Simulating Cosmic Reionisation

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Zwei Dinge erfüllen das Gemüt mit Bewunderung und Ehrfucht, der bestirnte Himmel über mir und das moralische Gesetz in mir.

Kant, Kritik der praktischen Vernunft

CHAPTER 1

Introduction

1.1 The epoch of reionisation

The first stars and galaxies formed a few hundred million years after the Big Bang, when the Universe was only a small fraction of its present age. Their radiation is thought to have transformed the previously cold and neutral hydrogen that filled intergalactic space into the hot and ionised cosmic plasma that is observed today. This milestone in the history of the Universe is called the epoch of reionisation.

When did reionisation occur? Was it a simple instantaneous event, or a complex transition of extended duration? Were the first stars in the first galaxies sufficiently powerful to reionise the Universe, or was an additional source of ionising radiation at play? Much about the cosmic reionisation transition is still unknown.

Theoretical studies of the epoch of reionisation are currently particularly timely because of the wealth of observational data of unparallelled quality that will soon be provided by a new generation of observatories. Radio interferometers like LOFAR[1], MWA[2] and SKA[3] will open a previously unexplored observational window by surveying the Universe at very low frequencies with unprecedented high resolution and sensitivity. The infrared space-based observatory JWST[4] and the optical ground-based adaptive optics telescope ELT[5] will even enable the direct imaging of the sources responsible for the reionisation process.

Radiative transfer simulations coupled to hydrodynamical simulations of the early Universe are one of the most promising techniques to study reionisation. Simulating reionisation is a challenging task that requires the radiation-hydrodynamical modelling of large representative volumes of the Universe at very high resolution. The main goal of this thesis is to present a radiative transfer method for use in this computationally demanding regime. To accomplish this goal, we will analyse the challenges posed by the desire to include the transfer of radiation in cosmological simulations of reionisation and show how they can be overcome.

The organisation of this chapter is as follows. In Sec. 1.2 we give a brief overview of the history of our Universe, sketch the physics behind the formation and evolution of the first stars and discuss some of the key aspects of the transition from the neutral to the ionised Universe they trigger. In Sec. 1.3 we review current observational constraints on the epoch of reionisation

[1] http://www.lofar.org
[2] http://www.haystack.mit.edu/ast/arrays/mwa/
[3] http://www.skatelescope.org
[4] http://www.jwst.nasa.gov/
[5] http://www.eso.org/sci/facilities/eelt/

and in Sec. 1.4 we discuss the main challenges encountered in simulating this important epoch. In Sec. 1.5 we present an outline of this thesis by summarising the content of its chapters, which concludes this chapter.

1.2 The first stars and the reionisation of the Universe

The theory of hierarchical structure formation constitutes one of the pillars of modern Big Bang cosmology. According to this theory, matter assembles to form increasingly larger structures, or *halos*, through the gravitational amplification of tiny primordial density fluctuations. The dilute cosmic gas accreted by these halos soon condensed to form the first generation of stars and galaxies. Their radiation photo-ionised and photo-heated the previously predominantly neutral intergalactic gas, causing a global phase transition that is referred to as reionisation.

In this section we give a brief overview of some of the most important physical processes behind reionisation. This overview is not intended to be exhaustive. Rather, we focus our discussion on a few key issues that are of direct relevance to the work presented in this thesis. The reader is referred to the excellent reviews by, e.g., Barkana & Loeb (2001), Ciardi & Ferrara (2005), Furlanetto, Oh, & Briggs (2006), and Fan, Carilli,& Keating (2006) and to the textbooks by, e.g., Peacock (1999), Kolb & Turner (1990), Peebles (1993) and Padmanabhan (1993) for more information.

1.2.1 The expanding Universe

The history of the expanding Universe (see, e.g., Kolb & Turner 1990) starts with its birth in the Big Bang about 13.7 billion years ago. Back then it was so dense and so hot that frequent collisions, for instance between protons, electrons and photons, prevented elements from being formed. It was only about 380000 yr after the Big Bang, corresponding to a redshift $z \approx 1100$, that the adiabatic expansion of space had cooled the hot primordial plasma down to temperatures $T \approx 3000$ K that allowed the formation of neutral atoms. This key event in the history of the Universe is known as cosmological recombination.

Cosmological recombination (see Sunyaev & Chluba 2008 for a recent review) freed most of the photons that were previously trapped by Thompson scattering off free electrons. Today, these photons - witnesses of the infancy of the Universe - constitute the Cosmic Microwave Background (CMB) radiation and offer a direct view on the conditions in the Universe at the time of their last scattering (for a review see, e.g., Hu & Dodelson 2002). Together with observations of redshift $z \sim 0.5$ Type Ia supernova explosions that indicate a late-time acceleration in the expansion of space (Riess et al. 1998; Perlmutter et al. 1999) and observations of the large-scale structure of the Universe (e.g., Percival et al. 2007), the CMB observations (e.g., Komatsu et al. 2009) support a concordance cosmological model that specifies the composition of the expanding Universe and provides the current framework for investigations into its evolution.

At present, about 74% of the energy content of the Universe is assumed to be in the form of an elusive fluid dubbed dark (or vacuum) energy (for a review, see, e.g., Carroll, Press, & Turner 1992; Frieman, Turner, & Huterer 2008), which drives the observed late-time accelerated expansion of space. The matter in the Universe, which accounts for about 26% of its present energy density, is mostly (about 83% of the total matter mass) in the form of a cold and dark, weakly interacting, non-baryonic substrate (for a review see, e.g., Bertone, Hooper, & Silk 2004; Bergström 2000). The existence of this dark matter component is firmly established through observations of its gravitational interaction with ordinary (baryonic and leptonic) matter (e.g., Clowe et al. 2006; for a review see, e.g., Trimble 1987).

Ordinary matter, which may be detected through its emission/absorption of radiation across the electromagnetic spectrum, accounts for only about 17% of the total matter mass. Most of this matter is in the form of gas (e.g., Fukugita, Hogan, & Peebles 1998). Its initial (primordial) composition is well-constrained by Big Bang nucleosynthesis (e.g., Tytler et al. 2000; Kolb & Turner 1990). Just after recombination, about 75% of its mass consisted of neutral hydrogen and about 25% consisted of neutral helium. It contained trace amounts of free electrons, hydrogen and helium ions, deuterium and molecular hydrogen (as well as trace amounts of other light elements, like lithium and beryllium). The last component of the Universe, radiation (CMB photons, neutrinos and other light relativistic relics), presently contributes only an insignificant amount of less than 0.1% to the total energy budget (e.g., Fukugita & Peebles 2004).

The expansion of the Universe, i.e. the observation that the physical separation between idealised observers at rest increases with time t in proportion to the expansion factor $a(t) = [1+z(t)]^{-1}$, is characterised by the Hubble parameter $H \equiv \dot{a}/a$, where the dot indicates the time derivative. From dimensional analysis one may expect that the Hubble parameter is closely related to age of the Universe, $t \sim H^{-1}$. With this notation, the composition of the Universe is conveniently specified in terms of the set of cosmological parameters $\Omega_\Lambda \equiv \bar{\rho}_{\Lambda,0}/\rho_{\rm c}$, $\Omega_{\rm m} \equiv \bar{\rho}_{\rm m,0}/\rho_{\rm c}$ and $\Omega_{\rm r} \equiv \bar{\rho}_{\rm r,0}/\rho_{\rm c}$, where $\bar{\rho}_{\Lambda,0}, \bar{\rho}_{\rm m,0}$ and $\bar{\rho}_{\rm r,0}$ are, respectively, the present mean densities of dark energy, total (dark + ordinary) matter and radiation, $\rho_{\rm c} \equiv 3H_0^2/(8\pi G)$ is the critical density, G is the gravitational constant, c is the speed of light and $H_0 = 100h$ km s^{-1} Mpc^{-1} is the Hubble constant, i.e. the present value of the Hubble parameter. The value of h is confirmed to be about 0.7 by several independent measurements (e.g., Riess et al. 2009; for a review see, e.g., Jackson 2007).

