Prediction of the 21-cm signal from reionization: comparison between 3D and 1D radiative transfer schemes

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ABSTRACT
Three-dimensional radiative transfer simulations of the epoch of reionization can produce realistic results, but are computationally expensive. On the other hand, simulations relying on one-dimensional radiative transfer solutions are faster but limited in accuracy due to their more approximate nature. Here, we compare the performance of the reionization simulation codes GRIZZLY and C2-RAY which use 1D and 3D radiative transfer schemes respectively. The comparison is performed using the same cosmological density fields, halo catalogues and source properties. We find that the ionization maps, as well as the 21-cm signal maps from these two simulations are very similar even for complex scenarios which include thermal feedback on low mass halos. The comparison between the schemes in terms of the statistical quantities such as the power spectrum of the brightness temperature fluctuation agree with each other within 10% error throughout the entire reionization history.

GRIZZLY seems to perform slightly better than the semi-numerical approaches considered in Majumdar et al. (2014) which are based on the excursion set principle. We argue that GRIZZLY can be efficiently used for exploring parameter space, establishing observations strategies and estimating parameters from 21-cm observations.

Key words: radiative transfer - galaxies: formation - intergalactic medium - cosmology: theory - dark ages, reionization, first stars

1 INTRODUCTION

The Epoch of reionization (EoR), when the primordial neutral hydrogen (H I) in the intergalactic medium (IGM) was ionized by the radiation from the first sources, is one of the milestone events in the evolution of the Universe. However, many important facts such as the exact timing of this event, the sources responsible for reionization, the impact of the EoR on the later stages of the structure formation, etc. are currently not or poorly known. Various probes of the EoR such as observations of high-redshift quasars (Becker et al. 2001; Fan et al. 2006; Goto et al. 2011; Mortlock et al. 2011; McGreer et al. 2015), the cosmic microwave background radiation (CMB) (Zaldarriaga & Seljak 1997; Komatsu et al. 2011; Planck Collaboration et al. 2016b,a), high-redshift galaxies (Kashikawa et al. 2011; Bouwens et al. 2015; Mitra et al. 2015) and Lyα emitters (McQuinn et al. 2007b; Dijkstra et al. 2011; Choudhury et al. 2015) have been used to constrain some of these unknown facts. However, these probes can only provide limited information. For example, combining the observations of high-redshift quasars and the CMB, one can constrain the probable period of the event to lie between redshifts 15 and 6 (Fan et al. 2006; Malhotra & Rhoads 2006; Choudhury & Ferrara 2006; Mitra et al. 2011, 2012).

The evolving redshifted 21-cm signal from the H I in the IGM has the potential to revolutionize our understanding of reionization (Furlanetto et al. 2006; Morales & Wyithe 2010; Pritchard & Loeb 2012). Therefore a range of low frequency radio telescopes such as the Giant Metrewave Radio Telescope (GMRT)1 (Ghosh et al. 2012; Paciga et al. 2013), the Precision Array for Probing the Epoch of Reionization (PAPER)2 (Parsons et al. 2014), the

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1 http://www.gmrt.tifr.res.in
2 http://eor.berkeley.edu/
Murchison Widefield Array (MWA)\(^3\) (Bowman et al. 2013; Tingay et al. 2013) and the Low Frequency Array (LOFAR)\(^4\) (van Haarlem et al. 2013; Patil et al. 2017) are attempting to detect this faint signal from the EoR. The primary aim of these first generation experiments is to detect the signal in terms of statistical quantities such as the variance, skewness, power spectrum, etc. However, future radio telescopes such as the Square Kilometre Array (SKA)\(^5\) should have enough sensitivity to produce image cubes of the signal (Mellema et al. 2015; Ghara et al. 2016).

A large number of theoretical models based on either analytic calculations (e.g., Furlanetto et al. 2004; Paranjape & Choudhury 2014), semi-numerical simulations (Zahn et al. 2007; Mesinger & Furlanetto 2007a; Santos et al. 2008; Choudhury et al. 2009), or numerical simulations with radiative transfer (Iliev et al. 2006b; Mellema et al. 2006; McQuinn et al. 2007a; Shin et al. 2008; Baek et al. 2009; Thomas et al. 2009; Ghara et al. 2015) have been used to study the redshifted 21-cm signal from the EoR. Through these works a fair amount of theoretical understanding of the impact of various physical processes on the signal has been achieved. Aspects which have been considered include the impact of different kind of sources to the redshifted 21-cm signal, thermal feedback and peculiar velocities of the gas in the IGM. The simulations are not only important to extract information from the observations, but also to design observation strategies.

One thing to keep in mind is that the 21-cm observations do not provide direct information about the properties of the sources responsible for ionizing the IGM, minimum mass of the dark matter halos forming stars, thermal feedback, the effect of peculiar velocities of the gas in the IGM, etc. Due to the complexity of the astrophysical effects, one needs to use simulations to extract this information from the observations. In principle, this can be done using parameter estimation techniques such as the Markov chain Monte Carlo (MCMC) (Greig & Mesinger 2015) or artificial neural networks (Shimabukuro & Semelin 2017) in which the observations expressed in quantities such as power spectrum, variance or skewness will be compared to the outputs of the simulations.

The various simulation methods each have their own advantages and drawbacks and when using their results to design observation strategies or to interpret the observational data, one needs to keep in mind the various assumptions made by the models. While simulations of the 21-cm signal from the EoR using 3D radiative transfer methods such as Iliev et al. (2006b); Mellema et al. (2006) are assumed to be the most accurate ones, these require supercomputer facilities to run. On the other hand, simulations performed with semi-numerical methods are orders of magnitudes faster, the simplifying assumptions needed for this may lead to accuracy issues. Thus, it is absolutely necessary to compare the performance of different simulation techniques with each other so as to identify the advantages and drawbacks of these methods. This will be useful for improving the methods and for correctly interpreting the observations.

