we can speak of the first galaxies in the Universe. Reionization really started once sufficient numbers of these had formed.

1.2.6 Heating of Intergalactic Medium

This thesis mainly focuses on methods for calculating the heating of the early Universe, specifically the evolution of the IGM temperature for the redshift
Figure 1.1: A density field slice of MassiveBlack cosmological hydrodynamic simulation (0.75 Gpc)$^3$ at $z = 5$. The overlaid panels show the zoom-ins on scale 20 Mpc/h and 2 Mpc/h. Figure from Di Matteo et al. (2012).

range $z > 6$. By the time our Universe became neutral when protons and electrons recombined to form hydrogen atoms, our Universe was extremely uniform as indicated by the highly isotropic CMB map. At that time it had a temperature of $\sim 3000$ K. Due to the expansion of the Universe one would expect the baryonic gas to cool adiabatically so that $T_{\text{baryon}} \propto (1 + z)^2$. However, even though matter and radiation had decoupled the low concentration of free electrons (the gas is not completely neutral) still allowed Compton scattering of CMB photons. This process transferred energy from the CMB photons to the baryons and initially kept them at the same temperature as the CMB photons with is given by $T_\gamma \propto (1 + z)$. Only after $z \approx 150$ the densities had dropped sufficiently for this process to become inefficient (Peebles 1993). After this the CMB temperature and baryonic temperature began to diverge as the baryons started to follow the adiabatic cooling relation, $T_{\text{baryon}} \propto (1 + z)^2$. This period of time, called the Dark Ages, came to an end when the first collapsed objects formed and the first sources of light inside them. The radiation produced could then start to modify the thermodynamic evolution of the IGM.

The IGM heating processes induced by radiation from the first generations of objects can be categorized into a global uniform heating and a local patchy heating (in a relative sense). Both types of heating were caused by ionizing photons emitted from the collapsed structures, the difference being due to the energy content of the ionizing photons contributing to the heating. The global uniform heating driven by X-ray photons. These photons have long mean free paths in the IGM, $\lambda_X \approx 4.9 x_{\text{HI}}^{-1/3} (\frac{1 + z}{15})^{-2} \left( \frac{E}{300 \text{ eV}} \right)^3$ Mpc, where $x_{\text{HI}}$ is the volume-average neutral hydrogen fraction and $E$ is the photon energy.
These long mean free paths have motivated a simplifying assumption that the X-ray photons heated the IGM uniformly on a large scale. The X-ray photons could increase the IGM temperature to $\sim 100$ K globally but did not cause the ionized fraction to increase by much.

Compared to the X-ray photons, UV photons have short mean free paths in the IGM. The UV-photons were absorbed by the gas close to the source, nearly fully ionized it and increased the IGM temperature inside these ionized regions to $\sim 10,000$ K. It is commonly believed that both types of heating occurred at the same time but the global uniform heating increased the IGM temperature to several 100 K before any larger fully ionized and heated regions formed. The reason is that X-rays can deposit their energy over large regions and only about $\sim 0.004$ eV per particle at $z \sim 10$ is adequate to raise the temperature of the IGM to 100 K (Ciardi & Madau 2003).

However, the properties of the sources of X-ray photons are not known with any certainty. They could be generated in inverse Compton scattering of CMB photons off supernova-accelerated electrons (Oh 2001), supernova remnant shocks (Johnson & Khochfar 2011), high-mass X-ray binaries (Power et al. 2009; Mirabel et al. 2011), mini-quasars (Madau et al. 2004), halo accretion shocks (Dopita et al. 2011; Wyithe et al. 2011), cosmic rays (Samui et al. 2005; Lacki 2013; Sazonov & Sunyaev 2015) or dark matter annihilations (Belikov & Hooper 2009). The sources of UV photons are thought to be high redshift quasars (See Section 1.3.2) and star forming galaxies (See Section 1.3.3). At the end of EoR, the hydrogen gas had become almost fully ionized and had acquired a temperature of $\sim 10,000$ K.

1.3 Observational understanding

Cosmological observations can help us to constrain the unknown parameters in the reionization model. We review five different observational probes in this section, namely the cosmic microwave background, high redshift quasar absorption spectra, star forming galaxies, the hydrogen 21-cm line from the EoR and temperature measurements in quasar near zones.

1.3.1 Cosmic Microwave Background

In the first 378,000 years after Big Bang, photons were trapped in an interacting soup of protons and electrons. After our Universe cooled down to 3000 K the protons and electrons recombined to form neutral atoms, the photons decoupled from the soup and traveled freely through space without interacting with any of the newly formed neutral atoms. After decoupling, matter and radiation evolved independently.
During the EoR, free electrons were produced by the ionization processes caused by the first stars and galaxies. Scattering of free flowing CMB photons from these free electrons caused an observable imprint on the photons. These are the smoothing out of temperature anisotropies on small scales and the production of polarization anisotropies on large scales (Hinshaw et al. 2013; Planck Collaboration et al. 2014b). The electron scattering is mainly important during the EoR because at later times the electron density became too low to affect the CMB significantly. For this reason, CMB observations provide us with information about the EoR.

The key parameter which can be measured is the total electron scattering optical depth for the CMB,

$$\tau_{es} = c \sigma_T \int n_e(z) \frac{dt}{dz} \, dz,$$

(1.2)

where \(c\) is the speed of light, \(\sigma_T = 6.65 \times 10^{-25} \text{cm}^2\) is the Thompson scattering cross section and \(n_e(z)\) is the electron number density. For a flat Universe, the integrand can be evaluated analytically (Loeb & Furlanetto 2013),

$$\tau_{es} = 4.44 \times 10^{-3} \times \{ \sqrt{\Omega_\Gamma} + \Omega_m (1 + z_{reion})^3 - 1 \}. \quad (1.3)$$

Note that the parameter \(\tau_{es}\) does not encode any temporal information about the reionization history. It gives only a constraint on the total electron optical depth along the line of sight. Equation 1.2 is often used to calculate the redshift when the reionization was complete assuming an instantaneous reionization model. The current best-fit value under this assumption is \(z_{reion} = 8.8_{-1.4}^{+1.7}\) (Planck Collaboration et al. 2015).

1.3.2 High Redshift Quasars

Important information about the EoR can be extracted from the spectra of high redshift quasars. In particular, the spectral region blueward of the Ly\(\alpha\) (\(\text{Ly}\alpha\)) line is affected. The absorption of photons that have redshifted to the \(\text{Ly}\alpha\) wavelength by the intervening neutral hydrogen gas in the IGM places constraints on the ionization state of the IGM along the line-of-sight (LOS). The fraction of \(\text{Ly}\alpha\) transmission (a function of wavelength) depends on the distribution of neutral gas along that LOS.

The first detection of complete \(\text{Ly}\alpha\) absorption, which is often called Gunn-Peterson trough (Gunn & Peterson 1965), was achieved by Becker et al. (2001). This measurement implies the existence of a substantial amount of neutral hydrogen gas close to this \(z = 6.28\) quasar and hence indicates that reionization may not have been complete by then. Investigation of high redshift quasar spectra in the redshift range \(5.7 < z < 6.4\) implies that reionized ended at
around $z \sim 6$ (Fan et al. 2002; White et al. 2003; Fan et al. 2006; Willott et al. 2007, 2010). Besides the ionization information, the thermal imprint on the IGM as a result of photoheating caused by the quasar itself can also be inferred from the spectra (Wyithe et al. 2008; Bolton et al. 2010, 2012).

1.3.3 Star Forming Galaxies

It is widely believed that star forming galaxies played a major role in reionizing our Universe. They are believed to have produced sufficient numbers of ionizing photons to counter-balance the recombination of ionized gas and free electrons in the IGM. One way of confirming this claim is via the observation of the ultra-violet luminosity function of the star forming galaxies at $z \approx 6$ (Stanway et al. 2003; Bouwens et al. 2004; Barkana & Loeb 2006; Bouwens et al. 2006, 2007, 2008; Castellano et al. 2010; Lorenzoni et al. 2013; Bouwens et al. 2014). These measurements provide an estimate of the star formation rates. However, it is still controversial whether the observed galaxy population at these redshifts is enough to keep our Universe ionized (Gnedin 2008; Yüksel et al. 2008; Pawlik et al. 2009). To fully address this problem, the uncertainties about the ionizing photon production rate per baryon and the escape fraction of ionizing photons have to be resolved (Srbinovsky & Wyithe 2010; Yajima et al. 2011; Mitra et al. 2013).

1.3.4 Hydrogen 21-cm Line

Another important observational probe of the EoR is the weak, low energy line transition in the neutral hydrogen associated with the relative spin directions of the proton and electron in the atom. When their spin directions change from parallel to antiparallel (spin-flip transition), a photon of wavelength 21 cm is emitted.

