COSMIC REIONIZATION ON COMPUTERS. I. DESIGN AND CALIBRATION OF SIMULATIONS

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ABSTRACT

Cosmic Reionization On Computers is a long-term program of numerical simulations of cosmic reionization. Its goal is to model fully self-consistently (although not necessarily from the first principles) all relevant physics, from radiative transfer to gas dynamics and star formation, in simulation volumes of up to 100 comoving Mpc, and with spatial resolution approaching 100 pc in physical units. In this method paper, we describe our numerical method, the design of simulations, and the calibration of numerical parameters. Using several sets (ensembles) of simulations in 20 $h^{-1}$ Mpc and 40 $h^{-1}$ Mpc boxes with spatial resolution reaching 125 pc at $z = 6$, we are able to match the observed galaxy UV luminosity functions at all redshifts between 6 and 10, as well as obtain reasonable agreement with the observational measurements of the Gunn–Peterson optical depth at $z < 6$.

Key words: cosmology: theory – galaxies: formation – intergalactic medium – large-scale structure of universe – methods: numerical

Online-only material: color figures

1. INTRODUCTION

The study of cosmic reionization has been highlighted by the last decadal survey as one of the most promising areas of astrophysical research in the current decade. Progress in this area directly influences many other fields of astrophysics, from thermal evolution of the Lyman forest to properties of early galaxies.

Because the observational constraints on reionization are limited, theoretical modeling, including numerical simulations, play a relatively larger part in reionization studies than in many other fields of modern astrophysics. Historically, simulations of reionization were mostly confined to two opposite limits: simulations of small spatial volumes with detailed treatment of relevant physics, or large volume simulations with simplified physical modeling (Iliev et al. 2009a; Aubert & Teyssier 2010; Friedrich et al. 2011; Ahn et al. 2012; Shapiro et al. 2012; Trac & Gnedin 2009 for a review of the earlier work). Both approaches suffer from serious limitations. Small-box simulations can model individual ionizing sources with sufficient physical detail, but fail to account for the large-scale correlations between them. Large-box simulations include these correlations, but, by ignoring gas dynamics, are not able to model ionizing sources self-consistently. The inability of the simulations to include all relevant scales resulted in a recent surge in semi-numerical and purely analytical approximate methods (Furlanetto et al. 2004, 2006; Furlanetto & Oh 2005; Choudhury & Ferrara 2005, 2006; Zahn et al. 2007, 2011; Mesinger & Furlanetto 2007; Alvarez & Abel 2007; Shull & Venkatesan 2008; Mitra et al. 2011, 2012; Venkatesan & Benson 2011; Mesinger et al. 2011; Kuhlen & Faucher-Giguère 2012; Alvarez & Abel 2012; Zhou et al. 2013; Battaglia et al. 2013; Robertson et al. 2013; Kauvar & Gnedin 2013; Sobeck & Mesinger 2014).

That is where Moore’s Law comes to the rescue. The unrelenting exponential increase in supercomputing power means that sooner or later the gap between small- and large-box simulations is going to be bridged. In fact, this time is now—the new generation of supercomputing platforms that have recently been and are planned to be deployed in the US,4 the so-called petascale platforms (since they get close to or exceed 10^{15} floating-point-operations per second), are particularly suitable for large-scale simulations of reionization that treat fully self-consistently the radiative transfer of ionizing radiation and gas dynamics.

Taking advantage of this technological progress, we have started a Cosmic Reionization On Computers (CROC) project that aims, over the course of several years, to produce numerical simulations of reionization that model fully self-consistently (although not necessarily from the first principles) all relevant physics, from radiative transfer to gas dynamics and star formation, in simulation volumes of up to 100 comoving Mpc and with spatial resolution approaching 100 pc in physical units.

In this first paper of a series, we focus primarily on the technical aspects of our simulations, such as the description of the numerical method, simulation design, and the calibration of simulation parameters. We will present the original scientific results from our simulations in subsequent publications.

2. NUMERICAL TOOLS

Our main simulation tool is the Adaptive Refinement Tree (ART) code (Kravtsov 1999; Kravtsov et al. 2002; Rudd et al. 2008). The ART code is an implementation of the adaptive mesh refinement technique with the Fully Threaded Tree data structure (Khokhlov 1998). It includes a wide range of physical processes that make it particularly suitable for modeling cosmic reionization. Specifically, the current version of the code includes the following physical ingredients (in addition to standard ingredients of gravity, dark matter, and gas dynamics).

Cooling and heating of hydrogen and helium is computed “on the fly,” taking into account all relevant processes in a time-dependent manner, without any assumptions of photoionization

4 For example, “Stampede” at Texas Advanced Computing Center, “Kraken” at Oak Ridge National Laboratory, “Hopper” and “Edison” at the Livermore-Berkeley Laboratory, “Mira” at Argonne National Laboratory, “Blue Waters” at NCSA, etc.
or collisional equilibrium. Abundance of heavy elements is tracked self-consistently in ART, but, in the most general case, computing the full dependence of the cooling and heating functions on the incident radiation field is a complex task in itself, and cannot be currently implemented exactly in cosmological simulations, unless the radiation field is constant in space (Kravtsov 2003; Wiersma et al. 2009).

Since the latter is not a reasonable assumption during reionization or in the ISM of galaxies, ART uses the approximate method of Gnedin & Hollon (2012) which allows the computation of the metallicity-dependent part of the cooling and heating functions for an arbitrary time-dependent and spatially variable radiation field. ART, thus, is able to account for several physical effects that are missed in most other cosmological simulations codes, such as suppression of cooling in strong radiation fields, dependence of the LTE temperature on the radiation spectrum, etc. (see Gnedin & Hollon (2012) for some representative examples).

Radiative transfer of ionizing and ultraviolet radiation is currently implemented in ART using the Optically Thin Variable Eddington Tensor (OTVET) approximation of Gnedin & Abel (2001). While OTVET is an approximation, it has been extensively tested against exact schemes (Iliev et al. 2006a, 2009b). The Iliev et al. tests underscored one undesirable feature of the original ART implementation of the OTVET method—excessive numerical diffusion around ionization fronts. The implementation of the OTVET scheme in ART was substantially revised after those tests, and the currently used approach eliminates numerical diffusion almost completely; a full description of our current implementation of OTVET is presented in Appendix C. Thus, OTVET remains a highly suitable method for modeling cosmic reionization (see Gnedin & Abel 2001, for detailed discussion of the limitations and inaccuracies of OTVET).