Studies such as Zahn et al. (2011) compared a reionization simulation obtained using a full 3D radiative transfer technique with the result from a semi-numerical one. It showed excellent agreement between these two. Similarly, Majumdar et al. (2014) compared semi-numerical simulations and conditional Press-Schechter models with a full 3D radiative transfer simulation performed with C\(^2\)-RAY (Mellema et al. 2006). That study showed that the semi-numerical simulations such as Zahn et al. (2007); Mesinger & Furlanetto (2007a); Choudhury et al. (2009); Santos et al. (2010), which use an excursion-set formalism to create the ionized bubbles, produce an ionization history very similar to the C\(^2\)-RAY provided that the halo lists from an N-body simulation are used. However, if the halos are found from a conditional Press-Schechter approach, as is for example done in Alvarez et al. (2009b); Mesinger et al. (2011a), the fit with the C\(^2\)-RAY results is considerably worse.

One-dimensional radiative transfer simulations such as B\(E\)ARS (Thomas et al. 2009), Ghara et al. (2015) (hereafter grizzly) assume that the effect of each source is perfectly spherical and use special recipes to deal with overlapping ionized and/or heated regions. Due to these simplifying assumptions they are fast but can also be expected to be less accurate than full 3D radiative transfer schemes. Previously, Thomas et al. (2009) performed a limited comparison between the 1D radiative transfer code B\(E\)ARS and the 3D radiative transfer code CRASH (Ciardi et al. 2001) for a simulation volume of size 12.5 h\(^{-1}\) comoving megaparsec. However, before considering these 1D schemes for parameter estimations (e.g., Patil et al. 2014), their performance for larger simulation volumes and larger numbers of sources is required.

In this paper we present a detailed comparison between the performance of the 1D radiative transfer code GR\(Z\)LY (Ghara et al. 2015) with the 3D radiative transfer code C\(^2\)-RAY. We use the same initial conditions such as the density fields, halo catalogues, source models, and compare the reionization history produced by these two schemes. We consider bubble size distributions as well as cross-correlations between ionization maps, while for the redshifted 21-cm signal we focus on statistical quantities such as the evolution of the power spectra. We consider two different models: (i) reionization with only large mass halos which do not suffer from thermal feedback, (ii) reionization with both high and low mass halos where the latter are assumed to be sensitive to thermal feedback. Case (i) is identical to the one used in Majumdar et al. (2014) to compare semi-numerical and full radiative transfer results which therefore allows the comparison between semi-numerical, 1D RT and 3D RT results.

Our paper is structured in the following way. In section 2, we describe the simulations used in this paper. In particular different subsections describe the N-body simulation and the source model used in this study as well as a brief description of the underlying algorithms of C\(^2\)-RAY and GR\(Z\)LY. In section 3, we present our results before we conclude in section 4. Throughout the paper, we have chosen the cosmological parameters \(\Omega_m = 0.27\), \(\Omega_\Lambda = 0.73\), \(\Omega_B = 0.044\), \(h = 0.7\) consistent with the Wilkinson Microwave Anisotropy Probe (W\(M\)AP) results (Hinshaw et al. 2013) and within the error bars consistent with Planck (Planck Collaboration et al. 2014).

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\(^3\) http://www.mwatelescope.org/
\(^4\) http://www.lofar.org/
\(^5\) http://www.skatelescope.org/
2 SIMULATIONS

Below we discuss the radiative transfer methods along with the source model and N-body simulation used in this study.

2.1 N-body simulation

Both radiative transfer methods considered in this study use the results of the same N-body simulation. This dark matter only N-body simulation was carried out using the publicly available code CUBEPM\(^6\) (Harnois-Déraps et al. 2013). The details of the simulations are: (i) the size of the simulation cube is 163 comoving megaparsec (cMpc), (ii) the number of dark matter particles is 3072\(^3\), (iii) the fine grid used by the particle-particle-mesh method is 6144\(^3\), (iv) the mass of the dark matter particles is 5.47 \times 10^6 M_\odot. The details of the simulation can also be found in Iliev et al. (2012). Although this N-body simulation is by now rather old, we use it to enable direct comparison to the results in Majumdar et al. (2014) who compared the performance of a semi-numerical method to C\(^2\)-RAY.

Snapshots of the density field are generated from redshift 20.134 to redshift 6 using equal time intervals of 11.5 megayears (Myr). The resolution of these gridded density fields is 256\(^3\). CUBEPM\(^6\) also produces dark matter halo lists using an on the fly halo finder based on the spherical overdensity method. The lowest mass halos produced have a mass of \sim 10^8 M_\odot, which corresponds approximately to the mass needed to initiate star formation driven by atomic cooling.

2.2 Source model

Our knowledge about the sources of reionization is very limited. Different efforts, both observational and modelling, have been undertaken to improve our understanding of the impact of various sources such as primordial galaxies (Wise et al. 2014; Xu et al. 2016), mini-quasars (Bromm & Loeb 2003; Zaroubi et al. 2007; Alvarez et al. 2009a; Tanaka et al. 2012) and high-mass X-ray binaries (Fialkov et al. 2014; Kaaret 2014; Kneivitt et al. 2014) on the expected 21-cm signal from the EoR. However, the individual contributions of these sources towards reionization remain quite uncertain.

In this study, we assume the sources of ionizing radiation formed in the dark matter halos. We further assume their spectral energy distribution can be approximated by a blackbody of an effective temperature of 50,000 K, which is appropriate for a massive population II star. We normalize the spectrum such that the rate of production of the ionizing photons is

\[ N_\gamma = g_\gamma \frac{M_h \Omega_B}{10 \text{ Myr} M_\odot m_p}, \]

where \( g_\gamma \) is the source ionization efficiency coefficient, \( M_h \) and \( m_p \) are the mass of the dark matter halo and proton mass respectively. For the fiducial model considered here, we choose \( g_\gamma = 21.7 \) for the sources formed in dark matter halos with mass \( M_h \geq 2.2 \times 10^9 M_\odot \), which will produce \( N_\gamma = 1.33 \times 10^{43} \times \frac{M_h}{10^9 M_\odot} \text{ s}^{-1} \). This is a similar choice as the L3 model in Iliev et al. (2012).