Neutral hydrogen atoms at high redshift will emit or absorb 21-cm photons. The large scale 21-cm background radiation emitted by the neutral hydrogen stores a wealth of information about the IGM during the EoR. The detection of these photons over a range of wavelengths on the entire sky in principle enables us to produce a three-dimensional 21-cm signal cube. Of the three dimensions, two correspond to the plane of the sky. The third one, parallel to the line of sight, is the temporal dimension represented by the observed wavelength of the redshifted 21-cm transition, as the light waves are stretched due to the cosmological expansion. Therefore the reionization history can be obtained from this time-axis.

In principle, the large scale (on scales between $\sim 15$ and 1000 comoving Mpc) 21-cm signal during the EoR can be detected by existing low-frequency
**Figure 1.2:** Top panel: The time-evolution of 21-cm brightness temperature fluctuations. The redshift range covers the dark ages (before the first stars has formed) to the end of the EoR. The blue and purple colors correspond to the 21-cm absorption (negative brightness temperature). The blue trough is a result of the decoupling of CMB photons and gas particles. Gas particles cool faster than the CMB photons, causing the spin temperature to drop below the CMB temperature. The purple trough is a result of the coupling of Ly$\alpha$ photons and gas particles. The Ly$\alpha$ temperature follows much the same as kinetic temperature which is less than the CMB temperature before the first stars have formed. Red color corresponds to 21-cm emission (positive brightness temperature). It happens when the bright sources begin to ionize and heat the IGM. The kinetic temperature becomes much higher than the CMB temperature and is the cause of the 21-cm emission. Bottom panel: The time-evolution of the spatially averaged 21-cm brightness temperature. Figure from Pritchard & Loeb (2010).
radio telescopes such as LOFAR\textsuperscript{1}, 21CMA\textsuperscript{2}, MWA\textsuperscript{3}, GMRT\textsuperscript{4} and PAPER\textsuperscript{5}. However, to date no detection has been achieved yet. The intensity of the detected signal is measured against the CMB signal and expressed in terms of the 21-cm brightness temperature $\delta T_b$ which depends on the neutral hydrogen density and the excitation or spin temperature $T_s$ of the neutral gas. The forthcoming telescope SKA\textsuperscript{6} is expected to have the sensitivity to image the 21-cm signal.

The 21-cm brightness temperature from the Cosmic Dawn and the Epoch of Reionization is a function of neutral hydrogen density, components of the gradient of the peculiar velocity parallel to the LOS and the relative population of the hydrogen atoms in the parallel spin direction, characterized by the spin temperature. The relation between them can be approximated by

$$
\delta T_b \approx 9x_{\text{HI}}(1 + \delta)\sqrt{1+z} \left[ 1 - \frac{T_{\text{CMB}}}{T_s} \right] \left[ \frac{H(z)/(1+z)}{dv/|dr|} \right] \text{mK},
$$

where $x_{\text{HI}}$ and $\delta$ are the neutral fraction of hydrogen and the overdensity of matter. The spin-temperature $T_s$ determines the relative abundance of the hydrogen atom in two different spin states,

$$
\frac{n_1}{n_0} = \left( \frac{g_1}{g_0} \right) \exp(-T_*/T_s),
$$

where $n_1$ and $n_0$ are the number density of hydrogen atoms with parallel spin direction and anti-parallel spin direction. $g_1 = 3$ and $g_0 = 1$ are their statistical weights and $T_* = 0.068 \text{ K}$ is the temperature corresponding to the 21-cm transition.

As shown by Equation 1.4, the value of the spin temperature determines whether the signal is seen in absorption ($T_s < T_{\text{CMB}}$) or in emission ($T_s > T_{\text{CMB}}$) against the CMB. The spin temperature is determined by a competition between different processes (see Pritchard & Loeb 2012, for a review). For high redshifts ($z > 30$) the densities are high enough for collisional excitation to dominate and $T_s$ will be given by the gas temperature. Since this is lower than $T_{\text{CMB}}$, the signal will be in absorption. Once collisions become inefficient, CMB photons dominate the excitation and the spin temperature becomes equal to $T_{\text{CMB}}$ which means that the signal disappears. This changes as soon as star

\textsuperscript{1}http://www.lofar.org
\textsuperscript{2}http://cosmo.bao.ac.cn/
\textsuperscript{3}http://www.haystack.mit.edu/ast/arrays/mwa
\textsuperscript{4}http://gmrt.ncra.tifr.res.in
\textsuperscript{5}http://astro.berkeley.edu/dbacker/eor/
\textsuperscript{6}http://skatelescope.org
formation produces sufficient amounts of non-ionizing UV photons which can redshift into the Ly\(\alpha\) transition. Due to their frequent scattering with neutral hydrogen atoms, these photons acquire an energy distribution characterized by the gas temperature and through the Wouthuysen-Field effect the spin temperature also acquires this value. As long as the IGM is unheated this implies an absorption signal but heating by early X-ray sources can cause the signal to show up in emission. See Figure 1.2 for an illustration of this evolution of the 21cm signal.

A wealth of cosmological and astrophysical information can in principle be extracted from the 21-cm signal. For example, the cosmological parameters which affect the matter density fluctuations in the EoR. Since the 21-cm brightness temperature is capable of constraining these fluctuations on different length scales, constraints on the cosmological parameters can thus be derived. In addition, the ionizing source properties are reflected in their induced hydrogen ionization patterns and thus in the 21-cm signal from the patchy neutral regions from the EoR. Figure 1.2 illustrates the time-evolution of 21-cm brightness temperature from a reionization model by Pritchard & Loeb (2012). The mean brightness temperature evolution relies on several important physical processes, such as the time instance of the ionization led by the first stars and their imposed ionization and heating onto the hydrogen gas. Properties of the first stars can thus be extracted from the 21-cm maps through careful analysis.

### 1.3.5 Direct Temperature Measurement in Quasar Near Zones

Bright quasars produce highly ionized regions around themselves which are called quasar near zones. These show up in quasar spectra as regions of low Ly\(\alpha\) absorption just blueward of the quasar Ly\(\alpha\) line. In the previous decade, the sizes of these zones were used to examine the ionization state of the IGM. The analysis modeled the scope and shape of the observed transmission to obtain a constraint of ionization state at \(z \approx 6\) (Fan et al. 2006, Mesinger & Haiman 2007, Alvarez & Abel 2007, Bolton & Haehnelt 2007, Wyithe et al. 2008, Maselli et al. 2009b).

As the spectra of quasar near zones show absorption lines caused by denser structures along the line of sight, it is possible to measure the temperature of the gas from the thermal broadening of these lines. Such measurements were first performed by Bolton et al. (2010) who attempted to directly measure the IGM temperature close to the quasar SDSS J0818+1722 (\(z = 6.02\)). Later, Bolton et al. (2012) applied the same method to seven quasars (\(z \approx 6\)) to improve the temperature measurements. Both used radiative transfer simulations to compute synthetic quasar spectra. These papers concluded that the thermal
state at $z \approx 6$ is $\log(T/K) = 4.21 \pm 0.03 \pm 0.06$ at 68(95) percent confidence.

1.4 From observations to astrophysics

These various observational probes measure specific properties of the intergalactic gas such as the ionization fraction or the temperature. However, these properties do not directly inform us about the physical processes that caused them. For example, the nature of the sources of reionization does not directly follow from the the distribution of the 21cm signal. In order to interpret the observations in terms of astrophysical processes we need to simulate these processes and compare the results of these simulations to the observations.

The most important processes to simulate for reionization are the photoionization and photoheating of the IGM. For this we need methods which give the local intensity of the radiation field, or in other words methods which solve the radiative transfer equation. In Chapter 3 we outline several existing radiative transfer methods. This description puts into perspective the new radiative transfer method (PYRAMID) described in Paper II.

Once the radiative transfer has provided the local intensity of the radiation field, we can derive the time evolution of the ionization fraction and the temperature by solving the coupled ionization and thermal equations. In Chapter 4 we describe some standard solvers for the ionization and thermal equations. The performance of these solvers are analyzed and compared in Paper III.

However, we start with a description of one specific radiative transfer and time-dependent photoionization code, namely $C^2$-RAY. This code is the subject of Paper I where we introduce two improvements necessary to accurate calculate the photoheating rates. Chapter 2 describes the $C^2$-RAY code in some more detail which helps to put Paper I into perspective.
2. C²-RAY - A cosmological radiative transfer code

C²-RAY (Mellema et al. 2006) is a cosmological radiative transfer code for photoionizing radiation which has been used extensively for reionization simulations (e.g., Iliev et al. 2006b; Datta et al. 2012; Iliev et al. 2011, 2014). It uses a short characteristics method to calculate the transfer of ionizing photons (See Chapter 3 and the C2R method to solve the photo-equations (See Chapter 4).