Dilution due to the expansion of space implies that the density of matter evolves according to $\bar{\rho}_{\rm m}(a) = m\bar{n}_{\rm m}(a) = a^{-3}\bar{\rho}_{\rm m,0}$, where $\bar{n}_{\rm m}$ is the mean number density of particles of mass m. The energy density of radiation evolves both because of dilution and because of the stretching of the wavelength λ_0 with the expanding space, yielding $\bar{\rho}_{\rm r}(a) = \bar{n}_{\rm r}(a)h_{\rm P}c/(a\lambda_0) = a^{-4}\bar{\rho}_{\rm r,0}$, where $\bar{n}_{\rm r,0}$ is the mean number density of the massless relativistic particles and $h_{\rm P}$ is Planck's constant. The energy density of the vacuum simply remains constant, $\bar{\rho}_\Lambda(a) = \bar{\rho}_{\Lambda,0}$.

The mathematical description of the expansion of the concordance Universe is provided by Einstein's theory of General Relativity and (curved) space-time (e.g., Wald 1984; Nabler 1989). A central role in this theory is played by Einstein's field equation, which relates the geometry and energy content of the Universe. Employing the postulated (and observationally supported) homogeneity and isotropy of space as well as the scalings of the (energy) densities of dark energy, matter and radiation that we have derived above, Einstein's field equation transforms into $H^2(a) = H_0^2(\Omega_{\rm r}a^{-4} + \Omega_{\rm m}a^{-3} + \Omega_\Lambda)$, a relation known as the Friedmann equation. Note that we assumed that space is flat, which is, both on theoretical and observational grounds, the preferred geometry of the Universe in the concordance model, and which manifests itself in the relation $\Omega_{\rm r} + \Omega_{\rm m} + \Omega_\Lambda = 1$. Hence, $\Omega_\Lambda \approx 0.74$, $\Omega_{\rm m} \approx 0.26$ and $\Omega_{\rm r} \sim 10^{-4}$ are, respectively, identical to the fractional contributions of dark energy, matter and radiation to the total energy content of the Universe given above.

The Friedmann equation encapsulates the dependence of the expansion of space on the composition of the Universe. At present, the expansion rate is dominated by the densities of dark energy and matter. The different redshift dependencies of the densities of dark energy, matter and radiation imply, however, that this was not always the case. Indeed, the expansion of space was dominated by the radiation density for redshifts $z \gtrsim z_{\rm eq}$, where $z_{\rm eq} = (\Omega_{\rm m}/\Omega_{\rm r}) - 1 \sim 5 \times 10^3$ marks the redshift at which the radiation density becomes equal to the matter density. The expansion was dominated by the matter density for redshifts $z_\Lambda < z < z_{\rm eq}$, where $z_\Lambda = (\Omega_\Lambda/\Omega_{\rm m})^{1/3} - 1 \approx 0.3$ marks the redshift at which matter density becomes equal to the dark energy density. The history of the expanding Universe may thus be divided into an early radiation-dominated epoch, an intermediate matter-dominated epoch and the current epoch of dark energy domination.

1.2.2 The formation of galaxies

The galaxies observed today evolved from tiny fluctuations in the matter distribution through gravitational amplification. The characteristic time-scale associated with galaxy formation is therefore given by the free-fall time $\sim (G\rho_{\rm m})^{-1/2}$, where $\rho_{\rm m}$ is the local density of matter (dark + ordinary).

Linear theory

The initial growth of matter fluctuations due to gravitational instability in the expanding Universe is well described by linear theory (for reviews see, e.g., Peebles 1980; Peacock 1999; Padmanabhan 1993; Loeb 2006). It crucially depends on the size of the fluctuation wavelength λ with respect to the size of the causally connected Universe, whose boundaries are marked by the (particle) horizon (e.g., Kolb & Turner 1990). The (proper) radius $\lambda_{\rm H}$ of the horizon is given by the physical distance light could have travelled since the Big Bang, i.e. $\lambda_{\rm H}(t) \sim ct \sim cH^{-1}$.

Linear theory describes the growth of fluctuations in terms of the density contrast $\delta(\mathbf{r}) \equiv \rho_{\rm m}(\mathbf{r})/\bar{\rho}_{\rm m} - 1$, where $\mathbf{r}$ is the spatial coordinate. Fluctuations grow at different rates during different epochs of the expansion history of the Universe. We will briefly review the growth of fluctuations in the different regimes to facilitate the understanding of the fluctuation power spectrum that we present further below.

Linear fluctuations on super-horizon scales grow in proportion to the square of the expansion factor, $\delta \propto a^2$, during radiation-domination and in proportion to the expansion factor, $\delta \propto a$, during matter-domination. A super-horizon fluctuation will eventually enter the horizon (at $\lambda_{\rm H} \sim \lambda$) and become a sub-horizon fluctuation. If the fluctuation enters the horizon during the radiation-dominated era, then its gravitational growth is suppressed by the rapid expansion of space caused by the high (with respect to the matter density) radiation density (Meszaros 1974).

Sub-horizon fluctuations in the weakly interacting dark matter may continue to grow, in proportion to the expansion factor, $\delta \propto a$, once the Universe enters the matter-dominated era. On the other hand, sub-horizon fluctuations in ordinary matter may only continue to grow (in proportion to the expansion factor) after recombination. Before recombination, frequent scatterings of photons off free electrons smooth the fluctuations in the free electron density and, through electromagnetic coupling of electrons and protons, in the proton density.

Fluctuations that enter the horizon during the matter-dominated era evolve in a slightly different manner. Fluctuations in dark matter that enter the horizon during matter-domination simply continue their super-horizon growth, $\delta \propto a$. Fluctuations in ordinary matter that enter the horizon during matter-domination but before recombination are washed out by the radiation pressure mediated by photon-electron scattering. These fluctuations may only grow (in proportion to the expansion factor) after recombination. Finally, fluctuations in ordinary matter that enter the horizon after recombination are not affected by radiation pressure and continue to grow in proportion to the expansion factor, $\delta \propto a$.

Jeans mass

Thermal gas pressure prevents the growth of sub-horizon fluctuations in ordinary matter if the sound-crossing time $\lambda/c_{\rm s}$ becomes smaller than the gravitational free-fall time, i.e. if $\lambda \leq \lambda_{\rm J} \equiv c_{\rm s}\pi^{1/2}(G\rho_{\rm m})^{-1/2}$, where $c_{\rm s}$ is the sound speed (and the additional factor $\pi^{1/2}$ results from a detailed linear theory analysis of the fluctuation growth). The sound speed $c_{\rm s}^2 = \gamma k_{\rm B}T/(\mu m_{\rm H})$, where μ is the mean gas particle mass in units of the hydrogen mass $m_{\rm H}$ and γ is the ratio of specific heats, which for an ideal, mono-atomic gas is $5/3$. The Jeans scale $\lambda_{\rm J}$ defines the Jeans mass $M_{\rm J} \equiv (4\pi/3)\rho_{\rm m}(\lambda_{\rm J}/2)^3$. Introducing the overdensity $\Delta \equiv \rho_{\rm m}/\bar{\rho}_{\rm m}$, the total (dark matter + gas) Jeans mass reads

$$M_{\rm J} \approx 6 \times 10^7\ {\rm M}_\odot\ \Delta^{-1/2} \left(\frac{T}{10^3\ {\rm K}}\right)^{3/2} \left(\frac{1+z}{10}\right)^{-3/2} \left(\frac{\mu}{1.22}\right)^{-3/2} \left(\frac{\Omega_{\rm m}h^2}{0.13}\right)^{-1/2}. \tag{1.1}$$

In fluctuations with masses greater than the Jeans mass, gravity cannot be supported by the gas pressure gradient, enabling the fluctuation to grow.