In addition, we consider a more complex reionization scenario where we use all halos of mass \( M_h \geq 10^9 M_\odot \). We divide these in two populations, low mass atomically cooling halos (LMACHs) in the mass range \( 10^8 \leq M_h < 10^9 M_\odot \) and high mass atomically cooling halos (HMACHs) in the mass range \( M_h \geq 10^9 M_\odot \). The LMACHs are assumed to be sensitive to thermal feedback and stop producing ionizing photons once they are located in an cell which is more than 10 percent ionized. The HMACHs are taken to be insensitive to thermal feedback. While still active the LMACHs produce ionizing photons with an efficiency \( g_\gamma = 130 \), whereas the HMACHs have \( g_\gamma = 8.7 \). The higher efficiency of the LMACHs is motivated by either a larger contribution from Pop III stars or a higher fraction of ionizing photons escaping. In the C\(^2\)-RAY results these parameters result in a rather early end of reionization around \( z = 8.5 \) and a Thomson optical depth value of 0.08, consistent with the value determined by WMAP and within the 2\(\sigma \) range of Planck. This scenario is identical to the L1 model of Iliev et al. (2012). The details of these scenarios are given in Table 1.

2.3 3D radiative transfer simulation C\(^2\)-RAY

The 3D radiative transfer method considered in this work uses the ‘Conservative Causal Ray-tracing method’ (C\(^2\)-RAY). The details of the method can be found in Mellema et al. (2006). The method is briefly described in the following steps.

- It starts with preparing the source list in a random order at each redshift.
- Given the SED of the sources, the total photo-ionization rate (\( \Gamma \)) is calculated at time \( t \) at each cell in the simulation box including contributions from all the sources. This step takes into account the time evolution of the neutral fraction of the cells during the time step which affects the optical depth from the sources.
- The history of the ionization fraction of hydrogen (\( x_{\text{HII}} \)) is estimated by solving the non-equilibrium equation,

\[ \frac{dx_{\text{HII}}}{dt} = (1 - x_{\text{HII}}) (\Gamma + n_e C_{\text{II}}) - x_{\text{HII}} C_{\text{II}}, \]

where \( n_e \) is the electron density at the cell, \( C_{\text{II}} \) and \( \alpha_{\text{II}} \) represent the collisional ionization and recombination coefficients for hydrogen respectively. The quantity \( C \) is the clumping factor (which can be defined as \( \langle n^2 \rangle / \langle n \rangle^2 \), where \( n \) is the baryon number density) which accounts the clumpiness of the IGM. Here we have taken \( C = 1 \) but in general it can be larger than 1 or even position dependent.

C\(^2\)-RAY was compared to other fully numerical radiative transfer codes in Iliev et al. (2006c) and Iliev et al. (2009) and was found to produce accurate results. In this study we do not consider the temperature evolution of the intergalactic gas, only its ionized state.

2.4 1D radiative transfer simulation GRIZZLY

The details of the one-dimensional radiative transfer method can be found in Ghara et al. (2015). The method mainly
follows the BEARS algorithm (Thomas et al. 2009) with a few changes compared to the original method. To express its relation to the original BEARS method, we have chosen to call it GRIZZLY. The basic idea of both methods is not to solve the one-dimensional radiative transfer equations on the fly while generating the ionization maps. Rather, they use pre-generated ionization profiles to construct the ionization maps. Here, we briefly summarize the most important steps of the algorithm.

• We start by choosing the range for the key source parameters: redshift, density contrast of the uniform background IGM, luminosity of the source, age of the source. We then generate a large number of ionization and kinetic temperature profiles around the sources for different combinations of these parameter values. Next we create a list of radii of the HII bubbles as a function of different parameters. We assume the radius of the HII region to be the radius at which the ionization fraction drops to 0.5 from the location of the source. This library of 1D profiles only needs to be compiled once for a given cosmology and spectral energy distribution of sources.

• For a given redshift and a certain halo position, we determine the luminosity and the age of the halo according to a source recipe, see Sect. 2.4.1. From this we determine the size of the HII bubble around it using the density field and the pre-generated list of the HII bubble radii. This step is done iteratively. We start with a small radius around the centre of the source, calculate the spherically averaged overdensity of the IGM within this radius and then estimate the radius of the HII bubble from the list. We change the initial choice of radius such that the estimated radius of the HII region matches with the chosen radius for the same overdensity. The parameter values corresponding to that radius are then associated with the source and the corresponding profiles will be used to generate the ionization and kinetic temperature maps.

• The procedure described in the previous step is performed for all halos at the redshift being considered. Although the number of overlaps between the individual HII regions around the halos are negligible during the initial stages of reionization, they become important at the later stages of reionization. To incorporate the effect of overlap, we estimate the unused ionizing photons for each overlapping HII region and distribute them around the overlapping regions such that each photon ionizes one hydrogen atom.

• Next, we use the pre-generated 1D ionization profiles corresponding to each halo to calculate the ionization fraction at the partially ionized region beyond the HII regions. The ionization fraction in the overlapping partially ionized regions is then expressed as

\[ x_{\text{HII}}(x) = \sum_i x_{\text{HII-1D}}(x) \times n_{\text{H-1D}} \times (1 - x_{\text{HII}}(x)) \]

where the summation symbol represents a sum over all overlapping sources. Here, \( x_{\text{HII}}(x) \) denotes the ionization fraction obtained after considering overlapping HII regions from \( i - 1 \) number of sources. We take \( x_{\text{HII}}(x) = 0 \). The term \( (1 - x_{\text{HII}}(x)) \) takes care of the fact that the \( i \)th source encounters an already partially ionized IGM, due to overlap between previous \( i - 1 \) number of sources, before contributing to ionization.

• Next, we generate the kinetic temperature maps using a correlation of the neutral fraction and the gas temperature in the partially ionized region (for details, see Ghara et al. 2015).