Friedrich et al. (2012) described an improved version of C²-RAY. This version includes multifrequency radiative transfer and the treatment of helium. However, Friedrich et al. (2012) showed that in order to achieve an accurate result for the photoheating calculation, a strict time-step limit has to be chosen which has a negative impact on the code performance. In Paper I (Lee et al. 2016) we have introduced two new methods to obtain accurate photoheating results in an efficient manner. The first method uses an adaptive time-step algorithm which calculates an optimal time-step considering only the relevant cells. The second method uses asynchronous evolution which allows different cells to evolve with different time-steps. We refer readers to Paper I for a detailed discussion of these methods.

This chapter serves to introduce the key aspects of C²-RAY for a better understanding of the code.

2.1 Numerical radiative transfer

C²-RAY is implemented on a three-dimensional Cartesian grid. The grid cells contain information on the number density of gas \( n \), the ionization fractions \( x_{\text{HI}}, x_{\text{HII}}, x_{\text{HeI}}, x_{\text{HeII}}, x_{\text{HeIII}} \) and the gas temperature \( T \). The cosmological radiative transfer equation is for example given by Norman et al. (1998),

\[
\frac{1}{c} \frac{dI_\nu}{dt} + \frac{\hat{n} \cdot \nabla I_\nu}{\bar{a}} - \frac{H(t)}{c} \left( \nu \frac{dI_\nu}{d\nu} - 3I_\nu \right) = j_\nu - \kappa_{\nu}^{\text{abs}} I_\nu.
\]

This equation takes into account the finite speed of light as well as cosmological redshifting due to the expansion of the Universe. In this equation, \( c \) is the
speed of light, $I_ν$ is the specific light intensity which is a function of frequency $ν$, $\hat{n}$ is the unit vector pointing in the propagation direction, $a$ is the cosmological scale factor, $H(t) \equiv \dot{a}/a$ is the Hubble parameter at time $t$, $\bar{a} \equiv \frac{1+z_{\text{em}}}{1+z}$ is the ratio of scale factors between the redshift of photon emission $z_{\text{em}}$ and the redshift which is being considered, $\bar{z}$. Finally, $j_ν$ is the emission coefficient and $κ^\text{abs}_ν$ is the absorption coefficient.

By assuming that the ionizing photon mean free path is much smaller than $c\Delta t$ where $\Delta t$ is the time step, and that any ionizing recombination radiation produced by the gas is all absorbed locally, Equation 2.1 can be simplified to

$$\hat{n} \cdot \nabla I_ν = -κ^\text{abs}_ν I_ν.$$  \hspace{1cm} (2.2)

The formal solution of Equation 2.2 is

$$I_ν = I_{0,ν} e^{-τ_ν},$$  \hspace{1cm} (2.3)

where $τ_ν$ is the frequency dependent optical depth due to neutral hydrogen. This is the equation which $C^2$-RAY solves.

$C^2$-RAY uses the short characteristics method, which is a ray-tracing method, to calculate the optical depths between the sources to the cells. The short characteristics method is further explained in Section 3.2. The optical depth values are then used to calculate the photoionization and photoheating rates as we explain in the next Section.

### 2.2 Photoionization and Photoheating rate calculation

After we have calculated the optical depths between a source and the cells, we know the rate at which ionizing photons enter and leave all cells. The difference between the incoming and outgoing rates is the ionizing photon absorption rate which is used to calculate photoionization rates $Γ_{\text{HI}}$, $Γ_{\text{HeI}}$, $Γ_{\text{HeII}}$ and photoheating rate $\mathcal{H}$. In the following, we use the parameter $i$ to denote the species (HI, HeI and HeII) and parameter $j$ to denote the photon frequency bin (the frequency domain is partitioned into 47 frequency bins). If we define $G^\text{total}_j$ to be the total ionization event rate per volume induced by the photons in frequency bin $j$, then

$$G^\text{total}_j = \frac{G_j(τ^\text{in}) - G_j(τ^\text{out})}{V_{\text{shell}}},$$  \hspace{1cm} (2.4)

where $V_{\text{shell}}$ is the volume of the spherical shell of which inner radius and outer radius coincide with the entrance and exit positions of the ray through the cell. The function $G_j(τ^\text{total})$ is defined by

$$G_j(τ^\text{total}) = \int_{ν_j}^{ν_j+1} \frac{L_ν}{hν} e^{-τ^\text{total}(ν)} dν,$$  \hspace{1cm} (2.5)
where $\tau_{\text{total}}(v) = \tau_{\text{HI}}(v) + \tau_{\text{HeI}}(v) + \tau_{\text{HeII}}(v)$ is the combined optical depth contributed by all absorbing species at frequency $v$, $L_v$ is the source luminosity and $h$ is the Planck constant. We approximate $\tau_{\text{total}}(v)$ by

$$\tau_{\text{total}}(v) = \tau_{\text{total}}^j \left( \frac{v}{v_j} \right)^{-\eta_j}. \quad \text{(2.6)}$$

which implies that $\tau_{\text{HI}}(v)$, $\tau_{\text{HI}}^j(v)$ and $\tau_{\text{HI}}(v)$ use the same power law index $\eta_j$ within frequency bin $j$ (Friedrich et al. 2012). The advantage of this approximation is that the value of $G_j$ is only controlled by one parameter, namely $\tau_{\text{total}}^j \equiv \tau_{\text{total}}(v_j)$. We can therefore pre-calculate the values $G_j$ for a large range of values for $\tau_{\text{total}}^j$ and the rates can be found through interpolation of these values. This way we avoid repeated evaluations of the expensive full photo-ionization integrals.

In frequency bin $j$, the photoionization rate $\Gamma^i_j$ for species $i$ is calculated using $S_j^{\text{total}}$ through

$$\Gamma^i_j = \frac{\tau^i_{\text{total}} j}{\tau^i_{\text{total}}} \frac{S_j^{\text{total}}}{n_i} . \quad \text{(2.7)}$$

Dividing by the number density $n_i$ changes the unit of photoionization rates from per volume to per particle. The ratio $\tau_{\text{total}}^i / \tau_{\text{total}}^j$ accounts for a correct distribution of the photo-ionization rates over the different species. The total photoionization rate $\Gamma^i$ of species $i$ is then found by summing over all relevant frequency bins,

$$\Gamma^i = \sum_j \Gamma^i_j. \quad \text{(2.8)}$$

The photoheating rate $\mathcal{H}$ is calculated in a similar way. The function $\mathcal{H}_j^i$ is defined as the rate of energy injected by photons in frequency bin $j$ to species $i$ per unit volume,

$$\mathcal{H}_j^i = \frac{H_j^i(\tau_{\text{total}}^\text{in}) - H_j^i(\tau_{\text{total}}^\text{out})}{V_{\text{shell}}}. \quad \text{(2.9)}$$

The function $H_j^i(\tau_{\text{total}})$ is given by

$$H_j^i(\tau_{\text{total}}) = \begin{cases} \int_{v_j}^{v_j+1} h(v - v_i) \frac{L_v}{h v} e^{-\tau_{\text{total}}(v)} d\nu & \text{if } v_j \geq v_i \\ 0 & \text{if } v_j < v_i \end{cases},$$

where $v_i$ is the ionization threshold frequency of species $i$. The $h(v - v_i)$ term forces us to calculate the values $H_j^i$ separately for each species. Similar to the photoionization rates, we pre-calculate each of these heating integrals $\mathcal{H}_j^i$ for a large range of values for $\tau_{\text{total}}^j$. The photoheating rate $\mathcal{H}_j$ in $j$th frequency bin
is the weighted sum of $\mathcal{H}_j$'s,

$$\mathcal{H}_j = \sum_{i=1}^{3} \frac{\tau_j^i}{\tau^\text{total}_j} \mathcal{H}_j^i,$$

(2.10)

where we use the same weighting factors as in Equation 2.7 for the correct distribution among the three photon-absorbing species. Finally, the total photoheating rate $\mathcal{H}$ is simply the sum over all frequencies

$$\mathcal{H} = \sum_j \mathcal{H}_j,$$

(2.11)

The free electrons produced by the ionization of species $i$ receive an energy $h(\nu - \nu_i)$. They collide with other particles (hydrogen, helium and electrons) and thermalize with them. As a result, the gas is heated. If the liberated electrons are energetic enough, they are capable of further ionizing HI, HeI and HeII. This process is known as secondary ionizations. How the kinetic energy of the free electrons is distributed over thermalization and secondary ionizations depends on the relative cross sections and the densities. We use the approximation from Ricotti et al. (2002) to calculate this.