In our simulations, we include ionizing radiation from stars fully self-consistently (in a time-dependent and spatially inhomogeneous manner), because it is the primary driver of the reionization process. We only include other sources of ionizing radiation (quasars, recombination radiation from helium that can ionize hydrogen, bremsstrahlung, etc.) in the cosmic background because these sources are either weakly clustered (helium recombination radiation) or too rare to significantly affect the radiation field in a typical region of the universe (bright quasars). Both components—the radiation from local sources and the radiation from distant sources (i.e., cosmic background)—are treated separately in ART and then combined together to derive a single solution of the radiative transfer equation (see Appendix C). The advantage of this approach is that it allows the contribution of rare sources (like quasars) to the cosmic background to be accounted for without actually requiring an impractically large simulation volume.

Contributions from helium recombination and bremsstrahlung can be easily computed exactly. Our model for the quasar contribution is presented in Appendix A.

Of course, the cosmic background is only important if the mean free path of ionizing photons is sufficiently large, so that the radiation field from distant sources is comparable to or above the radiation field from local sources at a typical location in the universe.

Since we are running several independent realizations for each set of numerical parameters, the post-reionization evolution of the intergalactic medium would not be captured correctly if we computed the mean free path for the cosmic background from within one simulation box—periodic boundary conditions will extend that box over the whole universe, whereas it is supposed to represent just one sub-volume of the universe, and only the full set of independent realizations should be treated as a numerical model for the whole universe. Hence, we use the fit from Songaila & Cowie (2010) to account for Lyman limit absorptions in the cosmic background; the background is then still subject to local absorptions inside shielded regions, as captured by the radiative transfer solver in Equation (C7). Radiation from local ionizing sources is absorbed fully self-consistently with the actual simulated gas distribution in the box (Equation (C4)).

Molecular hydrogen chemistry (both gas-phase and dust-based) can be followed in complete detail in ART (Gnedin & Kravtsov 2011). However, since the spatial resolution of our simulations (≳ 100 pc) is too coarse to resolve the scale heights of galactic disks, it would make little sense to use the full molecular chemistry module in this work. Instead, we use the fitting formulae of Gnedin & Draine (2014), derived from a large set of small-volume, high resolution simulations, to reliably account for the environmental dependence of the molecular gas on such ISM properties as dust-to-gas ratio or local interstellar radiation field. These fitting formulae are similar to the ones presented in Gnedin & Kravtsov (2011), but they also account for the overlap of damping wings of separate absorption lines in the Lyman–Werner band at high molecular column densities.

Star formation cannot yet be modeled from first principles in cosmological simulations and needs to be implemented with a phenomenological “sub-grid” model. In the last several years an important observational advance was made in understanding star formation on galactic scales. Both local (Leroy et al. 2008, 2012, 2013; Bigiel et al. 2008, 2011; Bolatto et al. 2011) and intermediate redshift (Genzel et al. 2010; Daddi et al. 2010; Tacconi et al. 2013) observational studies find that the star formation rate surface density on several hundred pc scales correlates well, and approximately linearly, with the surface density of molecular gas. We use this observed correlation to define our star formation recipe in an entirely empirical manner,

\[ \Sigma_{\text{SFR}} = \frac{\Sigma_{\text{H}_2}}{\tau_{\text{SF}}} \]  

(1)

where \( \Sigma_{\text{SFR}} \) is the star formation rate surface density, \( \Sigma_{\text{H}_2} \) is the surface density of the molecular gas (including the contribution of helium), and \( \tau_{\text{SF}} \) is the molecular gas depletion timescale.

We ignore the slightly sub- or super-linear slopes sometimes found in observations, since with our resolution we are only able to resolve a modest range of surface densities where the difference between an exactly linear and a slightly non-linear slope is negligible.

The current most widely accepted viewpoint is that the depletion timescale \( \tau_{\text{BW}} \approx 1–2 \) Gyr for normal star-forming galaxies. We use the value of \( \tau_{\text{SF}} = 1.5 \) Gyr as fiducial, and explore the effect of varying this parameter on our results below.

Stellar feedback is implemented in our simulations with the current industry standard “blastwave” or “delayed cooling” model (Stinson et al. 2009, 2013; Governato et al. 2010; Agertz et al. 2011, 2013; Brook et al. 2012). While this model is purely phenomenological, it is known to reproduce many of the observed properties of real galaxies well, and, hence, is an appropriate numerical tool at present. The delay timescale \( \tau_{\text{BW}} \) is a parameter that we vary as part of the simulation calibration.
procedure. Our fiducial value of $\tau_{BW} = 10$ Myr is consistent with the use of this feedback model in the field.

**Ionizing radiation from stars** is a dominant contributor to the global reionization process. The exact amount and spectrum of that radiation depend on stellar initial mass function (IMF) and on local absorption inside the galaxy (usually quantified by "escape fractions"). For our modeled stars we use a fixed Kroupa IMF; the shape of the ionizing spectrum is adopted from Starburst99 modeling (Leitherer et al. 1999) and is plotted in Figure 4 of Ricotti et al. (2002a). The total UV and ionizing luminosities of a single-age stellar population with mass $m_*$ and metallicity $Z_*$ can be computed with Starburst99; we fit numerical results with the following formula:

$$L_{UV} = \epsilon_{UV} \times 10^{-4} \frac{m_* c^2}{Z_*^0 \Gamma(1 + 0.27 Z_*)} f(t),$$

where $f(t)$ is such that

$$\int_0^t f(t) \, dt = \frac{x(0.8 + x^2)}{1 + x(0.8 + x^2)},$$

and $x = t/(3 \text{ Myr})$. At late times ($t \gg 10$ Myr) the ionizing emissivity from a single-age stellar population falls off with time more rapidly than UV light. Our fit behaves in between the ionizing and UV emissivities, since our OTVET implementation ignores the contribution of Pop III stars. This is, necessarily, a simplification. Recent studies of the transition from Pop III to Pop II star formation modes (Ricotti et al. 2002a, 2002b; Wise & Abel 2008; Wise & Cen 2009; Wise et al. 2012; Muratov et al. 2013a, 2013b) demonstrated that the transition is rapid and occurs early on, and hence the contribution of Pop III stars to the global reionization budget is small. However, if in the future these studies are shown to be incorrect, our simulations should then be considered as a strict lower limit that only accounts for ionizing radiation from the currently observed stars and quasars.