2.4.1 Implementation of source model

In the model scenarios considered in this paper, we assume that dark matter halos always have ongoing star formation, unless they are suppressed through thermal feedback, see Sect. 2.4.2. To select a one-dimensional profile from the library we need to specify a luminosity and age for the halo. The original BEARS code and Ghara et al. (2015) used a fixed age for the halos, typically \( \sim 10 \) Myr and also used a luminosity calculated from the instant mass of a halo at the redshift under consideration. Those models assume that the stars inside the galaxies efficiently emit hydrogen ionizing photons until an age of \( \sim 10 \) Myr.

However, we found this source model to be inconsistent with the one used by C2-Ray in terms of the cumulative number of ionizing photons being produced. We therefore implemented another source model. In this model we follow the growth of halos and find both the age of the halo as well as the time-averaged mass (to be called the effective mass \( M_{\text{eff}} \)). We then calculate the luminosity based on \( M_{\text{eff}} \) using Eq. 1 and use this together with the age to find the appropriate profile from the library. The GRIZZLY code thus does not track the history of the state of the IGM gas but rather uses the history of the halos to calculate the state of the IGM at a given redshift.

It is not entirely trivial to calculate the age of the halos accurately from the halo lists as halos can move to new cells or multiple halos can merge. In principle, one needs to track the halos using a merger-tree algorithm. However, as no merger tree is supplied with the halo lists, we have used a simple method to account for their growth. For every pair of redshifts \( z_1 \) and \( z_2 \) we first search for a halo at the same location and it is found, we associate the change in mass with the halo whose history we are tracking. If a halo disappears from its previous grid position in some time step, we inspect bordering grid cells. If we find a newly formed heavier halo in a bordering grid cells, we assume that the identified halo must be the present state of the halo which disappeared. If we are not able to find any newly formed

| Model      | Min. halo (M_☉) | Thermal feedback | \( g_\gamma \) \( \text{LMACH} \) | \( g_\gamma \) \( \text{HMACH} \) | Model used in |
|------------|-----------------|------------------|-----------------|-----------------|---------------|
| MODEL I (fiducial) | \( 2.2 \times 10^9 \) | No               | 0               | 21.7            | L3            |
| MODEL II   | \( 10^8 \)      | yes              | 130             | 8.7             | L1            |

Table 1. Details of the scenarios considered in this paper. LMACH and HMACH represent the low-mass and high-mass atomically cooling halo respectively.
halo in the neighbourhood, then we assume that a merger happened. In this case, we find previously existing heavier halo at the neighbour and set its age as the maximum of the ages of the identified and disappeared halo. Although this a posteriori reconstruction of the halo histories is rather crude, it does allow us to obtain the correct cumulative number of ionizing photons produced during reionization.

2.4.2 Implementation of thermal feedback
In the second C²-ray simulation we include LMACHs which are fully suppressed once their environment has been sufficiently ionized. The criterion used is that when the ionization fraction in the cell containing the LMACH is larger than 0.1, thermal feedback is assumed to stop the production of ionizing photons⁷.

To implement this recipe in GRIZZLY it is not trivial as the code only places ionized regions around active sources at the redshift of interest. We implemented the following simple prescription to take into account thermal feedback effects in GRIZZLY. We use the ionization map from the previous time step to select the active sources at a certain time step using the condition on the ionization fraction. We add to these the previously active sources which became inactive at the present time step but assign to them their effective mass and age corresponding to the last time they were active. In principle one needs to consider the recombination in the already ionized regions to correctly account for the suppression. However, it is not straightforward to implement recombination in an already ionized region in GRIZZLY. This is also true for other semi-numerical simulations such as models considered in Majumdar et al. (2014); Sobacchi & Mesinger (2014). However, recombinations play a minor role, especially since previously suppressed LMACH halos become active again after their halos have grown into HMACHs and the amount of time that recombinations act upon the relic H II regions will thus be limited.

Since the criterion for suppression is \( x_{\text{HI}} > 0.1 \), the treatment of partially ionized cells is important. We therefore implemented an improvement over the previous version of GRIZZLY when estimating the ionization fraction in cells containing an ionization front. We now assign the volume averaged ionized ionization fraction to these cells calculated from the higher resolution 1D profiles.

2.5 Differences between C²-ray and GRIZZLY
It is important to realise that C²-ray and GRIZZLY treat the calculation of the reionization history very differently. C²-ray follows the time evolution of the ionization fractions by taking the state at the end of the previously calculated time step as initial condition for the new time step. This means that any simulation has to be followed from the emergence of the first sources to a chosen end point, for example when the IGM reaches an average ionization fraction of 99 percent. The advantage is that any time-dependent effects such as recombinations and changes in the source luminosity or position are treated correctly.

The GRIZZLY as well as the related BEARS code do not use the previous state of the IGM as an initial condition for the next time step but instead construct the state of the IGM from scratch for every output. The time evolution is captured by considering the growth history of dark matter halos when calculating their luminosity and in the case of suppressed halos by using the recipe described above. This approach has as an advantage that it is not required to calculate the entire reionization history if this is not needed. The disadvantage is that time-dependent effects such as recombinations, radiative cooling and changes in the source properties have to be implemented in an approximate manner. These 1D radiative transfer reionization codes share this property with the semi-numerical methods based upon the excursion set approach such as 21cmFAST (Mesinger et al. 2011b).

2.6 21-cm signal
The differential brightness temperature \( \delta T_b \) of the 21-cm signal can be expressed as,

\[
\delta T_b(x, z) = 27 \, x_{\text{HI}}(x, z)[1 + \delta_n(x, z)] \frac{\Omega_m b^2}{0.023} \times \left( \frac{0.15}{\Omega_m b^2} \right)^{1/2} \left( 1 - \frac{T}{T_b} \right) \text{mK},
\]

where the quantities \( x_{\text{HI}}, \delta_n \) and \( T(z) = 2.73 \times (1 + z) \) K denote the neutral hydrogen fraction, baryonic density contrast and the CMB brightness temperature, respectively, each at position \( x \) and redshift \( z \). \( T_b \) represents the spin temperature of hydrogen in the IGM.