2.3 Recombination processes

In any ionized gas recombinations will take place. To calculate the evolution of the ionized fractions therefore requires including the recombination rates. The hydrogen recombination rates $\alpha_{\text{HII}}^A$ and $\alpha_{\text{HII}}^B$ and the helium recombination rates $\alpha_{\text{HeIII}}^A$ and $\alpha_{\text{HeIII}}^B$ are functions of temperature (Hui & Gnedin 1997). The helium recombination rates $\alpha_{\text{HeII}}^A$ and $\alpha_{\text{HeII}}^B$ are more complicated because dielectronic recombination dominates when the temperature is above $7 \times 10^4$ K. We use the fitting formula from Aldrovandi & Pequignot (1973) for $T > 9 \times 10^3$ K and fitting formula from Hui & Gnedin (1997) for $T \leq 9 \times 10^3$ K. In addition, the helium recombination rate to the first excited level, $\alpha_{\text{HeIII}}^2$, follows from the result of Osterbrock & Ferland (2006). We list the fits we use for the recombination rates below.

The recombination rates of HI are

$$\alpha_{\text{HII}}^A = 1.269 \times 10^{-13} \frac{(315608/T)^{1.503}}{[1 + (604613/T)^{0.470}]^{1.923}}$$

(2.12)

$$\alpha_{\text{HII}}^B = 2.753 \times 10^{-14} \frac{(315608/T)^{1.500}}{[1 + (115185/T)^{0.407}]^{2.242}}.$$  

(2.13)
The recombination rates of HeII ($T < 9 \times 10^3$) are

$$\alpha_{\text{HeII}}^A = 1.269 \times 10^{-13} \frac{(570662/T)^{1.503}}{[1 + (1093222/T)^{0.470}]^{1.923}}$$

$$\alpha_{\text{HeII}}^B = 2.753 \times 10^{-14} \frac{(570662/T)^{1.500}}{[1 + (208271/T)^{0.407}]^{2.242}}.$$ (2.14, 2.15)

The recombination rates of HeII ($T \geq 9 \times 10^3$) are

$$\alpha_{\text{HeII}}^A = 3 \times 10^{-14} \left(\frac{570662}{T}\right)^{0.654}$$

$$+ 1.9 \times 10^{-3} T^{-1.5} \exp\left(-\frac{4.7 \times 10^5}{T}\right)$$

$$\times [1 + 0.3 \exp\left(-\frac{9.4 \times 10^4}{T}\right)].$$

$$\alpha_{\text{HeII}}^B = 1.260 \times 10^{-14} \left(\frac{570662}{T}\right)^{0.750}$$

$$+ 1.9 \times 10^{-3} T^{-1.5} \exp\left(-\frac{4.7 \times 10^5}{T}\right)$$

$$\times [1 + 0.3 \exp\left(-\frac{9.4 \times 10^4}{T}\right)].$$ (2.16, 2.17)

The recombination rates of HeIII are

$$\alpha_{\text{HeIII}}^A = 2.538 \times 10^{-13} \frac{(1262990/T)^{1.503}}{[1 + (2419521/T)^{1.923}]^{1.923}},$$

$$\alpha_{\text{HeIII}}^B = 5.506 \times 10^{-14} \frac{(1262990/T)^{1.500}}{[1 + (460945/T)^{0.407}]^{2.242}},$$

$$\alpha_{\text{HeIII}}^2 = 8.540 \times 10^{-11} T^{-0.6}.$$ (2.18, 2.19, 2.20)

Recombination events produce at least one photon. The energy of the emitted photon depends on which electronic state the electron recombines to. Some of these recombination photons are energetic enough to ionize another atom or ion and should therefore be considered in the calculation of the ionization fractions. In principle this means that every ionized cell becomes a source of ionizing photons which can substantially complicate the radiative transfer calculation. An often used approximation is that these ionizing recombination photons are absorbed locally inside the region defined by the computational cell. This is known as the On The Spot (OTS) approximation. For example when in HII recombination the absorbed electron goes directly to ground state, an HI ionizing photon is emitted. Its rate is controlled by the recombination coefficient $\alpha_{\text{HII}}^1$. In the OTS approximation these photons are used to ionize...
the local HI atoms which means effectively that recombinations to the ground state are not considered. Since $\alpha_{\text{HI}}^B = \alpha_{\text{HI}}^A - \alpha_{\text{HI}}^1$, this can be implemented by using $\alpha_{\text{HI}}^B$ to calculate the HII recombination rates.

The situation becomes more complicated when helium is present. Photons from recombinations of HeII and HeIII can lead to ionization of HI, HeI and HeII. For HeII, recombination to the ground state (with recombination coefficient $\alpha_{\text{HeII}}^1$) results in a photon which can ionize both HI and HeI. In the OTS approximation a fraction $y$ of these photons will ionize HI while a fraction $1-y$ of these photons will ionize HeI. $y$ is determined by the fraction of relative optical depth of HI at the HeI ionization threshold frequency.

The recombination of HeII to other states emits photons which are not energetic enough to ionize HeI but a fraction $p$ of them can ionize HI. The fraction $p$ is determined by the electron density and critical electron density (Osterbrock & Ferland 2006). In a cosmological application, the electron density is always much smaller than the critical electron density and thus $p$ converges to 0.96.

The recombination of HeIII to the ground state (with recombination coefficient $\alpha_{\text{HeIII}}^1$) emits photons which can ionize HI, HeI and HeII. In the OTS approximation a fraction $y_a^2$ of these ionize HI, a fraction $y_b^2$ of these ionize HeI and a fraction $1-y_a^2-y_b^2$ of these ionize HeII. $y_a^2$ and $y_b^2$ are determined by the relative optical depths of HI and HeI at the HeII ionization threshold frequency.

The recombination of HeIII to the first excited state (with recombination coefficient $\alpha_{\text{HeIII}}^2$) produces a photon (HeII Balmer continuum photon) above the hydrogen ionization threshold. Therefore only local HI atoms absorb these photons.

The recombination of HeIII to any excited state (with recombination coefficient $\alpha_{\text{HeIII}}^B$) would eventually cascade to ground state with photon emission which are energetic enough to ionize both HI and HeI. A fraction $\nu$ of these leads to two-photon emission and a fraction $1-\nu$ of these leads to HeII Lyman-$\alpha$ emission. Here $\nu = 0.285(T/10^4)^{0.119}$ is a temperature-dependent parameter (Hummer & Seaton 1964). From the two-photon emission, $l = 1.425$ photons are energetic enough to ionize HI and $m = 0.737$ photons are energetic to ionize HeI. Therefore, for each two-photon emission, $(l-m+my)$ photons ionize HI and $m(1-y)$ photons ionize HeI. The HeII Lyman-$\alpha$ photons have a probability $(1-f)$ to escape without being absorbed locally, where $f$ depends on $x_{\text{HI}}$. A fraction $f$ of HeII Lyman-$\alpha$ photons are absorbed by both HI and HeI. A fraction $z$ of which ionize HI and a fraction $1-z$ of which ionize HeI. The factor $z$ is determined by the relative optical depth of HI and HeI at the HeII Lyman-$\alpha$ frequency.

The code contains this full version of the OTS approximation. This causes
the ionization equations of HI, HeI and HeII to be coupled. This complicates the solution of these equations, see Section 2.6 below.

2.4 Collisional ionization process

We also include collisional ionization in the ionization equations. Collisional ionization is the process in which free, thermalized electrons are energetic enough to collide and knock out bound electrons and therefore ionize the atoms/ions. Typically, collisional ionization only becomes important at temperatures above $20 \times 10^4$ K which means that they are rarely very important for pure photoionization cases. However, when coupled to hydrodynamics, they may become important.

We use the collisional photo-ionization rates fitted by Hui & Gnedin (1997), Janev et al. (1987) and Cox (1970).

$$C_{\text{HI}} = 5.835 \times 10^{-11} \sqrt{T_e} e^{-157804/T}$$ (2.21)

$$C_{\text{HeI}} = 2.710 \times 10^{-11} \sqrt{T_e} e^{-285331/T}$$ (2.22)

$$C_{\text{HeII}} = 5.707 \times 10^{-12} \sqrt{T_e} e^{-631495/T}$$ (2.23)

2.5 Cooling process

We include several cooling processes in the thermal equation. They are free-free and recombination coolings for species HII, HeIII (Hummer 1994), and HeII (Hummer & Storey 1998), collisional excitation cooling for HI (Aggarwal 1983), collisional ionization cooling for HeI (Hui & Gnedin 1997), collisional excitation, collisional ionization and dielectronic recombination cooling for HeII (Hui & Gnedin 1997). In cosmological simulations we also include Compton cooling with the cosmological microwave background radiation (Shapiro & Kang 1987) and adiabatic cooling due to the expansion of the Universe.