Another source of ionizing photons that we do not include is annihilation radiation from dark matter. We leave the exploration of this reionization source to future work.

### 3. DESIGN OF THE SIMULATIONS

#### 3.1. Resolution Requirements

The spatial resolution is constrained by the range of scales on which our star formation model is valid, hence we do not vary it in this paper. The mass resolution is a simulation parameter, and, hence, needs to be set carefully. There are several physical arguments that can be used to pick up important mass scales, but the eventual choice of the mass resolution must be done in a convergence study.

The strictest requirement is that all halos that can cool via atomic hydrogen line cooling ($M_{\text{tot}} \gtrsim (1–2) \times 10^6 M_\odot$) need to be resolved (Gnedin & Ostriker 1997; Gnedin 2000; Iliev et al. 2006b; Trac & Cen 2007; Zahn et al. 2007; McQuinn et al. 2007; Trac et al. 2008; Pawlik et al. 2009). That requirement may be an overkill, though, since dwarf galaxies in the Local Group contain only a few stars (e.g., Kravtsov 2009, and references therein)—if these galaxies are typical of dwarf galaxies at high redshift, the mass resolution requirements may be relaxed.

We present the detailed analysis of the mass convergence properties of our simulations in the Appendix D. The optimal resolution for our simulation, measured as the total "equivalent particle mass" $M_1$ (the sum of the masses of a single dark matter particle and an average mass of a baryonic cell in the absence of refinement, or the mass of a single dark matter particle compensated by the ratio of $\Omega_M/\Omega_{DM}$), would be about $10^4 M_\odot$, which is equivalent of resolving a, say, 20 h$^{-1}$ Mpc box (in comoving units) with 1024$^3$ dark matter particles. As Appendix D shows, such a simulation would account for 80% of all ionizing photons.

Unfortunately, such a resolution is still too computationally expensive at present, so as our fiducial mass resolution we adopt an eight times coarser resolution of $7 \times 10^4 M_\odot$ (resolving a 20 h$^{-1}$ Mpc box with 512$^3$ dark matter particles). With this coarser resolution we account for about 55% of all ionizing photons and for 70% of ionizing emissivity at $z = 6$. At present such precision is sufficient to match the existing observational data; by the time the James Webb Space Telescope significantly expands observational samples, faster supercomputing platforms will allow us to increase our mass resolution to the equivalent of 1024$^3$ particles in a 20 h$^{-1}$ Mpc box.

Because in ART the number of dark matter particles throughout the simulation remains fixed, while cells of the adaptive mesh are created and destroyed dynamically, it is more convenient to quantify the resolution in terms of the number of dark matter particles. Each simulation starts with the same number of adaptive mesh cells as dark matter particles to ensure the consistency of the mass resolution in two main gravitating components. As the simulation proceeds, the number of cells usually grows with time, so that by the end of the simulation the number of cells is a factor of several higher than the number of dark matter particles.

Our fiducial simulation series is presented in Table 1. Each of the simulations in the series is run with an additional six levels of refinement (except B20HR, which is run with five levels of refinement, to maintain the same spatial resolution as other runs), achieving the same cell size of 125 pc in proper units at $z = 6$ (145 pc at $z = 5$), with the actual spatial resolution being a factor of $\sim 3$ worse. Such resolution is well matched to the range of scales on which the star formation model given by Equation (1) is observationally tested.

| Run         | Box Size (comoving) | Resolution (proper at $z = 6$) | Number of DM Particles |
|-------------|---------------------|--------------------------------|------------------------|
| Fiducial series |                     |                                |                        |
| "B20"       | 20 h$^{-1}$ Mpc     | 125 pc                         | 512$^3$                |
| "B40"       | 40 h$^{-1}$ Mpc     | 125 pc                         | 1024$^3$               |
| "B80"       | 80 h$^{-1}$ Mpc     | 125 pc                         | 2048$^3$               |
| Convergence study |                 |                                |                        |
| "B20LR"     | 20 h$^{-1}$ Mpc     | 125 pc                         | 256$^3$                |
| "B20HR"     | 20 h$^{-1}$ Mpc     | 125 pc                         | 1024$^3$               |
In this paper we only present results from 20 \, h^{-1} \text{Mpc} and 40 \, h^{-1} \text{Mpc} boxes. A simulation with the 80 \, h^{-1} \text{Mpc} box is currently feasible to complete on the largest available machines, but it is sufficiently computationally expensive (requiring 20–30 million CPU hours depending on the platform); with the computational resources available to us, we will only be able to afford one per year beginning in 2014.

3.2. Running Sets of Simulations

Even our largest “B80” simulations, with the 80 \, h^{-1} \text{Mpc} box size, will be only marginally large enough for obtaining convergent results on the distribution of sizes of ionized regions or on observable properties of high-redshift galaxies. Thus, in order to extend the reach of our simulations, we run sets of independent realizations of initial conditions for each particular choice of box size and simulation parameters, accounting for the cosmic variance on the scale of the box size.

This variance is commonly referred to as the “DC mode.” The ART code supports the DC mode in arbitrary cosmology without any approximations, following the method described in Gnedin et al. (2011). In fact, as has been shown in that paper, if a set of independent realizations with a given box size properly accounts for the DC mode, it becomes statistically equivalent to a simulation with a several times larger box.

Table 2 lists all sets of simulations that we present in this paper. We have performed several sets of 20 \, h^{-1} \text{Mpc} that serve as our primary parameter exploration data. We extract most of the science results from two sets of three independent realizations of the 40 \, h^{-1} \text{Mpc} box. We highlight in boldface the fiducial set B20.sf1.uv2.bw10. One of the largest existing observational data sets on the sources of reionization are the UV luminosity functions of high-redshift galaxies. Matching them would validate our star formation model, which we delegate to Appendix B, as it has only a modest effect on our results (and no effect at all at \( z > 7 \)).