The temperature of the cosmic gas remains coupled to the temperature of the cosmic microwave background due to scattering off residual free electrons down to redshifts $1 + z_{\rm dec} \approx 160(\Omega_{\rm b}h^2/0.022)^{2/5}$ (e.g., Peebles 1993; Barkana & Loeb 2001), i.e. down to redshifts well after recombination. At present ($z = 0$), the distribution of energies of CMB photons is observed to be very close to that of photons emitted by a black body of temperature $T_{\rm CMB,0} = 2.73$ K (Fixsen et al. 1996). The temperature $T_{\rm bb}$ of a black body is related to the energy density $c^2\rho_{\rm bb}$ of the black-body radiation it emits through $aT_{\rm bb}^4 = c^2\rho_{\rm bb}$, where $a = 4\sigma_{\rm SB}/c$ is the radiation constant and $\sigma_{\rm SB}$ is the Stefan-Boltzmann constant. For $z > z_{\rm dec}$, the gas temperature therefore evolves according to $T = T_{\rm CMB} = T_{\rm CMB,0}(1 + z)$ and as a result, the Jeans mass becomes independent of redshift. At the mean density ($\Delta = 1$), $M_{\rm J} \approx 2.4 \times 10^5(\mu/1.22)^{-3/2}(\Omega_{\rm m}h^2/0.2)^{-1/2}$.

For redshifts $z < z_{\rm dec}$, the fraction of residual free electrons becomes so small that photon-electron scattering becomes improbable and the gas thermally decouples from the CMB. In the absence of other heating or cooling mechanisms, the gas then cools adiabatically, $T \propto (1 + z)^2$. The cosmological Jeans mass, i.e. the Jeans mass at density $\rho_{\rm m} = \bar{\rho}_{\rm m}$, then becomes

$$M_{\rm J} \approx 4 \times 10^3\ {\rm M}_\odot \left(\frac{1+z}{10}\right)^{3/2} \left(\frac{\mu}{1.22}\right)^{-3/2} \left(\frac{\Omega_{\rm m}h^2}{0.13}\right)^{-1/2} \left(\frac{\Omega_{\rm b}h^2}{0.022}\right)^{-3/5}. \tag{1.2}$$

Nonlinear collapse

Once $\delta \sim 1$, linear theory breaks down. An analytical approximation to the nonlinear growth of top-hat (i.e. spherical and homogeneous) sub-horizon fluctuations is provided by the spherical collapse model (Gunn & Gott 1972; for a textbook treatment see, e.g., Padmanabhan 1993). Near the linear regime, a fluctuation still grows approximately linearly with the expansion factor ($\delta \propto a$, assuming that the fluctuation becomes nonlinear well after recombination) while expanding with the Universe. Due to the pull-back from its self-gravity, the fluctuation then turns around, decoupling its dynamics from that of the expanding background. The fluctuation eventually becomes highly nonlinear and collapses to form a halo of density $\rho_{\rm coll}$.

The halo properties follow from the virial theorem, which relates the halo potential and kinetic energies. Accordingly, $v_{\rm vir}^2 \sim GM_{\rm vir}/r_{\rm vir}$, where $v_{\rm vir}$ is the halo velocity dispersion,

$M_{\rm vir}$ is the halo mass and $r_{\rm vir}$ is the halo radius. The latter two are related through $M_{\rm vir} = 4\pi/3\bar{\rho}_{\rm m}\Delta_{\rm coll}r_{\rm vir}^3$, where $\Delta_{\rm coll} \equiv \rho_{\rm coll}/\bar{\rho}_{\rm m}$ is the halo overdensity. Spherical collapse theory predicts a halo overdensity $\Delta_{\rm coll} \approx 180$ independent of halo mass and nearly independent of redshift. The collapse shock-heats the gas in the halo to temperatures $T_{\rm vir} \equiv \mu m_{\rm H} v_{\rm vir}^2/(3k_{\rm B})$. The virial mass is related to the viral temperature through

$$M_{\rm vir} \approx 2\times 10^6\ {\rm M}_\odot \left(\frac{T_{\rm vir}}{10^3\ {\rm K}}\right)^{3/2} \left(\frac{1+z}{10}\right)^{-3/2} \left(\frac{\mu}{1.22}\right)^{-3/2} \left(\frac{\Delta_{\rm coll}}{180}\right)^{-1/2} \left(\frac{\Omega_{\rm m}h^2}{0.13}\right)^{-1/2} \quad (1.3)$$

The fact that this is of the same order as the Jeans mass (Eq. 1.1), evaluated at the collapse overdensity, is not surprising, since both the virial and the Jeans mass are derived assuming similar balances between gravitational and thermal energy.

Hierarchical formation of galaxies in the concordance cosmology

The density fluctuations are thought to be seeded by the blow-up of quantum fluctuations during inflation, a theoretized brief (10^{-43} s $\lesssim t \lesssim 10^{-30}$ s) phase of accelerated expansion shortly after the Big-Bang (Guth 1981; for textbook treatments see, e.g., Linde 1990; Liddle & Lyth 2000). While our description so far considered fluctuations in real space $\mathbf{r}$, a description of fluctuations in Fourier space $\mathbf{k}$ is often more convenient mathematically (e.g., Barkana & Loeb 2001). Accordingly, a real space fluctuation $\delta(\mathbf{r})$ of wavelength λ is replaced by the corresponding Fourier space fluctuation $\delta(\mathbf{k})$ of wave number $k = |\mathbf{k}| = 2\pi/\lambda$. Standard models of inflation predict a Gaussian field of isotropic, scale-dependent random fluctuations, which are independent (in Fourier space) of each other. Their statistical properties are fully characterised by the scale-dependent variance, or power $P(k)$ at wave number k.

Standard inflationary theory predicts a primordial power spectrum $P(k) = k^{n_{\rm s}}$ with $n_{\rm s} \approx 1$. The scale-dependence of the (linearly evolving) fluctuation spectrum is modified due to the subsequent linear growth of fluctuations. The suppression of fluctuation growth during radiation-domination leads to a turn-over in the power spectrum at a comoving[6] scale of the order of the horizon at matter-radiation equality, $\lambda_{\rm H,com}(z_{\rm eq}) \sim a_{\rm eq}^{-1}cH^{-1}(z_{\rm eq}) \sim 100$ Mpc comoving, and implies a small-scale asymptotic scaling $P(k) \propto k^{n_{\rm s}-4}$. At comoving scales larger than $\lambda_{\rm H,com}(z_{\rm eq})$, the power spectrum preserves its primordial shape.

The overall amplitude of the (linearly evolved) power spectrum, which is commonly expressed in terms of the rms density variation σ_8 (extrapolated to redshift $z = 0$ using linear theory and averaged using a top-hat filter of radius $8\ h^{-1}$ Mpc), is not predicted by inflation and needs to be observationally determined. According to recent observational estimates, e.g. based on the analysis of CMB fluctuations (Komatsu et al. 2009), $\sigma_8 \approx 0.8$. Note that the shape of the power spectrum is also modified due to the nonlinear growth of fluctuations (e.g., Peacock & Dodds 1996).

The primordial shape of the power spectrum, together with its subsequent linear evolution, implies a fluctuation variance that increases with decreasing mass of the fluctuation. This mass-dependence is at the basis of the current paradigm of structure formation, the hierarchical formation of galaxies (White & Rees 1978; Blumenthal et al. 1984; White & Frenk 1991; for a review see, e.g., Baugh 2006). The lower the mass of a fluctuation, the larger its variance and the earlier (on average) it collapses. This bottom-up growth successfully explains for instance

[6] Comoving scales $\lambda_{\rm com}$ are related (by definition) to physical scales λ through $\lambda = a\lambda_{\rm com}$, where a is the expansion factor.

why galaxy-size halos are already observed at redshifts $z \lesssim 10$, while cluster-size halos, i.e. halos hosting hundreds of galaxies, do not assemble until much later, $z \lesssim 1$.