2.6 Solving Ionization and Thermal Equation

In this section we explain how we solve the set of photo-equations – three ionization equations and one thermal equation. The three ionization equations determine the evolution of the ionization fractions $x_{\text{HII}}$, $x_{\text{HeII}}$ and $x_{\text{HeIII}}$. We present the ionization equations in matrix form,

$$\frac{d}{dt} x = Ax + g$$ (2.24)
where

\[ x = \begin{pmatrix} x_{\text{HI}} \\ x_{\text{HeI}} \\ x_{\text{HeII}} \end{pmatrix}, \quad g = \begin{pmatrix} U_{\text{HI}} \\ U_{\text{HeI}} \\ 0 \end{pmatrix}, \quad \text{and} \]

\[
A = \begin{pmatrix}
-U_{\text{HI}} + R_{\text{HI}} \rightarrow \text{HeI} n_e & n_{\text{He}} R_{\text{HeII}} \rightarrow \text{HeI} n_e & n_{\text{He}} R_{\text{HeIII}} \rightarrow \text{HeI} n_e \\
0 & -U_{\text{HeI}} - U_{\text{HeII}} & -U_{\text{HeI}} + R_{\text{HeII}} \rightarrow \text{HeI} n_e \\
0 & U_{\text{HeI}} & R_{\text{HeIII}} \rightarrow \text{HeI} n_e
\end{pmatrix}
\]  

(2.26)

We explain our notation below.

\(U_i\) is the photo-ionization rate of species \(i\)

\[
U_{\text{HI}} = \Gamma_{\text{HI}} + C_{\text{HI}} n_e
\]  

(2.27)

\[
U_{\text{HeI}} = \Gamma_{\text{HeI}} + C_{\text{HeI}} n_e
\]  

(2.28)

\[
U_{\text{HeII}} = \Gamma_{\text{HeII}} + C_{\text{HeII}} n_e
\]  

(2.29)

and \(R_{i \rightarrow j}\) is the effective recombination rate corresponding to the ionization of the species \(j\) by recombination of species \(i\) using the OTS approximation explained in Section 2.3.

\[
R_{\text{HI}} \rightarrow \text{HeI} = -\alpha_{\text{HI}}^B
\]  

(2.30)

\[
R_{\text{HeII}} \rightarrow \text{HeI} = p \alpha_{\text{HeII}}^B + y \alpha_{\text{HeII}}^A
\]  

(2.31)

\[
R_{\text{HeII}} \rightarrow \text{HeI} = (1 - y) \alpha_{\text{HeII}}^A - \alpha_{\text{HeII}}^A
\]  

(2.32)

\[
R_{\text{HeIII}} \rightarrow \text{HeI} = (1 - y_a^2 - y_b^2) \alpha_{\text{HeIII}}^A + \alpha_{\text{HeIII}}^B
\]

\[+ [v(l - m + my) + (1 - v)fz] \alpha_{\text{HeIII}}^B
\]  

(2.33)

\[
R_{\text{HeIII}} \rightarrow \text{HeI} = y_b^2 \alpha_{\text{HeII}}^A + [vm(1 - y) + (1 - v)f(1 - z)] \alpha_{\text{HeIII}}^B
\]

\[+ \alpha_{\text{HeIII}}^A - y_a^2 \alpha_{\text{HeIII}}^A
\]

\[
R_{\text{HeIII}} \rightarrow \text{HeI} = y_a^2 \alpha_{\text{HeIII}}^A - \alpha_{\text{HeIII}}^A.
\]  

(2.34)

(2.35)

The thermal equation calculates the thermal evolution of the gas. We assume it follows the ideal gas law so that the internal energy density is proportional to the temperature,

\[
u = \frac{3}{2} k_B T (n_{\text{H}} + n_{\text{He}} + n_e).
\]  

(2.36)
The internal energy density \( u \) is subject to change by the heating and cooling processes. The thermal equation becomes

\[
\frac{du}{dt} = \mathcal{H} - C.
\]  

(2.37)

The four photo-equations are coupled due to the fact that the individual terms are non-trivial functions of both the ionization fractions and the temperature. The \( n_e \), \( \Gamma \)'s and \( \mathcal{H} \) are function of \( x_{\text{HI}}, x_{\text{HII}}, x_{\text{HeI}}, x_{\text{HeII}} \) and \( x_{\text{HeIII}} \). \( C_i \)'s, \( R_{i\rightarrow j} \) and \( C \) are functions of \( T \).

A numerical method is required to solve these coupled equations. We consider a time \( t \) and a time-step \( \Delta t \) and evolve the ionization fractions and thermal state to time \( t + \Delta t \). When we assume that the matrices \( \mathbf{A} \) and \( \mathbf{g} \) do not change during the time interval \( \Delta t \), it is possible to derive an analytical solution for the ionization equations [Friedrich et al. 2012]. This is not possible for the thermal equation which is instead solved using a first order Runge-Kutta method.

The key assumption of \( C^2\) Ray is that the matrices \( \mathbf{A} \) and \( \mathbf{g} \) should be evaluated for the time-averaged values of the ionization fractions and temperature. These depend of course on the solution we are trying to find which means that an iterative procedure is needed to find them. The time averaged value of a time-dependent parameter \( f \) is defined by

\[
\langle f \rangle = \frac{1}{\Delta t} \int_t^{t+\Delta t} f(t') \, dt'.
\]  

(2.38)

This integral can be evaluated because we have the analytical solutions for the ionization equations.

For the hydrogen only case, the analytical solution is quite simple and can be found in [Mellema et al. 2006]. When including helium and using the full version of the OTS approximation the expressions become substantially more complicated. The full analytical solutions of the ionization equations in this case are

\[
x_{\text{HII}}(t + \Delta t) = b_{11}c_1e^{\lambda_{1t}} + b_{12}c_2e^{\lambda_{2t}} + b_{13}c_3e^{\lambda_{3t}} + p_1,
\]  

(2.39)

\[
x_{\text{HeII}}(t + \Delta t) = b_{21}c_1e^{\lambda_{1t}} + b_{22}c_2e^{\lambda_{2t}} + b_{23}c_3e^{\lambda_{3t}} + p_2,
\]  

(2.40)

\[
x_{\text{HeIII}}(t + \Delta t) = b_{31}c_1e^{\lambda_{1t}} + b_{32}c_2e^{\lambda_{2t}} + b_{33}c_3e^{\lambda_{3t}} + p_3.
\]  

(2.41)

For the initial condition \( x_{\text{HII}}(0), x_{\text{HeII}}(0) \) and \( x_{\text{HeIII}}(0) \), we use coefficients \( S, K, R \) and \( T \) to define the above variables.

\[
S = \sqrt{A_{33}^2 - 2A_{33}A_{22} + A_{22}^2 + 4A_{32}A_{23}},
\]  

(2.42)

\[
K = 1/(A_{23}A_{32} - A_{33}A_{22}),
\]  

(2.43)
\[ R = 2A_{23}[A_{33}g_2 K - x_{\text{HeII}}(0)], \quad (2.44) \]
\[ T = -A_{32}g_2 K - x_{\text{HeIII}}(0). \quad (2.45) \]

The \( \lambda_i \)'s are given by
\[ \lambda_1 = A_{11}, \quad (2.46) \]
\[ \lambda_2 = 0.5(A_{33} + A_{22} - S), \quad (2.47) \]
\[ \lambda_3 = 0.5(A_{33} + A_{22} + S). \quad (2.48) \]

\( p_i \)'s are given by
\[ p_1 = -\frac{1}{A_{11}}[g_1 + (A_{33}A_{12} - A_{32}A_{13})g_2 K], \quad (2.49) \]
\[ p_2 = A_{33}g_2 K, \quad (2.50) \]
\[ p_3 = -A_{32}g_2 K. \quad (2.51) \]

\( B_{ij} \)'s are given by
\[ B_{11} = 1, \quad (2.52) \]
\[ B_{12} = \frac{-2A_{32}A_{13} + A_{12}(A_{33} - A_{22} + S)}{2A_{32}(A_{11} - \lambda_2)}, \quad (2.53) \]
\[ B_{13} = \frac{-2A_{32}A_{13} + A_{12}(A_{33} - A_{22} - S)}{2A_{32}(A_{11} - \lambda_3)}, \quad (2.54) \]
\[ B_{21} = 0, \quad (2.55) \]
\[ B_{22} = \frac{-A_{33} + A_{22} - S}{2A_{32}}, \quad (2.56) \]
\[ B_{23} = \frac{-A_{33} + A_{22} + S}{2A_{32}}, \quad (2.57) \]
\[ B_{31} = 0, \quad (2.58) \]
\[ B_{32} = 1, \quad (2.59) \]
\[ B_{33} = 1. \quad (2.60) \]

\( c_i \)'s are given by
\[ c_1 = \frac{2p_1 S - \left[R + (A_{33} - A_{22})T\right][A_{21} - A_{31}]}{2S} + x_{\text{HeII}}(0) + \frac{T}{2}[A_{21} + A_{31}], \quad (2.61) \]
\[ c_2 = \frac{R + (A_{33} - A_{22} - S)T}{2S}, \quad (2.62) \]
\[ c_3 = - \frac{R + (A_{33} - A_{22})S}{2S}. \]  

(2.63)