In this study we will adopt the high spin temperature approximation: \( T_b \gg T_z \). In this case \( \delta T_b \) becomes insensitive to the actual value of the spin temperature. This approximation is valid when the spin temperature is coupled to the IGM gas temperature through Lyα coupling and the IGM has been sufficiently heated (\( T_K \gg T_z \)) by the X-ray sources. Most reionization scenarios reach this state well before substantial ionized regions form (Cohen et al. 2017).

After generating the ionization fraction cubes as described in sections 2.3 and 2.4, it is straightforward to generate the differential brightness temperature cubes using Eq. 4. Below we will compare \( x_{\text{HI}} \) and \( \delta T_b \) results at fixed redshifts. We will not consider the effect of peculiar velocities in the IGM (leading to the so-called redshift-space distortions). The comparison of fully numerical and semi-numerical models in Majumdar et al. (2014) suggest that redshift-space distortions will not change the main conclusions of the comparison.

3 RESULTS
In this section, we compare the different outputs from the two simulation codes considered in this work, namely C²-ray and GRIZZLY. Before evaluating the different scenarios
listed in Table 1, we first consider two single source scenarios to test the impact of the fundamental difference between the two codes as described in Sect. 2.5.

3.1 Test scenarios: single sources

To gauge the basic differences between C$^2$-RAY and GRIZZLY we follow the growth of an ionized region for two single source scenarios. For both we take the IGM around the source to have a uniform density at the mean value of the Universe. We choose the size of the simulation box to be 20 h$^{-1}$ Mpc and use a grid of size 100$^3$. We assume that the source formed at redshift 15 and we follow the impact of the source on the IGM up to redshift 6 using time steps of 10 Myr.

- TEST A: The source is hosted by a dark matter halo with constant mass which we take to be 10$^9$ M$_\odot$. We choose an efficiency factor $g_r = 21.7$, as defined in Equation 1, which sets the rate of production of ionizing photons to $N_\gamma = 1.33 \times 10^{52}$ s$^{-1}$.
- TEST B: The source is hosted by a dark matter halo with a mass which changes exponentially with redshift as (see, e.g. Wechsler et al. 2002),

$$M_{\Delta}(z) = m_s \times \exp[\beta(z_i - z)],$$

(5)

where $m_s = 10^9$ M$_\odot$, $z_i = 15$, $\beta = 0.5$. This scenario mimics the typical growth of dark matter halos and thus will show the impact of capturing source evolution through an effective mass $M_{\Delta}$ in GRIZZLY. We choose the same efficiency $g_r$ as in Test A.

The performance of the methods for these test scenarios is shown in Figure 1. The left hand and middle panel shows the evolution of the neutral fraction in the simulation volume for TEST A and B respectively, whereas the right hand panel shows relative difference between the two codes. We see that they very similar results for both tests with differences less than 10 per cent. However, for TEST A the ionization front grows faster in the GRIZZLY results. The probable reason is that GRIZZLY underestimates the impact of recombinations. While placing the H II bubble around the sources, we assume that the source has been emitting ionizing photons at a constant rate determined by its effective mass ($M_{\Delta}$) during its entire age and we include the effect of recombinations using the densities at the redshift which we are considering. Since the expansion of the Universe causes densities to be higher at higher redshifts, this will underestimate the impact of recombinations over the age of the source. C$^2$-RAY calculates the recombination rates at every time step using the densities at that redshift and thus captures this evolution of the recombination rate.

Interestingly, the match between the two codes is better for TEST B where the halo mass is increasing in time (see the middle panel of Figure 1). Since in this case most photons are emitted at later times and the growth of the H II region is faster at later times, the effect of underestimating recombinations is less severe in this case. Below when considering more complex simulations with multiple sources we will see further demonstrations of the impact of recombinations.

We conclude that GRIZZLY is capable of approximating the expansion of an ionization front around a growing halo to within 10 per cent accuracy, giving confidence that the effective mass approach works well. When considering the multiple sources case below, larger differences than the ones found here will have to be due to how GRIZZLY deals with overlapping H II regions and source suppression.

3.2 Model I: Large halos only

Now, we will consider a model where the reionization is driven by halos with mass $M_\Delta \geq 2.2 \times 10^9$ M$_\odot$ in a volume 163 comoving Mpc across. These halos are never suppressed. This model is same as the L3 model in Iliev et al. (2012) and was also used in Majumdar et al. (2014) to compare semi-numerical simulation techniques with a fully numerical one.

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Comparison between $C^2$-RAY and GRIZZLY

Not taking into account the time needed to construct the library of 1D ionization profiles, the simulation run time for the whole reionization history is $\sim 5.5$ CPU hours$^8$ for GRIZZLY. This number is without generating the $T_K$ maps and Ly$\alpha$ flux maps which are not being used here. For comparison, the entire $C^2$-RAY simulation took $\sim 10^5$ CPU hours. So there is a factor $\sim 10^5$ gain in computing time when using GRIZZLY.

3.2.1 Reionization history

Using the source model described in section 2.2 and following the methods described in sections 2.3 and 2.4, we generate the ionization maps in the simulation box. The ionization histories from these two simulations are shown in the bottom panel of Figure 2. In this scenario, the first sources appear at redshift 19 and ends around $z \sim 8.4$. The Thomson scattering optical depth from the GRIZZLY and $C^2$-RAY simulations are 0.0696 and 0.0697 respectively. As can be seen from the figure, the evolution of the mass averaged neutral fraction as a function of redshift from these two simulations are very similar.

The top panel of Figure 2 shows the redshift evolution of the ratio of the volume and mass averaged neutral fraction for this reionization history. As the reionization scenario considered here is ‘inside-out’, high-density regions are ionized first. This leads to a higher volume averaged neutral fraction than the mass averaged neutral fraction. Also for this ratio we find very good agreement between the two codes. This suggest that the ionization maps from these two schemes will be very similar. The small differences may originate from the approximations that go into the implementation of the ionization and differences in the treatment of recombinations in the two schemes. This agreement is better than for any of the semi-numerical results from Majumdar et al. (2014), see figure 1 in that paper.