The mass-function of halos, i.e. the abundance of halos of a given mass, generally must be obtained using numerical simulations of the nonlinear structure formation process (see Sec. 1.4). Analytical approximate models help, however, to gain insight into the physical process at work. An excellent approximation to the mass function in numerical simulations is obtained from excursion set theory (Press & Schechter 1974; Bond et al. 1991; Sheth, Mo, & Tormen 2001; Maggiore & Riotto 2009), which combines the statistical description of the growth of fluctuations with the spherical (or its variant, the ellipsoidal) collapse model. The mass-function may be compared with observations by modelling the observed stellar luminosity distribution of (clusters of) galaxies as a function of halo mass. The stellar luminosities of galaxies depend on their star formation histories. The physics of star formation will be the subject of the next section.

1.2.3 The first stars

Stars form due to the gravitational collapse of gas in dark matter halos. The ability of a halo to contain gas is determined by the balance between the attractive gravitational forces and the repulsive pressure forces exerted on the gas. Only halos whose gravitational binding energy $\sim k_{\mathrm{B}}T_{\mathrm{vir}}$ per particle exceeds the gas thermal energy $\sim k_{\mathrm{B}}T$ may therefore retain accreted gas (e.g., Barkana & Loeb 1999). To form stars, the halo gas must efficiently cool (i.e. on cooling time scales smaller than the free-fall time; Rees & Ostriker 1977; Silk 1977) and reduce its thermal pressure to collapse to higher densities.

The ability of gas to cool efficiently depends on its density, temperature and composition. At temperatures $T < 10^4$ K, primordial gas cools mostly through radiative de-excitation of collisionally excited molecular hydrogen (e.g., Bromm, Coppi, & Larson 2002; Abel, Bryan, & Norman 2002). Cooling times smaller than the free fall time require gas temperatures $T \gtrsim 10^3$ K and molecular hydrogen fractions of $n_{\mathrm{H}_2}/n_{\mathrm{H}} \gtrsim 10^{-4}$ (e.g., Bromm & Larson 2004). Both these criteria are satisfied in halos with virial temperatures $T_{\mathrm{vir}} \sim 10^3$ K (Haiman, Thoul, & Loeb 1996; Tegmark et al. 1997; Yoshida et al. 2003). These *mini-halos*, which are expected to form as early as $z \gtrsim 10$ (see, e.g., the review by Barkana & Loeb 2001) and hence have masses $M_{\mathrm{vir}} \sim 10^6$ $\mathrm{M}_{\odot}$ (Eq. 1.3), constitute the first sites of star formation in the hierarchically evolving concordance Universe. Note that their mass is significantly larger than the cosmological Jeans mass (Eq. 1.2), which determines the ability of fluctuations to grow.

The details of stellar formation and evolution are not very relevant for the work presented in this thesis. We will therefore content ourselves with a brief presentation of (some) key aspects. Our discussions will be largely based on the recent reviews by Bromm & Larson (2004) and Ciardi & Ferrara 2005, to which the reader is referred for further details.

The birth of the first stars

Detailed three-dimensional simulations (Bromm, Coppi, & Larson 2002; Abel, Bryan, & Norman 2002) show that the gravitationally collapsing gas settles into a quasi-static configuration once it reaches temperatures $T \sim 200$ K and hydrogen number densities $n_{\mathrm{H}} \sim 10^4$ cm^{-3}. These characteristic values for the temperature and density are set by the physics of molecular hydrogen cooling (e.g., Bromm & Larson 2004). Below $T \lesssim 200$ K, molecular hydrogen cannot cool because of the lack of excitable transitions with correspondingly low energies. Above densities

$n_{\rm H} \gtrsim 10^4$ cm^{-3}, collisional excitations and de-excitations become so frequent that the population of the energy states of molecular hydrogen reaches its thermal equilibrium value, rendering radiative cooling inefficient. The gas only continues to collapse once the accumulated gas mass becomes larger than the Jeans mass, $M_{\rm J} \sim 700$ M$_\odot(T/200$ K$)^{3/2}(n_{\rm H}/10^4$ cm$^{-3})^{-1/2}$ (Bromm & Larson 2004). The collapse then proceeds to densities $n_{\rm H} \sim 10^{22}$ cm^{-3} at which the gas becomes optically thick to its cooling radiation and forms a hydrostatical proto-stellar core of mass $\sim 5 \times 10^{-3}$ M$_\odot$ (e.g., Omukai & Nishi 1998).

The final stellar mass will be determined by the physics of accretion. Dimensional analysis (Bromm & Larson 2004) suggests that the accretion rate is given by the ratio of Jeans mass and free-fall time, $\dot{M}_{\rm acc} \sim c_{\rm s}^3/G \propto T^{3/2}$. While the initial mass of the accreting proto-stellar core is comparable to the mass of proto-stellar cores in present-day star formation, a comparison of the temperatures of present-day star-forming regions ($T \sim 10$ K) and those in primordial ones ($T \sim 200$ K) indicates that primordial proto-stellar clumps may accrete gas at rates that are about two orders of magnitude higher than the rates at which present-day proto-stellar clumps accrete their gas. Although dimensional arguments certainly oversimplify the description of the accretion problem, it is thus generally expected that the first stars are typically much more massive (~ 100 M$_\odot$) than their present-day analogues (~ 1 M$_\odot$).

Life and death of the first stars

Being formed out of primordial gas, the first stars are metal-free. The nuclear fusion that powers the luminosities of stars must then proceed via proton-proton burning. Consequently, the first stars are much hotter than their present-day counterparts whose finite metallicity enables nuclear fusion to proceed via the more efficient CNO cycle. In fact, the first stars are found to resemble black-body emitters with black-body temperatures $T_{\rm bb} \approx 10^5$ K. As a result, the rate of emission of hydrogen (and helium) ionising photons by primordial stars may exceed that by present-day metal-enriched stars by more than an order of magnitude (e.g., Bromm, Kudritzki, & Loeb 2001; Schaerer 2002). The large masses of the first stars imply short stellar life-times. The final fates of the first stars depend on the precise values of their masses (e.g., Heger & Woosley 2002; for a review see Woosley, Heger, & Weaver 2002).

Stars with masses 10 M$_\odot \lesssim M \lesssim 30$ M$_\odot$ built up iron cores with masses in excess of the Chandrasekhar mass and hence collapse and explode as supernovae (SNe), enriching their surroundings with the products of their stellar nucleosynthesis. Stars with masses 30 M$_\odot \lesssim M \lesssim 140$ M$_\odot$ and masses $M > 260$ M$_\odot$, on the other hand, collapse into black holes that lock up most of the stellar material. The stellar black holes may provide the seeds for the massive ($10^5 - 10^9$ M$_\odot$) black holes observed as high-redshift quasars and at the centres of todays galaxies (e.g., Madau & Rees 2001; Volonteri & Rees 2005; Booth & Schaye 2009; Milosavljević et al. 2009). The death of stars in the mass-range 40 M$_\odot \lesssim M \lesssim 100$ M$_\odot$ is expected to be accompanied by a burst of gamma-rays. High-redshift gamma-ray burst are indeed observed and provide important observational probes of the epoch of reionisation (e.g., Ciardi & Loeb 2000; Salvaterra et al. 2009). For stars in the mass range 140 M$_\odot \lesssim M \lesssim 260$ M$_\odot$ no black hole is expected to form. These stars are instead disrupted in pair-instability SNe which leave no stellar remnants behind.

1.2.4 The transition to the ionised Universe

The first stars (and quasars) transformed the highly neutral post-recombination gas into a highly ionised plasma within only a few hundred million years (e.g., Sec. 1.1; Barkana & Loeb

2001). It is straightforward to see why the mere conversion of only trace amounts of gas into stars or black holes could have caused such a dramatic effect (Loeb & Barkana 2001): nuclear fusion releases $\sim 7 \times 10^6$ eV per hydrogen atom, and thin-disc accretion onto Schwarzschild black holes releases 10 times more energy. The ionisation of hydrogen requires, however, only 13.6 eV. It is therefore sufficient to convert a small fraction, i.e. $\sim 10^{-5}$, of the total baryonic mass into stars or black holes in order to reionise the Universe, at least if recombinations are unimportant.