The method produces the solutions at time \( t + \Delta t \) and also the time-averaged ionization fractions \( \langle x_{\text{HI}} \rangle, \langle x_{\text{HII}} \rangle, \langle x_{\text{HeI}} \rangle, \langle x_{\text{HeII}} \rangle \) and \( \langle x_{\text{HeIII}} \rangle \). Their analytical expressions are

\[ \langle x_{\text{HI}} \rangle = 1 - \langle x_{\text{HII}} \rangle \]  

(2.64)

\[ \langle x_{\text{HII}} \rangle = b_{11} c_1 \left( e^{\lambda_1 \Delta t} - 1 \right) + b_{12} c_2 \left( e^{\lambda_2 \Delta t} - 1 \right) + b_{13} c_3 \left( e^{\lambda_3 \Delta t} - 1 \right) \]  

(2.65)

\[ \langle x_{\text{HeI}} \rangle = 1 - \langle x_{\text{HeII}} \rangle - \langle x_{\text{HeIII}} \rangle \]  

(2.66)

\[ \langle x_{\text{HeII}} \rangle = b_{21} c_1 \left( e^{\lambda_1 \Delta t} - 1 \right) + b_{22} c_2 \left( e^{\lambda_2 \Delta t} - 1 \right) + b_{23} c_3 \left( e^{\lambda_3 \Delta t} - 1 \right) \]  

(2.67)

\[ \langle x_{\text{HeIII}} \rangle = b_{31} c_1 \left( e^{\lambda_1 \Delta t} - 1 \right) + b_{32} c_2 \left( e^{\lambda_2 \Delta t} - 1 \right) + b_{33} c_3 \left( e^{\lambda_3 \Delta t} - 1 \right) \]  

(2.68)

As described above, we use a first order Runge-Kutta method to solve the heating equation. The heating rate is taken to be constant during the time-step and is based on the time-averaged values of the ionization fractions. The cooling rate is however a rapidly varying function of the temperature. This forces us to use small sub-time-steps. We begin from the initial energy density \( u_0 = u(t) \) and proceed by a short sub-time-step to the next solution point. The sub-time-steps \( \Delta t_i \) are calculated before we proceed to the \( i \)th steps. The process stops when \( \Delta t = \sum_{i=1}^{n} \Delta t_i \). In each sub-time-step, intermediate solutions \( u_i \) and hence \( T_i \) are derived by

\[ u_i = \frac{3}{2} k_B T_i (n_H + n_e). \]  

(2.69)

\( T_i \) is then used to update the cooling rate \( C_i \). The sub-time-step of the \( i \)th step depends on the results of the previous step.

\[ \Delta t_i = f_{\text{thermal}} u_{i-1} / |\mathcal{H} - C_{i-1}|, \]  

(2.70)

where \( f_{\text{thermal}} \) is the maximum relative change in the energy density which we take to be 10%.

The temperature solution \( T_n = T(t + \Delta t) \) is then given by

\[ T(t + \Delta t) = \frac{2}{3k_B(n_H + n_e)} \left( u_0 + \sum_{i=1}^{n} (\mathcal{H} - C(T_{i-1})) \Delta t_i \right) \]  

(2.71)

and the time averaged temperature \( \langle T \rangle \) is

\[ \langle T \rangle = \frac{2}{3k_B(n_H + n_e)} \left( u_0 + \sum_{i=1}^{n} (\mathcal{H} - C(T_{i-1})) \Delta t_i^2 / \Delta t \right). \]  

(2.72)
2.7 Performance

$C^2$-RAY was extensively tested against analytical solution as well as against numerical solutions from other codes. The original paper describing $C^2$-RAY, Mellema et al. (2006), showed for a range of challenging photoionization problems that the method accurately calculates the growth of ionizing regions even when time-steps much larger than the ionization time were chosen. This property makes $C^2$-RAY a very efficient method for time-dependent photoionization calculations since it allows large time-steps with minimal loss of accuracy.

The code also participated in the Cosmological Radiative Transfer Comparison Project and showed excellent consistency with other codes when comparing ionization fractions and growth of ionized regions both in the photoionization tests (Iliev et al. 2006a) and in the tests with hydrodynamics (Iliev et al. 2009). However, careful consideration of the temperature results in Iliev et al. (2006a) for example, does reveal some discrepancies with other codes, made less obvious by the fact that the participating codes displayed a much larger spread in temperature results than in ionization results.

Also the updates version including helium was tested (Friedrich et al. 2012) although the lack of both analytical solutions and numerical benchmark results made thorough tests difficult, leaving only comparison to the photoionization equilibrium code CLOUDY as an option (Ferland et al. 2013). Friedrich et al. (2012) first showed the dependency of the heating rate on the choice of the time-step which motivated the development of the changes described in Paper I.
3. Radiative Transfer Methods

In this chapter, we summarize some radiative transfer methods commonly used in cosmological radiative transfer codes. In Chapter 2, we saw that the solution of the simplified radiative transfer equation is

\[ I_\nu = I_{0,\nu}e^{-\tau_\nu}. \]  

(3.1)

This simplified solution has greatly helped the numerical implementation of some radiative transfer codes as the problem can be reduced to finding the optical depth between the source and the target position. This optical depth needs to be calculated from the discretized gas information in the finite-sized computational cells. In this chapter we summarize some existing radiative transfer methods as well as our newly devised method - PYRAMID method.

3.1 Long characteristics method

The long characteristics method (Amanatides & Woo 1987) applies onto a Cartesian grid composed of rectangular cells (not necessarily cubic cells). The optical depth between the source cell and a target cell (which is not the source cell) depends on optical depths of cells which lie in between these two cells. The problem becomes identifying which cells lie in between and finding out their contribution to the source-target optical depth. This can be achieved by casting a ray from the source cell to the target cell. By tracing the trajectory of the ray, cells traversed by the ray can be identified and the intersection lengths of the ray and the traversed cells are then calculated. The left panel of Figure 3.1 illustrates the ray-tracing idea in the long characteristics method. The optical depth of each individual traversed cell, which depend on the intersection lengths, contributes cumulatively to the source-target optical depth. The source-target optical depth \( \tau \) is thus given by

\[ \tau = \sum_{i \in J} \sigma l_i n_i, \]  

(3.2)

where \( J \) is the index set of the traversed cells, \( \sigma \) is the ionization cross section, \( l_i \) is the intersection length of the ray and cell \( i \) and \( n_i \) are the number density of gas particles of the cell \( i \). The long characteristics method is very accurate
as Equation 3.2 gives the exact solution of the source-target optical depth assuming that each cell has a uniform density. However, the drawback of this method is that it is computationally expensive. The cells closer to the source are repeatedly traversed by rays which introduces redundant calculations.

3.2 Short characteristics method

A faster method was proposed by Kunasz & Auer (1988), namely, the short characteristics method. This method is more efficient than the long characteristics method while still retaining high accuracy. It starts from the cells that are closest to the sources and then proceeds radially outward. The source-target optical depth is the weighted sum of the source-neighboring optical depths where neighboring cells are those cells adjacent to the target cell are closer to the source cell than the target cell. The right panel of Figure 3.1 illustrates the ray-tracing idea in the short characteristics method. The source-target optical depth $\tau$ is thus given by

$$\tau = \sum_{i \in J} \omega_i \tau_i,$$  \hspace{1cm} (3.3)

where $J$ is the index set of the neighboring cells and $\tau_i$ is the optical depth between the source and cell $i$. The weight $\omega_i$ depends on the relative position between the source cell and target cell. Figure 3.2 illustrates the idea of how ray-tracing is used to identify the neighboring cells and their weight contribution.

Through the use of the optical depths of previously calculated cells, the short characteristics method is much more efficient than the long characteristics one. However, the required interpolation of optical depths introduces a
diffusivity in the results which shows up most clearly in shadowing tests.

3.3 Hybrid characteristics method

Both the long and short characteristics methods can be adapted to the structure of an adaptive mesh refinement (AMR) grid. However, if the grid is domain decomposed over multiple processors it is difficult to achieve an even distribution of work over the processors for these methods. To overcome this drawback, the hybrid characteristics method was developed.

The hybrid characteristics method (Rijkhorst et al. 2006) is a ray-tracing method that is neither classified as long nor short characteristics method, but uses properties from both methods. The cells are grouped into patches of $n^3$ cells of the same hierarchy. Within a patch, the long characteristics method is used twice. In the first case, each patch cell is assumed to be the target cell. The rays are sent from the source to the patch cells’ centers. The optical depths, which correspond to intersecting ray sections with the whole patch, are calculated. These optical depths are regarded as the local optical contribution within the patch. In the second case, none of the patch cells are the target cell, but the patch is located in the mid-way between the source and a target cell of the other patch. The patch cells thus contribute to the cumulative optical
Figure 3.3: Hybrid characteristics method. The top panel shows how the long characteristics method is used in patches of cells for calculating the local optical depths assuming the target cell is included in the patch. The middle panel is similar to the top panel but for calculating the cumulative optical depth contribution for a target not included in the patch. The bottom panel shows how the short characteristics method is used to interpolate the optical depths for the cumulative optical depth contribution of a target cell. Figure from Rijkhorst et al. (2006).