![Figure 1. Ultraviolet galaxy luminosity functions from a combination of simulation sets B20.sf1.uv2.bw10 and B40.sf1.uv1.bw10 at six different redshifts. Lines with bands show the average luminosity functions with the rms variation over our effective 3.75 \, h^{-1} \text{Mpc} boxes (the error of the mean is, respectively, a factor of \( \sqrt{3.75} = 1.9 \) smaller). Circles with error bars are a compilation of recent observational measurements (Bouwens et al. 2007, 2011; Oesch et al. 2012, 2013, 2014; Bradley et al. 2012; Schenker et al. 2013; Willott et al. 2013; Bowler et al. 2014). Different redshifts are shifted vertically by 1 dex for clarity. (A color version of this figure is available in the online journal.)](image)

4. CALIBRATION OF THE SIMULATIONS

4.1. Star Formation Model

One of the largest existing observational data sets on the sources of reionization are the UV luminosity functions of high-redshift galaxies. Matching them would validate our star formation and feedback models.

As our final simulation data, we combine the fiducial 20 \, h^{-1} \text{Mpc} and 40 \, h^{-1} \text{Mpc} sets (B20.sf1.uv2.bw10 and B40.sf1.uv1.bw10). Six independent realizations of the 20 \, h^{-1} \text{Mpc} box are equivalent, by volume, to 0.75 of a single 40 \, h^{-1} \text{Mpc} box, increasing our fiducial set from 3 to 3.75 40 \, h^{-1} \text{Mpc} boxes.

In order to predict UV luminosities of our model galaxies, we use the Flexible Spectral Population Synthesis (FSPS) code (Conroy et al. 2010; Conroy & Gunn 2010). One complication in computing stellar luminosities in far-UV is a proper account of cosmic dust. A fully self-consistent dust model would require a complex and computationally expensive ray tracing through the simulated galaxies, and is beyond the scope of this first paper. Instead, we adopt a simple but reasonable dust obscuration model, which we delegate to Appendix B, as it has only a modest effect on our results (and no effect at all at \( z > 7 \)).

Figure 1 presents the primary result of this paper, the evolution of the galaxy UV luminosity function between \( z = 10 \) and...
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Figure 2. Ultraviolet galaxy luminosity functions for simulation sets with varied parameters of the star formation model. The timescale for delayed cooling \( \tau_{\text{SF}} \) and the depletion time \( \tau_{\text{BW}} \) (i.e., star formation efficiency) do affect the computed luminosity functions, but not in a directly proportional way due to the well-known self-regulation of star formation.

(A color version of this figure is available in the online journal.)

\( z = 5 \) from our simulations, and its comparison with the existing observational measurements.\(^5\) The simple star formation model of Equation (1) is able to reproduce the observations for all \( z > 5 \). The agreement becomes worse at low luminosities at \( z = 5 \), and that is not particularly surprising—since our simulations maintain fixed resolution in comoving units, the spatial resolution degrades as simulations evolve, and the feedback model becomes progressively less accurate, especially in the low-mass galaxies.

The sensitivity of our star formation model to the numerical parameters \( \tau_{\text{SF}} \) and \( \tau_{\text{BW}} \) is explored in Figure 2. To compare apples and apples, we use only three independent realizations D–F from our fiducial set B20.sf1.uv2.bw10, and compare them with simulation sets B20.sf1.uv2.bw40, B20.sf2.uv2.bw10, and B20.sf2.uv2.bw40 (which only included three simulations, D–F, each, and were only continued to \( z = 5.7 \), to save computational resources). A longer timescale \( \tau_{\text{BW}} \) for delayed cooling does have a significant effect on the simulated galaxies, but not a directly proportional one—the luminosity functions for the set B20.sf1.uv2.bw40 match the fiducial set very well if shifted horizontally by about 0.5 magnitude, which corresponds to only a factor of 1.6. The sensitivity of our star formation model to the star formation timescale \( \tau_{\text{SF}} \) (or, equivalently, to star formation efficiency) is stronger—a change in \( \tau_{\text{SF}} \) by a factor of two makes a similar 0.5 magnitude change of the simulated luminosity functions, but the effect is still substantially sub-linear. Finally, since the two parameters have opposite effects, a higher star formation efficiency (lower \( \tau_{\text{SF}} \)) can always be compensated by stronger feedback (longer \( \tau_{\text{BW}} \), as illustrated by the set B20.sf2.uv2.bw40. That result should not be surprising at all; it is well established that stellar feedback “self-regulates” star formation on kiloparsec scales (Schaye et al. 2010; Agertz et al. 2011, 2013; Hopkins et al. 2011; Hopkins et al. 2013). The sensitivity of our star formation model to numerical parameters is somewhat higher than is usually found at lower redshifts, reflecting the fact that complete self-regulation takes some time to get established; that is also consistent with prior work (e.g., Schaye et al. 2010; Agertz et al. 2011).

Another observational constraint on our star formation model is offered by the observed UV continuum slopes of high-redshift galaxies. To measure the UV continuum slopes of model galaxies, we compute the monochromatic fluxes at 1300 Å, 1400 Å, 1500 Å, 1600 Å, and 1700 Å for our fiducial B20.sf1.uv2.bw10 set,\(^6\) and fit a power-law relation \( F_\lambda \propto \lambda^\beta \) using a simple least-squares fit in a log–log plane. In Figure 3 we show the average UV continuum slopes measured from our simulations and the rms scatter around them, as well as observational measurements at \( z = 5–7 \). Our simulations match the observed slopes at \( z = 5 \) rather well, but do not reproduce the trend of bluer spectra of brighter galaxies at \( z = 6 \) and \( z = 7 \).

The latter discrepancy is somewhat surprising, since by matching the whole evolution of luminosity functions our simulations reproduce not only star formation rates at a given redshift, but the whole prior star formation histories of galaxies. Nevertheless, it is possible to come up with several potential reasons for the discrepancy: our dust obscuration model (Appendix B) may be overly simplistic (since it is independent of the galaxy luminosity), the FSPS code may not be sufficiently accurate, as may the observational, broadband-based diagnostics for the true spectral slope; finally, our star formation and stellar feedback models may be too crude. For all these reasons, we leave resolving this apparent discrepancy to future work.

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\(^5\) The exact values of redshifts are matched to the Hubble filters used in the observations: \( z = 5.0, 5.9, 6.8, 8.0, 9.0, 10.0 \).