Because of the spatially clustered distribution of stars and galaxies, the reionisation process is expected to have occurred in a highly inhomogeneous manner. The neutral gas in and around the overdense regions that host the first star-forming halos is generally ionised first. The low-density gas far away from the these first sites of star formation, on the other hand, only becomes reionised once the stellar ionising radiation is channelled into the large-scale underdense voids (Ciardi, Stoehr, & White 2003). Consequently, reionisation starts from the inside-out (e.g., Lee et al. 2008). The ionised regions powered by individual star-forming halos would then grow until they overlap. Thereafter, the reionisation process would reverse to proceed from the outside in, with ionising radiation slowly carving its way from the highly ionised voids into remaining dense pockets of neutral gas (Miralda-Escudé, Haehnelt, & Rees 2000).

Reionisation is therefore a (geometrically) highly complex process whose detailed understanding requires the use of radiative transfer simulations (Sec. 1.4). These simulations are, however, computationally extremely demanding. As an alternative, (semi-) analytical models (e.g., Madau, Haardt, & Rees 1999; Valageas & Silk 1999; Chiu & Ostriker 2000; Furlanetto, Zaldarriaga, & Hernquist 2004; Benson et al. 2006; Choudhury, Haehnelt, & Regan 2009; for a review on the semi-analytical treatment of galaxy formation see Baugh 2006) that go beyond the type of order of magnitude estimates presented in the beginning of this section may be employed. Two parameters crucially determine the predictions of such models: the average fraction $f_{\rm esc}$ of ionising photons that escape star-forming galaxies to ionise the intergalactic medium and the average recombination rate of the intergalactic gas, $\langle \alpha_{\rm rec}(T) n_{\rm e} n_{\rm HII} \rangle$, where $\alpha_{\rm rec}$ is the recombination rate coefficient (e.g., Osterbrock 1989), $n_{\rm e}$ is the electron number density and $n_{\rm HII}$ is the number density of ionised hydrogen. Note that the average recombination rate is proportional to the average of the square of the gas density if the gas is highly ionised and hence is highly sensitive to density fluctuations (Sec. 1.2.5). The fact that the values of both the escape fraction (e.g., Wise & Cen 2009; Gnedin, Kravtsov, & Chen 2008; Inoue, Iwata, & Deharveng 2006; Razoumov & Sommer-Larsen 2006) and the average recombination rate (e.g., Madau, Haardt, & Rees 1999; Pawlik, Schaye, & van Scherpenzeel 2009) are highly uncertain, currently presents one of the most severe obstacles for a quantitative modelling of the reionisation epoch.

1.2.5 Feedback from star formation

The first stars affect the properties of the surrounding intergalactic gas through the emission of radiation and the ejection of mass and metals, which may change the initial conditions for the formation of subsequent generations of stars and galaxies. This *feedback* from star formation on star formation may be both positive, i.e. it may facilitate the formation of subsequent stellar populations and/or the reionisation of the cosmic gas, and negative, i.e. it may impede subsequent star formation and/or reionisation. Stellar feedback may be broadly classified as thermal, radiative, mechanical and chemical. In this section we will present an outline of these four types of feedback. Detailed discussions may be found in the extensive reviews by, e.g., Barkana & Loeb 2001, Ciardi & Ferrara (2005) and Ciardi (2008).

The ionising radiation emitted by the first stars (and quasars) photo-heats the intergalactic gas to temperatures $T \sim 10^4$ K (e.g., Miralda-Escudé & Rees 1994; Hui & Haiman 2003; Tittley & Meiksin 2007), raising the cosmological Jeans mass (Eq. 1.1 with $\Delta = 1$) to values $\sim 10^9$ $\mathrm{M}_{\odot}$ (Eq. 1.1 with $\Delta = 1$). This *Jeans filtering* (Shapiro, Giroux, & Babul 1994; Gnedin & Hui 1998; Okamoto, Gao, & Theuns 2008) prevents the further assembly of gas in halos with virial temperatures $T_{\rm vir} \lesssim 10^4$ K, corresponding to virial masses $M_{\rm vir} \lesssim 10^8$ $\mathrm{M}_{\odot}$ (Eq. 1.3). Photo-heating furthermore evaporates gas that already assembled in halos of such low masses, significantly reducing the halo gas fractions (e.g., Thoul & Weinberg 1996; Barkana & Loeb 1999; Kitayama & Ikeuchi 2000; Shapiro, Iliev, & Raga 2004; Dijkstra et al. 2004; Susa & Umemura 2004; Iliev, Shapiro, & Raga 2005; Pawlik & Schaye 2009). Both effects lead to a strong suppression of star formation and hence provide a negative feedback on reionisation.

Photo-ionisation heating provides, however, also a positive feedback on reionisation, because the suppression of small-scale gas density fluctuations due to Jeans filtering reduces the average recombination rate of the intergalactic gas (e.g, Haiman, Abel, & Madau 2001; Wise & Abel 2005; Pawlik, Schaye, & van Scherpenzeel 2009). Less photons are then required to keep the intergalactic gas ionised, which facilitates the reionisation of the Universe. In Chapter 2 we will demonstrate that this positive feedback is, in fact, very strong. The evaluation of the net thermal feedback from photo-heating will require the use of radiation-hydrodynamical simulations.

In addition to copious amounts of ionising radiation, the first stars emit radiation in the Lyman-Werner absorption band of molecular hydrogen, characterised by frequencies 11.2 eV $\lesssim h_{\rm P}\nu \lesssim 13.6$ eV. This soft ultra-violet (UV), non-ionising radiation may propagate un-absorbed by neutral hydrogen and dissociate the molecular hydrogen in nearby star-forming regions. Because molecular hydrogen is the main coolant in halos with virial temperatures $T_{\rm vir} \sim 10^3$ K, which present the first sites of star formation in the hierarchical Universe, the presence of a photo-dissociating background is expected to substantially suppress early star formation (Haiman, Rees, & Loeb 1997). The efficient formation of stars may only continue with the (hierarchical) build-up of halos with virial temperatures $T_{\rm vir} \gtrsim 10^4$ K, in which the gas cools through the emission of de-excitation radiation from collisionally excited atomic hydrogen (e.g., Barkana & Loeb 2001).

Ionising radiation may, on the other hand, increase the ability of primordial gas of temperatures $T \sim 10^3$ K to cool. This is because the formation of molecular hydrogen is catalyzed by free electrons, whose abundance is increased by the presence of an ionising background. If the ionising spectrum is sufficiently hard (e.g. X-rays), then ionising photons may penetrate into the dense star-forming regions and counteract the photo-dissociations by soft UV photons. Stellar photons may therefore provide a positive feedback on star formation in halos with virial temperatures $T_{\rm vir} \sim 10^3$ K (e.g., Haiman, Rees, & Loeb 1996; Ricotti, Gnedin, & Shull 2002; Glover & Brand 2003; Machacek, Bryan, & Abel 2003). Note, however, that photo-ionisation reduces the ability of primordial gas to cool radiatively in halos with virial temperatures $T_{\rm vir} \gtrsim 10^4$ K (Efstathiou 1992; Wiersma, Schaye, & Smith 2009), because it reduces the abundance of neutral hydrogen, their main coolant.

SN explosions of massive stars typically inject a few solar masses of gas with velocity of $\sim 10^4$ km s^{-1}, corresponding to a kinetic energy of $\sim 10^{51}$ erg. The ejected material sweeps up and shock-heats the surrounding gas, entraining outflows sufficiently powerful to, at least temporarily, substantially reduce the gas fractions for low-mass halos (e.g., Yepes et al. 1997; Tassis et al. 2003; Scannapieco et al. 2006; Dalla Vecchia & Schaye 2008; Whalen et al. 2008). Since this leads to a suppression of the star formation rate, the mechanical feedback from SN explosions, like photo-evaporation, provides a negative feedback on reionisation. As shown in Pawlik & Schaye (2009) and in Chapter 3 of this thesis, the negative feedback from SN explosions may, moreover, be amplified by the presence of a photo-evaporating UV background.