To illustrate the similarity between the reionization his-
Figure 4. Top panel: Scale dependence of the cross-correlation coefficient of the redshift of reionization maps from C$^2$-RAY and grizzly simulations for Model I. Bottom panel: Same as the top panel but for the neutral fraction maps at different stages of reionization.

Figure 5. Images of the neutral fraction for the same slice through the simulation box as in Fig. 3. Black is ionized, white is neutral. The top and bottom panels show the results from C$^2$-RAY and grizzly respectively. The results are for Model I, $z = 9.026$ when the mass averaged neutral fraction is $\sim 0.5$.

To compare two different maps, we define the cross-correlation coefficient of a quantity $Q (R^Q_{AB})$ as given below.

$$R^Q_{AB}(k) = \frac{P_{AB}(k)}{\sqrt{P_{AA}(k)P_{BB}(k)}},$$

where $P_{AA}$ and $P_{BB}$ are the auto power spectrum of the fields $A$ and $B$ respectively and the $P_{AB}$ is the cross power spectrum between them. Here, we will consider $A$ and $B$ as grizzly and C$^2$-RAY respectively. The quantity $Q$ could be the redshift of reionization, neutral fraction, brightness temperatures, etc.

The cross-correlation coefficient for the redshift of reionization cubes $R_z$ is found to be larger than 0.95 for scales with $k \lesssim 1$ Mpc$^{-1}$ (see top panel of Figure 4). This suggests that the reionization histories from these two simulations are very similar at large scales. Although the correlation drops at scales correspond to $k \gtrsim 1$ Mpc$^{-1}$, it is clearly still better than the semi-numerical schemes considered in Majumdar et al. (2014) (see Figure 3 of their paper).
3.2.2 Morphology of H\textsc{ii} regions

Next we compare the morphology of the ionized regions from the two simulations using maps of the neutral fraction. We show the same slice from the neutral fraction cubes from C\textsuperscript{2}-RAY and GRIZZLY in the two panels of Figure 5. Visually, the maps are quite similar. The Pearson cross-correlation coefficient calculated for these two slices is 0.93. One can notice that the ionized bubbles in the slice from GRIZZLY simulation appear to be more spherical than those from C\textsuperscript{2}-RAY. This is due to the application of 1D radiative transfer which erases the directional dependence of the H\textsc{ii} bubbles. However, the shapes of the bubbles become irregular once there is a significant amount of overlap between the H\textsc{ii} regions.

The scale dependent cross-correlation coefficients for maps of the neutral fraction at different stages of reionization from GRIZZLY and C\textsuperscript{2}-RAY are shown in the bottom panel of Figure 4. One can see very high correlation at large length scales, which are the ones of prime interest to the first generations of radio telescopes. We find that the cross-correlation coefficient of the neutral maps remains very close to unity (within $\sim 5$ per cent) at scales $k \leq 1$ Mpc$^{-1}$ until the universe is 50% ionized. There is a consistent shift to smaller $k$ values in the scale at which the correlation coefficient reaches 0.9 as reionization progresses. Although the correlation of the ionization fields drops for small length scales, the values actually remain higher than those for the semi-numerical models considered in Majumdar et al. (2014). For example, the cross-correlation coefficients of the neutral fractions between C\textsuperscript{2}-RAY and different semi-numerical schemes were found to be smaller than $\sim 0.4$ at a scale $k \sim 2$ Mpc$^{-1}$ at a stage with neutral fraction $x_{\text{HI}} \sim 0.5$, while the corresponding value for GRIZZLY is $\sim 0.6$.

3.2.3 Size distribution of H\textsc{ii} regions

We next compare the H\textsc{ii} bubble size distribution (BSD) from these two simulations. BSDs can provide valuable information about the growth of the ionized regions (Friedrich et al. 2011). However, due to the complex morphologies of the ionized regions, there is no unique way to define the sizes of the irregularly shaped H\textsc{ii} regions in simulation volume. Therefore different size determination methods have been developed and each address different aspects of the size distributions (Giri et al. 2017). In this study, we have use two such methods, namely the Friends-of-friends (FOF; Iliev et al. 2006a) and mean-free-path (MFP; Mesinger & Furlanetto 2007b).

First, we discuss our bubble size statistics from the FOF method. This algorithm considers two neighbouring cells with ionization fraction larger than 0.5 to be the part of the same ionized bubble and in the process finds the volume of each ionized region. This BSD algorithm focuses on connectivity. As shown in Furlanetto & Oh (2016) the percolative nature of reionization leads to the development of one dominant connected region which contains most of the ionized volume. This large connected region is known as the percolation cluster. The single percolation cluster is invisible in the normalized histogram of the volumes ($V dP/dV$) as this quantity gives the number of ionized bubbles of volume $V$. Instead we plot $(V/V_{\text{ion}}) V dP/dV$ which shows the fraction of the ionized volume ($V_{\text{ion}}$) contained in regions of volume $V$. Once the percolation cluster has formed it will have a value close to 1 in this quantity.

The top panel of Figure 6 shows the FOF-BSDs from the two simulations at three different stages of reionization. The volume of the percolation cluster is identical in both the simulations. One can observe that the number and size distribution of smaller ionized regions also match quite well during the early and late stages of reionization. However, we find that GRIZZLY produces a few larger bubbles during

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure6.png}
\caption{Top panel: The volume distribution of the H\textsc{ii} bubbles calculated by the FOF method at three different stages of reionization in Model I. The left to right curves (with colours green, red and blue) correspond to redshift 9.5, 9 and 8.7 when the neutral fractions are 0.7, 0.5 and 0.3, respectively. The solid and dashed curves represent C\textsuperscript{2}-RAY and GRIZZLY simulations respectively. Bottom panel: The PDF of the H\textsc{ii} bubble size calculated by the mean-free-path method. The line styles and colours have the same meaning as in the upper panel.}
\end{figure}
the intermediate stages. However, compared to the different semi-numerical models considered in Majumdar et al. (2014) (as shown in Figure 5 of that paper), the FOF-BSD from GRIZZLY matches the C²-RAY results better.