\(^6\) Such calculations would be too computationally expensive for all B40.sf1.uv1.bw10 simulations, and are not really needed.
4.2. Ionizing Emissivity

Our star formation model, specified by parameters $\epsilon_{\text{SF}}$ and $\epsilon_{\text{BW}}$, appears to work reasonably well. The last remaining parameter in the simulations that needs to be calibrated is the escape fraction up to the simulation resolution limit $\epsilon_{\text{UV}}$. This parameter can be calibrated with the observed spectra of high-redshift quasars—ionizing emissivity of our sources is proportional to $\epsilon_{\text{UV}}$, and, therefore, the whole process of reionization and its aftermath—the Ly$\alpha$ forest at $z = 5$–6—is affected by $\epsilon_{\text{UV}}$.

In order to model absorption spectra of high-redshift quasars, we compute synthetic Ly$\alpha$ spectra along 1000 totally random lines of sight at several simulation snapshots. Since simulations use periodic boundary conditions, we extend each line of sight to twice the simulation box size—random lines of sight in a periodic universe are only weakly affected by the artificial periodicity if they do not extend beyond twice the box length. For the $20\, h^{-1}$ Mpc box that corresponds to about $\Delta z = 0.15$ at $z = 6$, which is a typical redshift resolution for averaging properties of Ly$\alpha$ spectra in observed spectra (Fan et al. 2006b).

In Figure 4 we show the evolution of the mean Gunn–Peterson optical depth and the volume-weighted H$\alpha$ fraction in four of our simulation sets: three $20\, h^{-1}$ Mpc boxes with $\epsilon_{\text{UV}} = 0.1$, 0.2, and 0.4, and our fiducial $40\, h^{-1}$ Mpc box. There are several conclusions that can be drawn from that figure.

First, changing ionizing emissivity by a factor of two changes the moment of overlap of ionizing bubbles, indicated by the sharp drop in the volume-weighted mean H$\alpha$ fraction (Gnedin 2000, 2004; Gnedin & Fan 2006), by about $\Delta z \approx 0.5$.

Second, the opacity of the post-reionization Ly$\alpha$ forest are best matched by $\epsilon_{\text{UV}} = 0.2$ value independently of the box size.

Third, and most importantly, we do not yet reach numerical convergence at the box size of $40\, h^{-1}$ Mpc; the fact that our fiducial sets B20.sf1.uv2.bw10 and B40.sf1.uv1.bw10 have different values of the $\epsilon_{\text{UV}}$ parameter, but similar reionization histories, indicates that even three independent realizations of a $40\, h^{-1}$ Mpc box are not enough to obtain an accurate prediction for the mean Gunn–Peterson optical depth or the volume-weighted mean neutral fraction.

Finally, our simulations do not match the observational points at $z \gtrsim 6$ particularly well. However, we do not consider that a serious problem exactly for the third reason above: our sets of simulation boxes sample the Ly$\alpha$ forest at each redshift interval way better than the observational measurements, and yet they are still far from convergence. Hence, the observational values are not the converged results either, and the discrepancy between the observational constraints and our simulations does not necessarily imply a major failure of our physical model, but may also be due to just cosmic variance.

Large cosmic variance is further illustrated in Figure 5, where we show the average Gunn–Peterson optical depth and the volume-weighted mean H$\alpha$ fraction for all six independent realization of our fiducial B20.sf1.uv2.bw10 set. As one can see, the variations from realization to realization are very large (recall that the $20\, h^{-1}$ Mpc box is well-matched to the redshift bin of observational measurement of $\Delta z \approx 0.15$), and two of our realizations go through the observational points reasonably well.

The reason for such a large sensitivity to cosmic variance is in the extreme non-linearity of the relationship between the Gunn–Peterson optical depth $\tau_{\text{GP}}$ and the gas density, which makes $\tau_{\text{GP}}$ extremely sensitive to outliers. For example, consider $N$ lines of sight at some redshift during reionization, of which only one has non-zero transmitted flux $F_1$. The average flux over $N$ lines is $F_1/N$, and the corresponding Gunn–Peterson optical depth is

$$\tau_{\text{GP}} = -\ln (F_1/N) = \tau_1 + \ln N,$$
where $\tau$ is the Gunn–Peterson optical depth along that one line of sight with partial absorption. In observations, typically only a few lines of sight contribute to a given redshift bin, i.e., $N = 3–5$. Hence, a single line of sight with $\tau_1 = 10$ (an observational value at $z = 6.2$) results in the measured “average” of $T_G \approx 11.1–11.6$, only slightly above $\tau_1$.

Based on this reasoning, we use only post-reionization Ly$\alpha$ data ($z < 6$) for calibrating our simulations, and rely on the derived volume-weighted mean H i fraction from Fan et al. (2006b) as preferred calibration data, even if the Gunn–Peterson optical depth is a directly observed quantity—$(X_{HI})_V$ is, effectively, a convolution over the whole distribution function of observed Ly$\alpha$ fluxes in individual spectral pixels, just like $\tau_{GP}$, but it is more sensitive to typical values of the transmitted flux, while $\tau_{GP}$ is heavily weighted toward the tail of the distribution. In that sense it is a less biased, even if less direct, observational probe.

Hence, our preferred value for the parameter $\epsilon_{UV}$ is between 0.1 and 0.2 (with 0.2 matching observations better); the computational expense of simulations (and lack of convergence between $20 h^{-1}$ Mpc and $40 h^{-1}$ Mpc boxes) prevents us from actually fitting for the value of $\epsilon_{UV}$ to higher precision.

5. CONCLUSIONS

The CROC project is a long-term simulation campaign for modeling the process of cosmic reionization in sufficiently large simulations volumes (above 100 Mpc) with detailed physical modeling and spatial resolution better than $0.5$ kpc (simulation cell size of less than 150 pc).

A simple model of star formation and feedback, based on the linear Kennicutt–Schmidt relation in the molecular gas and a widely used “delayed cooling” or “blastwave” feedback, is able to reproduce the observed galaxy UV luminosity functions in the whole redshift range $z = 6–10$ with a value for the molecular gas depletion time of $\tau_{eff} = 1.5$ Gyr, consistent with observations at $z \sim 0$ and $z = 1–2$.