SN explosions (in particular, pair-instability SN explosions) also provide a chemical feedback on the subsequent star formation process by enriching the intergalactic gas with the metals synthesised in the first stars. It is well-known that gravitationally collapsing metal-enriched gas clouds may cool more efficiently than their metal-free counterparts and hence become more easily unstable to fragmentation into low-mass proto-stellar clumps (e.g., Bromm et al. 2001). In fact, enrichment to metalicities as low as $Z \sim 10^{-4}\ Z_{\odot}$, where $Z_{\odot}$ is the solar metalicity, may be sufficient to trigger the transition from the high-redshift ($z \sim 10$) massive (~ 100 $M_{\odot}$, see Sec. 1.2.3) star formation mode to the more standard low-mass (~ 1 $M_{\odot}$) star formation mode observed today (e.g., Bromm et al. 2001; Schneider et al. 2002).

Thermal, radiative, mechanical and chemical stellar feedbacks will likely occur simultaneously and give rise to complicated non-linear interactions between very different physical processes (we already mentioned the interplay between SN mechanical feedback and photo-heating). Different feedback processes are, moreover, expected to affect the properties of the cosmic gas over very different scales. Radiative transfer effects like self-shielding will play a critical role in determining the efficiencies of the radiative/thermal feedbacks. Because of these complexities, investigations of stellar feedback generally require the use of numerical simulations (Sec. 1.4).

1.3 Observing the epoch of reionisation

The epoch of reionisation is one of the last missing links in the story of the formation and evolution of galaxies. Evidence for reionisation is circumstantial - reionisation has, to date, not been directly observed. The detection and analysis of reionisation signatures in the highly ionised, post-reionisation Universe already provide, however, many interesting constraints on the duration and character of this important epoch. We summarise some of these constraints here and briefly discuss the prospective of direct observations of reionisation. The reader is referred to the recent reviews by Fan, Carilli,& Keating (2006) and Furlanetto, Oh, & Briggs (2006) for more information.

Observations of the absorption of light from quasars by intervening gas put strong constraints on the ionisation state of the Universe. Residual neutral hydrogen imprints a forest of Ly-α absorption lines in the spectra of background quasars (see Rauch 1998 for a review). The fraction of light transmitted by the intergalactic gas rapidly decreases with increasing redshift until, at redshift $z \gtrsim 6$, complete absorption troughs appear. The first clear-cut detection of such Gunn-Peterson troughs (Gunn & Peterson 1965) was reported by Becker et al. (2001). The strong evolution in the transmissivity of the high-redshift gas indicates a qualitative change in the ionisation state of the Universe and is consistent with results of models and simulations in which reionisation ends at redshifts $z \gtrsim 6$ (e.g., Fan, Carilli,& Keating 2006).

CMB photons scatter off free electrons produced during reionisation. This smooths fluctuations in the CMB temperature anisotropies and, if the CMB temperature shows a quadrupole anisotropy, generates a polarisation signal on angular scales $\lesssim 10^{\circ}$ corresponding to the scale of the horizon at reionisation (e.g., Zaldarriaga 1997; Hu & White 1997; Kaplinghat et al. 2003; Komatsu et al. 2009). At very small angular scales ($< 0.1^{\circ}$), scattering off free electrons additionally generates anisotropies due to the Sunyaev-Zeldovich effect (Sunyaev & Zeldovich

1980), the Ostriker-Vishniac effect (Ostriker & Vishniac 1986; Vishniac 1987) and patchy reionisation (e.g., Santos et al. 2003). Observations of the CMB and its polarisation may therefore provide important constraints on the reionisation process. Indeed, the most recent analysis of CMB temperature fluctuations (using the observed fluctuations in the polarisation signal to break the degeneracy between the damping of CMB fluctuations due to reionisation and the amplitude of the primordial fluctuation power) that have been measured with the WMAP[7] satellite implies a best-fit reionisation redshift $z = 11.0 \pm 1.4$ (Komatsu et al. 2009; assuming complete instantaneous reionisation).

Observational estimates of the ultra-violet (UV) luminosity density at redshifts $z \gtrsim 6$ (e.g., Stanway, Bunker, & McMahon 2003; Bouwens et al. 2004; Sawicki & Thompson 2006; Bouwens et al. 2008) provide a potential probe of the types of sources that reionised the Universe. At present, it is controversial whether the observed population of galaxies is capable of keeping the Universe at redshifts $z \lesssim 6$ in a highly ionised state (e.g., Gnedin 2008; Bouwens et al. 2008; Yüksel et al. 2008; Pawlik, Schaye, & van Scherpenzeel 2009 and Chapter 2 of this thesis). The ability of galaxies to keep the intergalactic gas ionised depends on the rate at which these galaxies produce ionising photons (which is inferred from their UV luminosity), the fraction of ionising photons that escape into the intergalactic medium and the average recombination rate in the intergalactic gas (Madau, Haardt, & Rees 1999). All these quantities are currently highly uncertain, both from an observer's and from a theorist's perspective. A contribution from quasars and other ionising sources (e.g., Rees 1986; Tegmark, Silk, & Evrard 1993; Mapelli, Ferrara, & Pierpaoli 2006; Dijkstra 2006; Srbinovsky & Wyithe 2007; Loeb 2009), though likely sub-dominant (e.g., Faucher-Giguère et al. 2008; but see Volonteri & Gnedin 2009), can therefore not yet be excluded.

In the (near) future, the detection of the redshifted 21 cm signal from neutral hydrogen will provide a direct view on reionisation (Scott & Rees 1990; Madau, Meiksin, & Rees 1997; Furlanetto, Oh, & Briggs 2006 for a review). Ly-α absorption studies only probe the very last stages of reionisation (when the gas is highly ionised), because the Ly-α optical depth saturates already for trace amounts ($n_{\mathrm{HI}}/n_{\mathrm{H}} \gtrsim 10^{-4}$) of neutral hydrogen. The analysis of CMB fluctuations provides, on the other hand, mostly integral constraints on the reionisation process, because the electron scattering optical depth towards reionisation is insensitive to the details of the reionisation history. The detection of emission in 21 cm allows, at least in principle, to map out the neutral hydrogen density as a function of redshift in spheres around the observer. Several low-frequency radio arrays (LOFAR, MWA, 21CMA) are now being constructed to measure the statistical properties of the redshifted 21 cm signal. Eventually (~ 2020), SKA will provide high-resolution tomographic images of the spatial distribution of the neutral hydrogen during reionisation.

1.4 Simulating the epoch of reionisation

Cosmological simulations of reionisation are amongst the most promising techniques to study the epoch of reionisation. These simulations combine prescriptions for the gravitational growth of density fluctuations in the expanding Universe and prescriptions for the hydrodynamical evolution of the cosmic gas with recipes for star formation and associated feedback and also follow the propagation of ionising radiation emitted by the first ionising sources (see, e.g., the reviews by Yepes et al. 1997; Bertschinger 1998; Dolag et al. 2008). Unlike analytical or

[7] http://map.gsfc.nasa.gov

semi-analytical models, which often rely on the presence of symmetries and which are mostly designed for application with specific scenarios or certain limiting regimes, cosmological simulations enable the investigation of three-dimensional problems in all their complexity. Cosmological simulations therefore constitute the prime choice for investigations into the epoch of reionisation, promising the modelling of the formation and evolution of stars and galaxies and the reionisation of the intergalactic hydrogen from first principles.

It is, however, important to realise that our current ignorance of many of (the details of) the physical processes that determine the formation and evolution of galaxies and their interactions with the surrounding intergalactic gas implies that cosmological simulations often suffer from some of the same systematic limitations as (semi-) analytical models (e.g., Furlanetto, Oh, & Briggs 2006). In fact, most reionisation simulations employ *sub-resolution* models that encode complex physics in an often simplified, sometimes heuristic, manner (e.g., Dolag et al. 2008). This introduces free parameters that require careful calibrations with results from other simulations and/or observations, just as is the case for (semi-) analytical models. Numerical simulations are, moreover, often compromised because of the lack of sufficiently powerful computational algorithms and resources. Simulating reionisation remains a computationally demanding task. In the following we will discuss some of the main challenges posed by the desire to incorporate the transport of ionising radiation into cosmological simulations of structure formation and reionisation.