Depth between the source and the target cell. This cumulative optical depth is calculated via two steps. In the first step, rays are drawn from the source to the every patch cell’s corners at the three patch surfaces where the rays leave the patch. The optical depths corresponding to this traversed ray sections are calculated and stored in the similar way as the first case. In the second step, a ray is drawn from the source to the target cell. This ray passes through the patch and leaves the patch at one of the three patch surfaces. The intersection position of the ray and the patch surfaces is recorded. The cumulative optical depth contributed by the patch is calculated by interpolating among the four pre-calculated optical depths corresponding to the nearest four cell’s corners from the intersection position.

3.4 Adaptive ray-tracing method

Another method used for AMR grids is called adaptive ray-tracing. It can be applied both to regular Cartesian grids (Abel & Wandelt 2002) or AMR grids (Wise & Abel 2011). In the adaptive ray-tracing method, 12 rays are sent out from a source and initially proceed radially outward. When the ray density becomes too low to sufficiently sample the cells, the rays are split using the Hierarchical Equal Area isoLatitude Pixelization algorithm (HEALPix; Górski 2005).
Figure 3.4: HEALPix orthogonal visualization. The four different layers of pixelization show the same property - each pixel at each layer has the same area. Figure from Górski et al. (2005).

et al. (2005)). Figure 3.4 shows an orthographical view of the HEALPix partition of a sphere. Along the clock-wise direction and starting from the top left corner the figure shows the 0th, 1st, 2nd and 3rd level of refinement of pixelization. One property of HEALPix is that each pixel in all level of refinement has the same area. This symmetrical property ensures even sampling in all directions and therefore each ray carries an equal photon flux in the case of isotropic sources. Figure 3.5 illustrates how the process of progressively splitting the rays results in a quad-tree structure.

3.5 SIMPLEX method

The SIMPLEX method is a radiative transfer method which uses an unstructured Delaunay grid (Paardekooper et al. 2010). Instead of following straight lines, photons propagate through the medium following a zig-zag trajectory constrained by the three possible modes of transport. These modes are scattering transport, ballistic transport and direction conserving transport. Figure 3.6
shows graphically the idea of these three modes of transport. In the scattering process, the photons are evenly distributed to all the neighboring cells. Ballistic transport distributes the photons to their two most straightforward neighboring cells with respect to the photon incoming direction. Direction conserving transport is similar to ballistic transport but refers back to the original direction of the photons in order to pick the next cells to send the photons to. It ensures the photons maintain more or less retain their original direction.
3.6 PYRAMID method

The PYRAMID method is a newly devised radiative transfer method. We outline the basic idea in this section. The PYRAMID method works on a Cartesian grid which for the radiative transport is transformed to the pyramidal grid as shown in Figure 3.7. The pyramidal cells point naturally toward the source. The alignment of pyramidal cells conforms to a ray-tracing method as schematically depicted in Figure 3.8. For complete discussion of PYRAMID method, we refer the readers to consult Paper II.

3.7 Moment methods

While some radiative transfer codes require the knowledge of optical depth between the source and the cells in their algorithms, some solve the cosmological radiative transfer equation based on the moment formulation. For this method, it is important to specify the form Eddington tensor in order to close the set of moment equations. Interested readers can consult the work of [Gnedin & Abell (2001)] which compute the Eddington tensor assuming an optically thin medium and [Aubert & Teyssier (2008)] which applies the "M1 approximation" to handle the case of optically thick medium.
Figure 3.8: Ray-tracing implementation of PYRAMID method.
4. Photoionization and Photoheating Algorithm

The previous chapter described how the transfer of radiation can be calculated. The determination of the local photon intensity allows to compute the photoionization and photoheating rates (collectively we refer to them as photo-rates). These rates determine the evolution of the ionization and thermal states of the gaseous medium. The photo-rates are the necessary ingredients of the ionization and thermal equations (henceforth collectively called the photo-equations). However, the photo-equations are coupled to each other and the complexity of this coupling makes it impossible to derive an analytical solution. Similar to the radiative transfer equation, the photo-equations have to be solved numerically.

There exists several methods that can be used to solve the photo-equations. We mention a few well-known examples, namely, the Forward Euler method (used in Ciardi et al. 2001; Maselli et al. 2003; Pierleoni et al. 2007; Pawlik & Schaye 2008; Maselli et al. 2009a; Pierleoni et al. 2009; Pawlik & Schaye 2011; Wise & Abel 2011; Graziani et al. 2013), the Backward Euler method (used in Anninos et al. 1997; Rosdahl et al. 2013), the Mid-Point method (used by Mackey 2012a,b) and the C²-RAY method (used by Mellema et al. 2006; Altay et al. 2008; Paardekooper et al. 2010; Cantalupo & Porciani 2011; Friedrich et al. 2012; Lee et al. 2016). Comparisons among these methods in terms of accuracy and the impact of the choice of time-step were first conducted by Mackey (2012a) (excluding the Backward Euler method). However, this comparison was rather qualitative and addressed only the case of a monochromatic source. In Paper III we have developed a quantitative tool to compare these methods which furthermore allows a multi-frequency source. The latter is especially important when considering the temperature evolution.

In this chapter, we briefly summarize these four methods. For simplicity, we assume a gaseous medium only consisting of atomic hydrogen and consider only one zone. Furthermore, we consider a simplified ionization equation which does not consider recombinations, which therefore can be written as

\[
\frac{dx_{\text{HI}}}{dt} = -\Gamma x_{\text{HI}},
\]

(4.1)
where \( x_{\text{HI}} \) is neutral hydrogen fraction of the gas, \( t \) denotes time and \( \Gamma \) is the photoionization rate. Note that \( \Gamma \) depends on \( x_{\text{HI}} \) which in its turn depends of \( t \). We assume these four methods use the same time-step \( \Delta t \).

### 4.1 Forward Euler method

The Forward Euler method, or the first order Runge-Kutta method, uses information at \( t = 0 \) to calculate the right hand side of Equation 4.1. Therefore equation 4.1 can be rewritten as

\[
\frac{x_{\text{HI}}(\Delta t) - x_{\text{HI}}(0)}{\Delta t} = -\Gamma(x_{\text{HI}}(0))x_{\text{HI}}(0).
\]  

(4.2)

The Forward Euler solution is thus given by

\[
x_{\text{HI}}(\Delta t) = x_{\text{HI}}(0) - \Gamma(x_{\text{HI}}(0))x_{\text{HI}}(0)\Delta t.
\]  

(4.3)

The Forward Euler method is not symmetrical - the solution is advanced by a time-step \( \Delta t \) but only uses information from the beginning of the time interval. It is generally not recommended for use because of its low accuracy and, for non-linear equations, its tendency to become unstable (Press et al., 1986). It is a fully explicit method in the sense that no iterations are needed and its simplicity makes it very efficient.

### 4.2 Backward Euler method

The Backward Euler method is an implicit method which utilizes iteration to achieve a converged solution. The method uses information from \( t = \Delta \) for the right hand side of Equation 4.1. Equation 4.1 is thus rewritten as

\[
\frac{x_{\text{HI}}(\Delta t) - x_{\text{HI}}(0)}{\Delta t} = -\Gamma(x_{\text{HI}}(\Delta t))x_{\text{HI}}(\Delta t).
\]  

(4.4)

However, we cannot solve this equation because \( \Gamma \) is a complicated function of \( x_{\text{HI}} \). We instead start with the guess \( \Gamma(x_{\text{HI}}(\Delta t)) = \Gamma(x_{\text{HI}}(0)) \) and put it into Equation 4.4. By rearranging terms we have

\[
x_{\text{HI}}(\Delta t) = \frac{x_{\text{HI}}(0)}{1 + \Gamma(x_{\text{HI}}(\Delta t))\Delta t}.
\]  

(4.5)

The calculated \( x_{\text{HI}}(\Delta t) \) is then used to update the value of \( \Gamma(x_{\text{HI}}(\Delta t)) = \Gamma(x_{\text{HI}}(0)) \) which is subsequently put back into Equation 4.4. A new \( x_{\text{HI}}(\Delta t) \) is calculated with the updated \( \Gamma(x_{\text{HI}}(\Delta t)) \). This iterative process continues until the value \( x_{\text{HI}}(\Delta t) \) converges.
The Backward Euler method is one of the most basic numerical methods for solving differential equations. It is in many ways similar to the Forward Euler method but the Backward Euler method is implicit while the Forward Euler method is explicit. The iterative property makes the Backward Euler method more stable and especially suitable for solving stiff equations (Butcher 2003).