A reasonable choice for the $\epsilon_{UV}$ parameter, a quantity that describes photon losses on scales unresolved in our simulations, of $\epsilon_{UV} = 0.1–0.2$ results in reionization history that is reasonably consistent with the observed opacity of the $\tau_{GP}$ forest in the spectra of Sloan Digital Sky Survey quasars at $z < 6$. An even better consistency can be achieved by fitting the simulations to the data, albeit at (presently unrealistically) large computational expense.

The observed increase in the Gunn–Peterson optical depth at $z > 6$ (Fan et al. 2006b) has been interpreted by several groups (including ours) as evidence for the reionization overlap (Becker et al. 2001; White et al. 2003; Gnedin 2004; Fan et al. 2006a; Gnedin & Fan 2006). That increase is, however, subject to large cosmic variance; with six independent realizations, each corresponding to multiple lines of sight, we find a spread in the redshift of overlap of about $\Delta z \approx 1$. Since the observational constraints have even less statistical power than our simulations, they have not yet converged on the true evolution of the average Gunn–Peterson optical depth, and may, therefore, be significantly biased.

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Simulations used in this work have been performed on the Joint Fermilab-KICP cluster “Fulla” at Fermilab, on the University of Chicago Research Computing Center cluster “Midway,” and on National Energy Research Supercomputing Center (NERSC) supercomputers “Hopper” and “Edison.”

APPENDIX A

MODEL FOR QUASAR SOURCES

For the intrinsic quasar spectral energy distribution we use our own fit to the Richards et al. (2006) model,

\[
\nu L_\nu \approx \frac{9.5 \times 10^{-5}}{(1 + (h \nu/300 eV)^{1/2})^6 e^{-h \nu/500 keV}} + \frac{10 eV/h \nu}{(1 + (9 eV/h \nu)^{3/2})^6} + 5.8 e^{-h \nu/0.2 eV}.
\]

The evolution of the bolometric quasar luminosity function has been determined by Hopkins et al. (2007). We fit the quasar bolometric luminosity density as a function of redshift as

\[
L_{QSO}(z) = 10^{7.7} L_{\odot} \frac{Mpc^3}{\text{h}^{-3} \text{Mpc}^3} \left(10^{1.2(z-4)} / \text{h} \right)^{1/3} + \left[3e^{-2.7z} \right]^{1/3} \text{dex},
\]

and we use a $k$-correction of $k_{Cor} = 3.9$ to translate from the bolometric to ionizing quasar luminosity.

APPENDIX B

DUST OBSCURATION MODEL

In this work we adopt a simple, but reasonable, dust obscuration model for our simulated galaxies, in which the dust optical depth at wavelength $\lambda$ is estimated as

\[
\tau_\lambda = \sigma_D(\lambda) Z_\star N_{eff}.
\]

where $N_{eff}$ is a parameter to be calibrated from the observational data, $Z_\star$ is the stellar metallicity in solar units, and $\sigma_D(\lambda)$ is the dust cross-section at solar metallicity. For the specific extinction law, we take the Small Magellanic Cloud (SMC) dust (Weingartner & Draine 2001), since most of our simulated galaxies at $z = 5–6$ have metallicities similar to SMC, and normalize it to solar metallicity by assuming the SMC metallicity of $-0.7$ dex (see Gnedin et al. 2008, for details),

\[
\sigma_D(\lambda) = 1.76 \times 10^{-21} \text{cm}^2 \left(\frac{1500 \text{ Å}}{\lambda}\right)^{1.1}.
\]

Figure 6 shows the observational constraints on the dust abundance in $z = 5$ and $z = 6$ galaxies from Bouwens et al. (2009). Our simple dust obscuration model can roughly match these constraints with the value of $N_{eff} \approx 5 \times 10^{21}$ cm$^{-2}$. At $z > 7$ the observational constraints are consistent with no dust obscuration (Bouwens et al. 2009, 2011); to account for that we adopt an extremely crude but simple ansatz for $N_{eff}$:

\[
N_{eff} = 5 \times 10^{21} \text{cm}^{-2} \text{min}(1, \text{max}(0, 0.5(8-z)))
\]

($N_{eff} = 5 \times 10^{21}$ cm$^{-2}$ for $z \leq 6$, $N_{eff} = 0$ for $z \geq 8$, and is linearly interpolated in between to avoid discontinuities). With that ansatz the dust obscuration at $z = 7$ is not identically zero, but is small enough to be unimportant and undetectable observationally.
The frequency dependence of $\bar{\nu}$ where

$\bar{\nu}$ is the spatially and angle-averaged specific intensity, $k_{\nu}$ is the absorption coefficient (per unit comoving distance), and $S_{\nu}$ is the source function (in appropriate units).

Equation, the source function (in appropriate units).

Applying the ansatz (C2) to Equation (C2). That particular form, however, ensures that $f_{\nu}$ and $g_{\nu}$ always remain non-negative, which is a desirable property for a numerical implementation (as it avoids numerical loss of precision).

Equation (C2) is nothing more than an ansatz, we replaced one unknown function with two, hence we can impose a condition on these two functions. The condition we impose is that terms with $f_{\nu}$ and $g_{\nu}$ cancel out separately. In the following we drop the frequency subscripts for brevity; all quantities except $\rho_S$ remain functions of frequency. In addition, we adopt a Newtonian approximation for $f$ and $g$, omitting terms with the Hubble
parameter for them, but retaining cosmological terms for $\tilde{J}$, (see Gnedin & Abel 2001, for more detailed description of this approximation). With these simplifications, one obtains

$$
\tilde{f}[-\tilde{k}\tilde{J} + \tilde{S}] - Lf \frac{a}{c}\frac{\partial \tilde{g}}{\partial t} + (\tilde{J} - L\tilde{g}) \frac{Df}{dt} + L \frac{Dg}{dt}
= - (\tilde{J} - L\tilde{g}) \tilde{k}f - Lkg + L\rho_S,
$$

(C3)

where we use a shorthand

$$
\frac{D}{dt} \equiv \frac{a}{c}\frac{\partial}{\partial t} + n\frac{\partial}{\partial x}
$$

for the derivative along the light cone.