Representative models of the Universe during reionisation require simulation boxes with sizes of several tens to hundreds of comoving Mpc (e.g., Barkana & Loeb 2004; Iliev et al. 2006). In simulations with smaller boxes, cosmic variance may give rise to results that are not representative of the cosmic mean. For example, the mass of the most massive halo clearly cannot exceed the total mass of the simulated volume. Large simulation boxes are also needed to capture statistically significant samples of ionised regions, which have typical sizes of up to tens of comoving Mpc (e.g., Furlanetto, Zaldarriaga, & Hernquist 2004; Furlanetto, McQuinn, & Hernquist 2006). Simulation boxes must, moreover, be sufficiently large to account for the modulation of density fluctuations by long wavelength modes. This means that the box size must be chosen such that density fluctuations averaged at the scale of the box remain negligible. Large simulation boxes are also important for predictions of the performance of future epoch-of-reionisation observatories, whose field of view will comprise large parts of the sky (e.g., Mellema et al. 2006a).

The hierarchical character of structure formation (Sec. 1.2.2) makes simulating reionisation in large boxes a very computationally demanding task. If cooling by molecular hydrogen is important, the first stars form in halos with masses as small as $\sim 10^6\ \mathrm{M}_\odot$ (Sec. 1.2.3). Even if one assumes that most of the molecular hydrogen is quickly destroyed by Lyman-Werner photons from the very first stars, the mass of the first star-forming halos is only increased to $\sim 10^8\ \mathrm{M}_\odot$ (Sec. 1.2.5), which is still very small. Simulations that aim to resolve the first sites of star formation in large simulations consequently require a large number of resolution elements, which is computationally expensive. The only way to perform such simulations is then to employ simulation methods that are parallelised for use with distributed memory machines.

In addition to very high mass resolution, simulating reionisation requires very high spatial resolution. The first star-forming halos exhibit structure on scales of the order of 10 (proper) kpc and less. Fluctuations in the intergalactic gas may occur on equally small scales (although it helps that Jeans filtering due to reionisation heating erases most of them, see Sec. 1.2.5). Simulating large representative cosmological volumes at such high spatial resolution while keeping the number of resolution elements low to ensure affordable computation times requires the use of spatially adaptive simulation techniques. Fortunately, such techniques, which comprise Adaptive Mesh Refinement (AMR; Berger & Colella 1989) and Smoothed Particle Hydrodynamics (SPH; Gingold & Monaghan 1977; Lucy 1977), are now routinely employed in state-of-the-art cosmological hydrodynamical simulations. We note in passing that SPH currently is arguably the most widely employed technique for large-scale structure formation simulations (see, e.g., Monaghan 2005 and Agertz et al. 2007 for discussions of the advantages and disadvantages of SPH and AMR).

The most severe challenge for simulating reionisation is probably the need to incorporate the transport of ionising radiation into the large spatially adaptive cosmological simulations described above. Computing the ionising intensity throughout the simulation box requires solving the seven-dimensional (three space coordinates, two directional coordinate, frequency and time) radiative transfer equation. This is a formidable task, not only because of the high dimensionality of the problem, but also because of the large number of ionising sources contained in typical cosmological volumes. To accomplish it, existing approaches (e.g., Gnedin & Abel 2001; Ciardi et al. 2001; Nakamoto, Umemura, & Susa 2001; Maselli, Ferrara, & Ciardi 2003; Razoumov & Cardall 2005; Mellema et al. 2006b; Susa 2006; Ritzerveld & Icke 2006; McQuinn et al. 2007; Semelin, Combes, & Baek 2007; Trac & Cen 2007; Pawlik & Schaye 2008; Aubert & Teyssier 2008; Altay, Croft, & Pelupessy 2008; Petkova & Springel 2009; Finlator, Özel, & Davé 2009) to solve the radiative transfer equation in cosmological simulations of reionisation often resort to a number of approximations.

Recently, the accuracy of several existing radiative transfer codes has been assessed in test simulations performed as part of a series of comparison projects (Iliev et al. 2006; Iliev et al. 2009). The results of the comparisons are encouraging, indicating that the participating codes have reached a certain level of maturity and reliability (Iliev et al. 2009). It should, however, be kept in mind that the design of most of the test simulations was kept rather simple in order to facilitate comparisons between different radiative transfer codes. Whether or not the approximations employed by current radiative transfer codes allow the accurate treatment of the radiative transfer problem in the complex setting of large-scale simulations of reionisation thus remains to be seen.

Radiative transfer codes that are both spatially adaptive and parallel on distributed memory are still rare (see Table 1 in Iliev et al. 2006 and Table 1 in Iliev et al. 2009). Most of even the most advanced reionisation simulations are therefore performed on uniform grids that contain relatively few grid points. Combined with the fact that large simulation boxes are necessary to model representative volumes of the Universe, this means that the spatial resolution of state-of-the-art radiative transfer simulations of reionisation is typically far below that of the underlying spatially adaptive hydrodynamical simulations. In fact, many radiative transfer simulations of reionisation ignore hydrodynamical effects altogether and assume the gas traces the dark matter. Small-scale structure in the cosmic gas is therefore often hardly accounted for.

This lack of adequate spatial resolution affects, for instance, the computation of recombination rates, whose precise knowledge is crucial to the understanding of the progress and topology of reionisation (e.g., Choudhury, Haehnelt, & Regan 2009; Chapter 6 of this thesis). At present, the effects of small-scale gas clumpiness on the recombination rate of the intergalactic gas are, at best, only included in a statistical manner by using pre-compiled sets of clumping factors obtained from high-resolution (re-)simulations of small parts of the original cosmological volume (e.g., Iliev et al. 2007; Kohler, Gnedin, & Hamilton 2007). Note that the lack of adequate spatial resolution also implies that the fraction of ionising photons that escape the star-forming galaxies to ionise the intergalactic gas, i.e. the escape fraction, is not computed self-consistently and hence constitutes an additional free parameter. The fact that the escape fractions of star-forming galaxies are degenerate with their ionising luminosities renders estimates of, for instance, the number of photons required to reionise the Universe difficult, if not impossible, and prevents tight constraints on the nature of the ionising sources.

Cosmological simulations typically contain millions of stellar ionising sources (e.g., Iliev et al. 2006). Large numbers of ionising sources pose a challenge to simulations of reionisation because most of the existing radiative transfer methods require computation times that scale linearly with the source number. The usual practice of reducing the number of ionising sources by combining sources that fall into the same cells of a superimposed mesh renders reionisation simulations feasible, but also reduces the spatial resolution at which the radiative transfer is performed. Note that the inclusion of diffuse radiation emitted by recombining ions further increases the number of ionising sources. It is then common to treat this recombination radiation using the on-the-spot approximation (e.g., Osterbrock 1989), assuming it is re-absorbed in the immediate vicinity of the recombining ion. The validity of this approximation in the context of large-scale reionisation simulations remains to be assessed (e.g., Ritzerveld 2005).

Radiative transfer simulations of reionisation are typically performed by post-processing pre-computed static density fields. This static approximation is appropriate for simulating the initial phase of rapid growth of ionised regions, which often proceeds at speeds close to the speed of light, or the propagation of ionisation fronts on cosmological scales (see, e.g., the discussion in Iliev et al. 2006). Once the speed of ionisation fronts becomes comparable to the sound speed of the ionised gas, the static approximation becomes, however, inapplicable and a full radiation-hydrodynamical treatment is required. In any case, the static approximation breaks down after about a sound-crossing time, as the Jeans filtering of the gas can then no longer be ignored. Although thermal feedback from reionisation is known to play a key role (see Sec. 1.2.5), its effects are ignored in almost all of the current large-scale reionisation simulations. Some simulations try to include the effects of reionisation heating at the expense of a detailed treatment of the radiative transfer problem by employing photo-heating rates computed in the optically thin limit (e.g., Gnedin & Abel 2001; Pawlik, Schaye, & van Scherpenzeel 2009 and Chapter 2 of this thesis). The main drawback of such an approach is that it ignores the ability of gas to shadow and self-shield (e.g., Kitayama & Ikeuchi 2000; Susa & Umemura 2004; Dijkstra et al. 2004).