The second BSD method that we use is MFP which is built on a Monte-Carlo inference of the sizes. This method selects random cells in the ionized regions and traces a ray in a random direction until it hits a neutral cell. In this case, we consider a cell to be ionized if its ionization fraction is larger than 0.5 and neutral if it is less than that. We repeat the ray tracing for enough number of times (in this case 10⁷ times) and record the lengths of the rays. This provides the estimate of the size distribution of the ionized regions, here expressed in radii instead of volumes.

The MFP-BSDs for GRIZZLY and C²-RAY show good agreement as can be seen in the bottom panel of Figure 6. The peaks of the curves at the different stages of reionization appear at the same radius which suggests that the most probable sizes of ionized regions in both simulations are identical. Majumdar et al. (2014) did not calculate MFP-BSDs and therefore we cannot compare to their results in this case.

3.2.4 Differential brightness temperature maps

The next quantity that we compare for the two simulations is the expected 21-cm signal. Figure 7 presents δT_b maps of the same slice at three different redshifts 9.5, 9 and 8.7 which correspond to the neutral fractions 0.7, 0.5 and 0.3 respectively. Visually the δT_b maps are quite similar. The Pearson-cross-correlation coefficients for these maps are 0.92, 0.9 and 0.9 respectively. However, the small-scale features are different due to the spherical nature of the bubbles around isolated sources in the 1D radiative transfer scheme. This was also seen in section 3.2.2 when we considered the morphology of ionized regions.

To check the level of similarity, we again use the scale-dependent cross-correlation between the two δT_b maps, see Figure 8. The large values of the cross-correlation coefficients R_{δT_b} suggest that the δT_b maps from these two schemes are very similar. However, we do find that the value of R_{δT_b} decreases at small scales which indicates mismatches between the δT_b maps at small scales. Still, R_{δT_b} is larger than 0.7 at scales such as k ≥ 1 Mpc⁻¹. This suggests that δT_b maps from GRIZZLY are more similar to the maps from C²-RAY than the maps from the semi-numerical models considered in Majumdar et al. (2014). For example, R_{δT_b} is less than...
0.7 at $k \geq 1$ Mpc$^{-1}$ for the semi-numerical models used in Majumdar et al. (2014) while $R_{2\delta T_b} \sim 0.85$ for grizzly. We also find the $R_{2\delta T_b}$ value to be larger than the $R_{2\delta T_b}$ at scales $k \geq 1$ Mpc$^{-1}$ (see Figure 4). This is due to the fact that the $\delta T_b$ signal is dominated by the density fluctuation at small scales and these are identical between the two simulations.

3.2.5 Spherically averaged power spectrum of the signal

Next we compare the outputs of these two schemes in terms of the power spectrum of the $\delta T_b$ fluctuations. The spherically averaged power spectrum $P(k)$ of the $\delta T_b$ fluctuations is defined as

$$\langle \delta T_b(k)\delta T_b^*(k') \rangle = (2\pi)^3 \delta_D(k-k')P(k),$$

(8)

where $\delta T_b(k)$ represents the Fourier transform of $\delta T_b(x)$. Here, We present the results in terms of the spherically averaged dimensionless power spectrum $\Delta^2(k) = k^3P(k)/2\pi^2$.

The top panel of Figure 9 presents the scale dependence of $\Delta^2(k)$ estimated from these two simulations at different stages of reionization, together with the ratio of the two results. While the power spectrum is dominated by the density fluctuations at the early stages of reionization, it starts to deviate from the background dark matter density power spectrum as reionization progress. The power spectra from these two schemes agree with each other to within 10 percent for most stages and scales. Only at the largest scales for $x_{HI} = 0.7$ the difference exceeds 20 percent. The overall features of the power spectra are very similar between the two codes.

The bottom panel of the figure compares the redshift evolution for the $k \sim 0.1$ Mpc$^{-1}$ mode of the power spectrum. The ratio between the $C^2$-RAY and GRIZZLY results starts to deviate from unity at redshift 14 and remains between 0.9 and 1.1 during the later stages of reionization once again indicating excellent agreement. Compared to the semi-numerical methods from Majumdar et al. (2014) the GRIZZLY results match the $C^2$-RAY ones equally well, or better.
3.3 Model II: Including low mass halos and thermal feedback

Finally we consider a more complex model for reionization and study the similarities of the outcomes of these two codes. While our fiducial model does not incorporate the contributions from LMACHs, these low-mass halos can provide a significant contribution to the overall ionizing photon budget. As explained in section 2.2, in Model II we take the minimum mass of halos which contribute to reionization to be $10^8 \, M_\odot$, and we suppress star formation in halos of masses (below $10^9 \, M_\odot$) in ionized regions. This scenario is same as the L1 model in Iliev et al. (2012). The details can be found in Table 1. Majumdar et al. (2014) did not study this model in their comparison between semi-numerical and numerical methods, so unlike for the results of Model I we are here not able to compare to semi-numerical methods.

Although GRIZZLY has to apply simplifying approximations in order to include thermal feedback, the reionization history it generates is very similar to that from $C^2$-RAY as shown in the bottom panel of Figure 10. The Thomson scattering optical depths for $C^2$-RAY and GRIZZLY are 0.08 and 0.081 respectively. The redshift evolution of the ratio of the volume and mass averaged neutral fraction from these two simulations also matches very well as shown in the top panel of the figure. This suggests that the neutral fraction maps from these two simulations for this complex model are also very similar. We do not show these here but below will show the 21-cm images from which the morphology of the ionized regions can also be seen.

The FOF-BSDs obtained for Model II as shown in the top panel of Figure 11 have mostly very similar shapes. At the early stages (with neutral fraction 0.7), GRIZZLY is seen to produce more large ionized regions, although this difference is likely due to small size differences among the larger
regions. However, this possible bias vanishes once the H\textsc{ii} regions start percolating during the middle and later stages of reionization. The distributions of the sizes of the H\textsc{ii} regions calculated using the MFP method for this scenario also display good agreement (as shown in the bottom panel of Figure 11). We find that there is no prominent peak feature in the MFP-BSD curves during the early stages of reionization. This is due to the fact that the size of the ionized regions are very small and mostly fall within the resolution limit of the simulation.