The condition we impose is then

$$
\frac{Dg}{dt} = -kg + \rho_S,
$$

(C4)

which, in the Newtonian limit (ignoring terms with 1/c), has a simple solution,

$$
g(t, x, n) = \int_0^\infty \rho_S(t, x + nl)e^{-\tau(x, x + nl)} dl,
$$

(C5)

where $\tau(x_1, x_2)$ is the optical depth between points $x_1$ and $x_2$,

$$
\tau(x_1, x_2) = |x_1 - x_2| \int_0^1 ds \, k(x_1 + s(x_1 - x_2)).
$$

An even more familiar form is the angle average of $g$,

$$
\langle g \rangle(t, x) = \frac{1}{4\pi} \int d^3x' \, \rho_S(x') e^{-\tau(x, x')},
$$

which is simply an integral of $\rho_S/(4\pi r^2)$ over all sources, diminished by the opacity between the source and the current location. In particular, $g$ is manifestly positive everywhere in the computational domain.

Using Equation (C4) in Equation (C3), we find

$$
(\tilde{J} - L\tilde{g}) \left[ \frac{Df}{dt} + kf \right] = f[\tilde{k}\tilde{J} - L\tilde{\rho}_S] + Lf \frac{a}{c}\frac{\partial \tilde{g}}{\partial t}.
$$

(Averaging Equation (C4) over space and angle results in

$$
\frac{a}{c}\frac{\partial \tilde{g}}{\partial t} = -(kg) + \tilde{\rho}_S.
$$

Combining the last two equations together, we find

$$
(\tilde{J} - L\tilde{g}) \left[ \frac{Df}{dt} + kf \right] = f[\tilde{k}\tilde{J} - L(kg)].
$$

(C6)

Finally, we can use Equation (C2) to compute the average absorption,

$$
\tilde{k}\tilde{J} \equiv \langle J \rangle = (\tilde{J} - L\tilde{g})(kg) + L(kg).
$$

Substituting $\langle k \rangle$ from the above equation into Equation (C6), we obtain the final equation for the function $f$,

$$
\frac{Df}{dt} = -kf + f(kf).
$$

(C7)

Equations (C4) and (C7) are our master equations for the cosmological radiative transfer. At this point no approximations have been made except for the assumptions A1 and A2 above.

One undesirable property of Equation (C7) is that it numerically unstable. To see that, we can average it over space and angle,

$$
\frac{a}{c}\frac{\partial \tilde{f}}{\partial t} = (kf)(\tilde{f} - 1).
$$

(C8)

Value $\tilde{f} = 1$ is indeed a solution of this equation, but an unstable one: $(\partial \tilde{f}/\partial t) > 0$ for $\tilde{f} > 1$ and $(\partial \tilde{f}/\partial t) < 0$ for $\tilde{f} < 1$. To circumvent this problem, we multiply the last term in Equation (C7) by a function $q(\tilde{f})$,

$$
\frac{Df}{dt} = -kf + q(\tilde{f})f(kf),
$$

(C9)

where $q(1) = 1$. It is easy to show that, if $q'(1) < -1$, then Equation (C9) is numerically stable.

A fiducial choice for $q$ is

$$
q(x) = \frac{2}{x} - 1,
$$

but, in the future, other forms for that function need to be explored.

C.2. OTVET Approximation in the Two-field Ansatz

Gnedin & Abel (2001) show how to derive a single diffusion-like equation for the angle average of fields $f$ and $g$. Namely, if

$$
F_f(t, x) = \frac{1}{4\pi} \int d\Omega f_f(t, x, n),
$$

$$
G_f(t, x) = \frac{1}{4\pi} \int d\Omega g_f(t, x, n),
$$

then (again omitting the frequency dependence for brevity)

$$
\frac{\partial G}{\partial \xi} = \frac{\partial}{\partial \xi} \left( \frac{1}{k} \frac{\partial F}{\partial x^j} \right) - kG + \rho_S,
$$

(C10)

$$
\frac{\partial F}{\partial \xi} = \frac{\partial}{\partial \xi} \left( \frac{1}{k} \frac{\partial G h_{\nu j}^{\nu}}{\partial x^i} \right) - kF + q(\tilde{F})F(kF),
$$

(C11)

where $d\xi = \hat{c} dt/(2a)$, $\hat{c} \leq c$ is the “reduced speed of light” (Gnedin & Abel 2001), and averaging in Equation (C11) is done over the space (obviously, $\tilde{F} = \bar{F}$).

We choose different Eddington tensors in Equations (C10) and (C11): for a cosmological simulation in a periodic box, $h_{\nu j}^{\nu}$ is chosen as the optically thin Eddington tensor from all sources inside a periodic box, while the Eddington tensor for the background radiation is taken to be isotropic, $h_{\nu j}^{\nu} = \delta^{ij}/3$.

C.3. Elliptic Solver for OTVET Diffusion-like Equation

Consider an OTVET-type equation for some function $E(\xi, x)$ and some tensor $h^{ij}(\xi, x)$,

$$
\frac{\partial E}{\partial \xi} = \frac{\partial}{\partial \xi} \left( \frac{1}{k} \frac{\partial E h^{ij}}{\partial x^i} \right) - kE + s,
$$

(C12)

where $k(\xi, x)$ is the absorption coefficient and $s(\xi, x)$ is the source term. This equation is discretized in some fashion in
space on a set of indices \( I \), where \( I \) may be an smoothed particle hydrodynamics (SPH) particle number, a set of indices \( (i, j, k) \) on a regular mesh, or any other discretization. We assume that the discretization is such that all quantities on a regular mesh, or any other discretization. We assume that the discretization is such that all quantities \( E_i, h_{i,j,k} \), and \( s_i \) are co-located in space on the same set of resolution elements \( I \).

The discretization scheme is associated with a spatial scale \( \Delta x \) (cell size on a regular mesh, SPH kernel size, etc.). Each cycle of the OTVET solver (for example, a time step of a hydro scheme) consists of the set of consecutive iterations, which we label as \( E^{(n)} \), where \( n = 0, 1, 2, \ldots \).

The second-order term in Equation (C12) is discretized as

\[
\frac{\partial}{\partial x^j} \left( \frac{1}{k} \frac{\partial E h^j}{\partial x^j} \right) \approx \frac{1}{\Delta x} \hat{D}_I [E; a],
\]

where \( a_I \equiv k_I \Delta x \) is the dimensionless absorption coefficient and \( \hat{D}_I [E; a] \) is a linear operator on the set of all values \( E_I \),

\[
\hat{D}_I [E; a] = \sum_J w_{I,J} E_J,
\]

with the sum being over all indices \( J \). Dimensionless weights \( w_{I,J} \) depend on various \( a_I \) as appropriate, and most \( w_{I,J} \) are zero because the second-order term only has a finite support.