4.3 Mid-Point method

The Mid-Point method, or the second order Runge-Kutta method, uses information from \( t = \Delta t/2 \) for the right hand side of Equation 4.1:

\[
\frac{x_{HI}(\Delta t) - x_{HI}(0)}{\Delta t} = -\Gamma(x_{HI}(\Delta t/2))x_{HI}(\Delta t/2).
\] (4.6)

The value of \( x_{HI}(\Delta t/2) \), and hence \( \Gamma(x_{HI}(\Delta t/2)) \) is obtained via the Forward Euler solution but for a time-step \( \Delta t/2 \). It is given by

\[
x_{HI}(\Delta t/2) = x_{HI}(0) - \Gamma(x_{HI}(0))x_{HI}(0)\Delta t/2.
\] (4.7)

Figure 4.1 graphically shows the difference between the Forward Euler method and the Mid-Point method, or in other words the difference between the Runge-Kutta methods of the first and second order. This method is generally more accurate than the previous two methods but has not been used much for time-dependent photoionization calculations. Its use was first promoted by Mackey (2012a).

4.4 C²-RAY method

The C²-RAY method uses time-averaged value \( \langle x_{HI} \rangle \) for the argument of \( \Gamma \) on right hand side of Equation 4.1

\[
\frac{dx_{HI}}{dt} = -\Gamma(\langle x_{HI} \rangle)x_{HI}.
\] (4.8)

We will define \( \langle x_{HI} \rangle \) later and for the moment we will assume it is a constant. Equation 4.8 can then be solved analytically, the solution being given by

\[
x_{HI}(\Delta t) = x_{HI}(0)e^{\Gamma(\langle x_{HI} \rangle)\Delta t}.
\] (4.9)

By defining the function \( x_{HI}(t) = e^{\Gamma(\langle x_{HI} \rangle)t} \), the time-averaged value \( \langle x_{HI} \rangle \) is thus given by

\[
\langle x_{HI} \rangle = \frac{x_{HI}(0)(1 - e^{-\Gamma(\langle x_{HI} \rangle)\Delta t})}{\Gamma(\langle x_{HI} \rangle)\Delta t}.
\] (4.10)
Figure 4.1: Graphical representation of the Forward Euler method and the Mid-Point method. The top panel shows an example of the Forward Euler method - one single step is taken to advance the system by one time-step. The bottom panel shows an example of the Mid-Point method - two steps are required to advance the system by one time-step. Figure from Press et al. (1986).
Note that the recursive form of $\langle x_{\text{HI}} \rangle$ is handled by an iterative procedure. First, put $\langle x_{\text{HI}} \rangle = x_{\text{HI}}(0)$ to the right hand side of Equation 4.8 and solve it analytically. Then, update $\langle x_{\text{HI}} \rangle$ by putting $\langle x_{\text{HI}} \rangle = x(0)$ to the right hand side of Equation 4.10. This updated value of $\langle x_{\text{HI}} \rangle$ is inserted in the right hand side of Equation 4.8. The updated solution is used to compare against the first solution. If these two solution do not coincide, the whole process repeats itself until the solutions have converged.

The use of $\langle x_{\text{HI}} \rangle$ in the C$^2$-RAY method allows for an integration time-step much larger than the ionization time-scale while achieving high degree of accuracy. This leads to a considerable speed-up of the computation time. An further advantage of this method is that it always yields solutions for $x_{\text{HI}}$ in the range $[0, 1]$, which is not guaranteed for the other three methods.

4.5 Prospective

We have presented in this chapter four different numerical methods for solving the simplest form of the ionization equation. We must emphasize that all the methods, except C$^2$-RAY method, are applicable to a wide range of differential equations. The accuracy of solutions for different methods can vary substantially depending upon the differential equations to be solved. The C$^2$-RAY method was designed to solve the ionization equation and usually includes the recombination and collisional ionization rates. Its use for other types of differential equations has to our knowledge not been explored, although it should apply to similar differential equations.

When considering the use of these methods, both their accuracy and their computational cost should be considered. For a given amount of computational time a intrinsically less accurate but faster method may still yield more accurate results through the use of shorter time-steps. In a relative sense the Forward Euler method has the simplest form as its solution requires only one explicit computational step. Next comes the Mid-Point method which requires two computational steps - one for advancing to the half time-step and another for advancing a full time-step. The Backward Euler method and the C$^2$-RAY methods are more complicated because they are implicit and require iteration to arrive at the solution. Each iteration is equivalent to one computational step. However, the number of iterations required depends on the imposed convergence criteria. Mackey (2012a) presented a joint analysis of both accuracy and computational efficiency for the Forward Euler, Mid-Point and C$^2$-RAY methods. He concluded that the latter two are always superior over the first method and that for some problems C$^2$-RAY is to be preferred over the Mid-Point method and whereas other problems show the reverse behaviour. However, he only considered monochromatic radiation and an evaluation for
the case of multi-frequency radiation would be useful.
5. Summary of Publications

5.1 Paper I

This paper describes two novel improvements to the C²-Ray code developed for dealing with photoheating in an efficient and accurate way. These two improvements are an adaptive time-step algorithm and asynchronous evolution. The adaptive time-step algorithm calculates an optimal time-step for the next computational step. Our method uses a fast ray-tracing scheme to quickly locate the relevant cells for this time-step calculation. While the time-step calculation cost scales linearly with the number of cells involved, our algorithm is efficient because a relatively large amount of irrelevant cells are discarded for the time-step calculation. Asynchronous evolution allows different cells to evolve with different time-steps. The asynchronized clocks of the cells will become synchronized for the times when the intermediate evolution results are produced or the total evolution time has been reached. This synchronization guarantees that the evolution results are physical. Asynchronous evolution implicitly implies that most of the computational resources are allocated to the heating-relevant cells and it thus makes the calculation substantially more computationally efficient than employing the same time-step over the whole grid.

5.2 Paper II

We propose a novel radiative transfer method - PYRAMID. It makes use of a newly devised pyramidal geometry. This pyramidal geometry inherits important properties of both Cartesian geometry and spherical geometry. In a typical radiative transfer simulation, the radiative transfer parameters are stored in Cartesian grid cells whereas the radiative transfer for a radially emitting source conforms to the spherical geometry. The combination of properties from the Cartesian and spherical geometries grants PYRAMID a great advantage in ray-tracing application. PYRAMID has unique features over the traditional ray-tracing methods. In this paper, we show how PYRAMID method is applied to calculate the photoionization and photoheating rates of hydrogen atoms by ionizing sources. We compare the performance of the PYRAMID
method with two traditional radiative transfer methods - long and short characteristics ray-tracing methods. We show that all methods produce a spherical photo-rate distribution around a single source. The numerical values of the photo-rates computed with the PYRAMID method are consistent with the two characteristics methods. The shadowing test shows that both PYRAMID and long characteristics methods generate sharp shadows behind an obstacle, while short characteristics produces a diffusive shadow. However, the PYRAMID method requires less computation time than long characteristics method.

5.3 Paper III

We present the first mathematical analysis of the performance of a series of existing methods which solve the coupled photoionization and thermal equations for a hydrogen gas in the case of multi-frequency radiation. The methods considered are the forward Euler, backward Euler, mid-point and $C^2$-RAY methods. Our analysis applies to a variety of density environments such as the IGM and star formation regions. In our analysis, we consider only the photoionization and photoheating processes during one time-step. Our mathematical work analyzes the accuracy of each of the methods quantitatively. It shows that the errors for each method depends on two initial parameters, namely the initial optical depth and the dimensionless time-step given by the product of the time-step and the initial photoionization rate. We conclude that $C^2$-RAY performs best for all initial conditions, followed by mid-point method.
Sammanfattning


I Artikel II utvecklar vi en ny ray-tracing-metod - PYRAMID. Eftersom en radiellt strålande källa inte kan representeras väl i kartesiska celler använder PYRAMID en ny, pyramidformad geometri, som delar egenskaper med såväl ett vanligt kartesiskt som ett sfäriskt koordinatsystem. Kombinationen av dessa egenskaper får de pyramidformade cellerna, som är mycket kompatibla med kartesiska celler, att anpassa sig till den radiellt strålande källan på ett naturligt sätt.

I Artikel III analyserar vi flera lösningsläkar för kopplad jonisering och termiska ekvationer. Dessa lösningsläkar används i stor utsträckning inom olika kosmologiska strålningstransportsmodeller. Vi utför en detaljerad och kvantitativ jämförelse mellan noggrannheten hos fyra olika standardlösare när det gäller valet av tidssteg. Vi finner också att de allmänna egenskaperna hos den analytiska lösningen återfinns i samtliga numeriska lösningar. Detta har förenklat vårt arbete avsevärt, eftersom resultatet av alla numeriska lösningar endast beror
på en kombination av två strålningsparametrar.
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