Current cosmological simulations provide invaluable insights into the physics of reionisation and enable first predictions for future observational campaigns. These simulations also reveal the limitations of the currently employed numerical techniques, triggering the exploration of novel approaches to address the numerical challenges outlined above. Several methods are now available to accomplish the transport of ionising radiation in a spatially adaptive manner (e.g., Gnedin & Abel 2001; Susa 2006; Ritzerveld & Icke 2006; Razoumov & Sommer-Larsen 2006; Trac & Cen 2007; Pawlik & Schaye 2008; Altay, Croft, & Pelupessy 2008; Petkova & Springel 2009). Other methods have been designed to avoid the scaling of the computation time with the number of ionising sources (e.g., Gnedin & Abel 2001; Cen 2002; Pawlik & Schaye 2008; Petkova & Springel 2009). Still other radiative transfer methods are available for direct use in step with hydrodynamical simulations (e.g., Gnedin & Abel 2001; Pawlik & Schaye 2008; Altay, Croft, & Pelupessy 2008; Petkova & Springel 2009), and some of these methods even include the radiation-hydrodynamical feedback (Gnedin & Abel 2001; see also table 1 in Iliev et al. 2009). The application of these methods in large-scale cosmological simulations of reionisation is likely to lead to new discoveries and to significantly advance our understanding of one of the last unknown epochs in the history of the Universe.

1.5 THESIS OUTLINE

In this section we give brief summaries of the contents of Chapters 2-7 of this thesis. The main scientific contribution of this thesis is the development of a novel method to solve the radiative transfer problem in large cosmological smoothed particle hydrodynamics simulations (Chapters 4 and 5). This scheme - TRAPHIC (TRAnsport of PHotons In Cones) - is designed to address and overcome the main challenges posed by simulations of reionisation: the huge dynamic range they exhibit, requiring the simultaneous simulation of the physics on both very small and very large scales, and the large number of ionising sources they contain. It is one of the first of a new generation of radiative transfer schemes that are developed to incorporate the spatially adaptive transport of ionising radiation into large-scale structure formation simulations of our Universe in an efficient and accurate manner.

Chapter 2. The critical star formation rate density required to keep the intergalactic hydrogen ionised depends crucially on the average rate of recombinations in the intergalactic medium (IGM). This rate is proportional to the clumping factor $C \equiv \langle\rho_{\rm b}^2\rangle_{\rm IGM}/\langle\rho_{\rm b}\rangle^2$, where $\rho_{\rm b}$ and $\langle\rho_{\rm b}\rangle$ are the local and cosmic mean baryon density, respectively and the brackets $\langle\rangle_{\rm IGM}$ indicate spatial averaging over the recombining gas in the IGM. We perform a suite of cosmological smoothed particle hydrodynamics simulations that include radiative cooling to calculate the volume-weighted clumping factor of the IGM at redshifts $z \geq 6$. We focus on the effect of photo-ionisation heating by a uniform ultra-violet background and find that photo-heating strongly reduces the clumping factor because the increased pressure support smoothes out small-scale density fluctuations. Because the reduction of the clumping factor makes it easier to keep the IGM ionised, photo-heating provides a positive feedback on reionisation. We demonstrate that this positive feedback is in fact very strong: even our most conservative estimate for the clumping factor ($C \approx 6$) is five times smaller than the clumping factor that is usually employed to determine the capacity of star-forming galaxies to keep the $z = 6$ IGM ionised. Our results imply that the observed population of star-forming galaxies at $z \approx 6$ may be sufficient to keep the IGM ionised, provided that the IGM was reheated at $z \gtrsim 9$ and that the fraction of ionising photons that escape the star-forming regions to ionise the IGM is larger than ≈ 0.2.

Chapter 3. Photo-heating associated with reionisation and kinetic feedback from core-collapse supernovae (SNe) have previously been shown to suppress the high-redshift cosmic star formation rate. Here we investigate the interplay between photo-heating and SN feedback using a set of cosmological, smoothed particle hydrodynamics simulations. We show that photo-heating and SN feedback mutually amplify each other's ability to suppress the star formation rate. Our results demonstrate the importance of the simultaneous, non-independent inclusion of these two processes in models of galaxy formation to estimate the strength of the total negative feedback they exert. They may therefore be of particular relevance to semi-analytic models in which the effects of photo-heating and SN feedback are implicitly assumed to act independently of each other.

Chapter 4. We present TRAPHIC, a novel radiative transfer scheme for Smoothed Particle Hydrodynamics (SPH) simulations. TRAPHIC (TRAnsport of PHotons In Cones) is designed for use in simulations exhibiting a wide dynamic range and containing a large number of light sources. It is adaptive both in space and in angle and can be employed for application on distributed memory machines. The (time-dependent) radiative transfer equation is solved by tracing individual photon packets in an explicitly photon-conserving manner directly on the unstructured grid traced out by the set of SPH particles. To accomplish directed transport of radiation despite the irregular spatial distribution of the SPH particles, photons are guided inside cones. The expensive scaling of the computation time with the number of light sources that is encountered in conventional radiative transfer schemes is avoided by introducing a source merging procedure.

Chapter 5. We present and test a parallel numerical implementation of our radiative transfer scheme TRAPHIC, specified for the transport of mono-chromatic hydrogen-ionising radiation, in the smoothed particle hydrodynamics code GADGET-2. The tests comprise several radiative transfer problems of increasing complexity. Some of these tests have been specifically designed to investigate TRAPHIC's ability to solve the radiative transfer problem in the large cosmological reionisation simulations that it was developed for, while others have been designed to demonstrate that TRAPHIC can also be employed in more general contexts. The results of all tests are in excellent agreement with both analytic solutions and numerical reference results obtained with state-of-the-art radiative transfer codes.

Chapter 6. Radiative transfer (RT) simulations coupled to cosmological hydrodynamical simulations are one of the most promising numerical tools to study reionisation, a key epoch in the high-redshift Universe. Current generations of RT schemes are, however, often limited for use with uniform and relatively coarse grids that imply a spatial resolution far below that of state-of-the-art spatially adaptive hydrodynamical simulations. Small-scale structure in the cosmic gas is then, at best, only statistically accounted for. Here we use the spatially adaptive RT scheme TRAPHIC (Chapter 4) to investigate the implications of this approximate approach. We contrast RT simulations performed on spatially adaptive smoothed particle hydrodynamics density fields with RT simulations performed on density fields that are defined on a uniform grid. Comparisons of the evolution of the mean ionised fraction, of the dependence of the ionised fraction on the local gas density and of power spectra of the 21 cm signal from neutral hydrogen reveal substantial differences caused by the difference in the dynamic range employed by the two types of RT simulations. Our results underpin earlier suggestions that ignoring the inhomogeneous distribution of gas on small scales, as is typically done in current RT simulations of reionisation, can give rise to misleading conclusions about the spatial distribution of the ionised gas and hence affect the interpretation of current and the predictions of future observations of reionisation.

Chapter 7. The temperature of the cosmic gas is a key astrophysical observable. The detailed modelling of its evolution with cosmological hydrodynamical simulations requires the use of radiative transfer methods to accurately compute the effects of photo-ionisation and photo-heating on the relevant cooling and heating rates. We extend our implementation of TRAPHIC to compute the non-equilibrium evolution of the temperature of gas exposed to hydrogen-ionising radiation. We verify this extension by comparing TRAPHIC's performance in thermally coupled radiative transfer test simulations with reference solutions obtained with other radiative transfer codes.

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