For example, for a regular mesh with \( I = (i, j, k) \),

\[
\hat{D}_I [E; a] = \frac{U^x_{i+1,j,k} - U^x_{i,j,k}}{a_{i+1/2,j,k}} + \frac{U^x_{i-1,j,k} - U^x_{i,j,k}}{a_{i-1/2,j,k}} + \frac{U^y_{i,j+1,k} - U^y_{i,j,k}}{a_{i,j+1/2,k}} + \frac{U^y_{i,j-1,k} - U^y_{i,j,k}}{a_{i,j-1/2,k}} + \frac{U^z_{i,j,k+1} - U^z_{i,j,k}}{a_{i,j,k+1/2}} + \frac{U^z_{i,j,k-1} - U^z_{i,j,k}}{a_{i,j,k-1/2}},
\]

where \( a_{i+1/2,j,k} = (a_{i,j,k} + a_{i+1,j,k})/2 + \epsilon \), and a small offset \( \epsilon = 10^{-3} \) is added to avoid division by zero (we have verified that it has no effect on the actual solution). Fluxes \( U^j \) are defined as

\[
U^y_{i,j,k} = E_{i,j,k} h^y_{i,j,k} + \frac{1}{4}(E_{i+1,j,k} h^y_{i+1,j,k} + E_{i-1,j,k} h^y_{i-1,j,k} + E_{i,j+1,k} h^y_{i,j+1,k} + E_{i,j-1,k} h^y_{i,j-1,k} + E_{i,j+1,k} h^y_{i,j+1,k} + E_{i,j-1,k} h^y_{i,j-1,k}),
\]

\[
U^z_{i,j,k} = E_{i,j,k} h^z_{i,j,k} + \frac{1}{4}(E_{i+1,j,k} h^z_{i+1,j,k} + E_{i-1,j,k} h^z_{i-1,j,k} + E_{i,j+1,k} h^z_{i,j+1,k} + E_{i,j-1,k} h^z_{i,j-1,k} + E_{i,j+1,k} h^z_{i,j+1,k} + E_{i,j-1,k} h^z_{i,j-1,k}),
\]

et.

Let us define two new, iteration-independent, discretized quantities,

\[
A_I \equiv \frac{\gamma}{1 + \gamma (\beta a_I - w_{I,I})} \quad \text{and} \quad B_I \equiv s_I \Delta x - (1 - \beta) a_I E^{(0)}_I,
\]

where \( \alpha, \beta, \gamma \) are constants.

Then one iteration of the OTVET elliptic solver consists of computing

\[
d^{(n+1)}_I = \hat{D}_I [E^n; a] - \beta a_I E^n_I + B_I,
\]

for all \( I \), followed by updating \( E_I \) as

\[
E^{(n+1)}_I = E^{(n+1)}_I + \alpha A_I d^{(n)}_I.
\]

Numerical stability requires \( \alpha < 1 \). A set of values that works particularly well is

\[
\alpha = 0.8, \quad \beta = 0.1, \quad \gamma = 1.
\]

The left panel of Figure 7 shows the error in the propagation of the ionization front as a function of time in Test 1 of Iliev et al. (2006a). This is the most sensitive to the iteration count of all tests presented in Iliev et al. (2006a) and Iliev et al. (2009b). As one can see, about 30 iterations are sufficient to achieve 2% precision in the ionization front evolution, and a mere 10 iterations already give 5% precision. The right panel of the same figure shows the improvement in tracking the ionization front with the new scheme. It should be compared with Figure 6.
of Iliev et al. (2006a); now the quality of OTVET solution approaches that of the best ray-tracing schemes.

**APPENDIX D**

**MASS CONVERGENCE TEST**

In order to test mass convergence in our simulations, we compare three 20 $h^{-1}$ Mpc runs with different particle counts (and, hence, mass resolutions): the lowest resolution B20LR.sf1.uv2.bw10 (256$^3$ particles, total equivalent particle mass $M_1 = 5 \times 10^5M_\odot$), the fiducial B20.sf1.uv2.bw10 (512$^3$ particles, total equivalent particle mass $M_1 = 7 \times 10^6M_\odot$), and the highest resolution B20HR.sf1.uv2.bw10 (1024$^3$ particles, total equivalent particle mass $M_1 = 9 \times 10^7M_\odot$). Figure 8 shows the luminosity functions at $z = 6$–10 (except for B20LR.sf1.uv2.bw10) on the left panel and the cumulative star formation rate density on the right panel.

In numerical analysis it is customary to extrapolate the results at finite resolution in order to estimate the convergence. We extrapolate the cumulative star formation rate density $\rho_\ast(<M_h|M_1)$ as a function of the simulation resolution $M_1$ to the limit $M_1 \to 0$ by adopting the functional form

$$\rho_\ast(<M_h|M_1) = \rho_\ast(<M_h|0) \exp(-\alpha(M_h)M_1^\beta(M_h)) \quad (D1)$$

and fitting three parameters $\rho_\ast(<M_h|0)$, $\alpha(M_h)$, and $\beta(M_h)$ from the three simulation values for $M_1 = 9 \times 10^5M_\odot$, $7 \times 10^6M_\odot$, and $5 \times 10^7M_\odot$ in each bin of halo mass $M_h$. Admittedly, the adopted functional form is somewhat arbitrary; we checked several different functional forms and found this one to provide the best fits to the simulation results. It can also be justified by noticing that extrapolation is often more precise in logarithmic space, and the ansatz (D1) is a simple power-law extrapolation in the log space.

With such extrapolation, we can estimate the completeness of our simulations for the total star formation rate as a function of redshift. The highest resolution B20HR.sf1.uv2.bw10 accounts for 90% of all star formation at $z = 6$ and for 60% at $z = 10$. Our fiducial runs include 70% of all star formation at $z = 6$ but only 20% of all star formation at $z = 10$. For the total, integrated over time production of ionizing radiation, the highest resolution run B20HR.sf1.uv2.bw10 misses 20% of all ionizing photons, while the fiducial runs miss 45%.

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