The differential brightness temperature maps from these two simulations also visually very similar at different stages of reionization as shown in Figure 12. The Pearson-cross-correlation coefficient calculated for the slices shown in Figure 12 are 0.7, 0.75 and 0.77 at reionization stages with neutral fraction 0.7, 0.5 and 0.3 respectively. The scale-dependent comparison of the $\delta T_b$ cubes from these two simulations is also shown in terms of the cross-correlation coefficient at different stages of reionization in Figure 13. One can see that the $\delta T_b$ cubes from these two simulations are highly correlated at the large scales with $k \lesssim 0.5$ Mpc$^{-1}$ (within 10 percent error), while the correlation drops at smaller scales.

We present the comparison between the spherically averaged power spectrum from these two simulations of Model II in Figure 14. The redshift evolution of the spherically averaged power spectrum at scale $k \sim 0.1$ Mpc$^{-1}$ are quite similar to each other as shown in the bottom panel of Figure 14. Although the power spectrum estimated from these two schemes are very similar, there are small differences too. For example, we find that the power spectra deviate from each other around redshift 10.5 when the neutral fraction is 0.7. Up to this time the LMACHs contribute substantially to reionization, so the differences are most likely connected to the way their suppression is implemented. Still, the differences are small and except at the very largest scales do not exceed 10 percent.

When comparing these results for Model II to the ones for Model I we see that GRIZZLY performs somewhat less well in the former case. However, the results are still very close to the numerical ones and definitely fall within the expected measurement errors from the observations.

Overall, we find that the results from these two simulations agree well with each other even for this more complex scenario. This suggest that the 1D radiative transfer can be used for the complex scenarios as well without a substantial loss of accuracy. Specifically, the 3D and 1D radiative trans-
fer schemes match quite well at scales $k \lesssim 1 \text{ Mpc}^{-1}$ which are the prime target of the current radio interferometers. This suggests that 1D radiative transfer codes such as BEARS or GRIZZLY can be efficiently used for predicting the expected signal for various source models as well as to find new observation strategies and possibly for parameter estimation.

4 SUMMARY AND DISCUSSION

In this paper, we have compared the performance of the 1D radiative transfer code GRIZZLY to the 3D radiative transfer code C$^2$-RAY in the context of a large scale reionization simulation. While C$^2$-RAY simulates the process more accurately, by performing both the full 3D radiative transfer and following the evolution of the ionization fractions and the source in time, this accuracy comes at a considerable computational cost. The GRIZZLY code simplifies the calculation by placing pre-generated 1D profiles of ionization fraction around the sources and using the halo growth history to approximate the evolutionary effects, which makes it approximately a factor $\sim 10^5$ faster.

We have used same sets of initial conditions, i.e. the same density fields, halo catalogues and source models for both simulations. We limit our comparison to the calculation of the ionization fraction. Beside comparing results around a single source, we consider two models to compare the outcomes of these simulations in detail. In Model I (also our fiducial model), we assume that the reionization is driven by massive halos with masses larger than $2.2 \times 10^9 \, M_\odot$. This model was also used in Majumdar et al. (2014) to evaluate the performance of semi-numerical reionization codes which rely on the excursion set formalism. We also consider a more complex model (Model II) which includes low mass halos (down to $10^8 \, M_\odot$) and suppression of star formation in halos with mass smaller than $10^9 \, M_\odot$ due to thermal feedback. For all the models considered in this paper, we have used the same SED which in this case is a blackbody spectrum. When calculating the the differential brightness temperature of the 21-cm signal we assume that $T_S \gg T_y$. Our findings from this comparison are the following.

- When comparing the reionization history due to an isolated source, we observe that GRIZZLY underestimates the effect of recombinations. Since this is a cumulative effect, the impact is largest at the later stages. Still, we find that the differences between the neutral fractions estimated from the two methods for the isolated sources remain less than 10 percent.
- For our fiducial simulation, the reionization histories in
terms of the evolution of the mass averaged neutral fraction and ionization maps are very similar between both simulations. The cross-correlation coefficient of the neutral fraction maps remains close to unity (within 5-10 percent) at scales \( k \lesssim 1 \) Mpc\(^{-1}\) before the universe reaches 50 percent ionization and somewhat worse after this.

- We have considered two different methods to characterize the size distribution of ionized regions, namely the friends-of-friends and mean-free path methods. For both methods the size distributions match very well between the C\(^2\)-RAY and GRIZZLY results. However, visual inspection of the ionization fraction maps does show that GRIZZLY produces more spherically shaped regions compared to C\(^2\)-RAY.

- Visually, the differential brightness temperature maps from the two simulations look very similar. The cross-correlation coefficients at large scales, \( k \lesssim 0.1 \) Mpc\(^{-1}\), are close to unity. We find that the correlation coefficients at small scales are higher for the \( \delta T_\text{b} \) maps than for the ionization maps. This is due to the density fluctuations in the neutral medium.

- The spherically averaged power spectra from the two simulations agree with each other within 10 percent.

- For the more complex scenario Model II, we find that the differences between the GRIZZLY and C\(^2\)-RAY are generally somewhat larger than for the simpler Model I but remain small. We conclude that GRIZZLY is capable of handling more complex source models where sources are not always “on”.

- The results from GRIZZLY are more similar to those from C\(^2\)-RAY compared to the different semi-numerical simulations considered in Majumdar et al. (2014). We find for example that the various cross-correlation coefficients are higher for GRIZZLY, especially for smaller scales. Furthermore, for the semi-numerical models the source efficiency was adapted at each redshift in order to reproduce the ionization history from C\(^2\)-RAY, whereas GRIZZLY is able to produce an excellent match for the reionization history without varying the source efficiency parameter.

These results imply that the faster 1D radiative transfer codes such as BEARS or GRIZZLY can be efficiently used for exploring parameter space, determining observational strategies or developing parameter estimation pipelines. Once the 1D profiles have been generated, these simulations are fast enough to be used for parameter estimation using techniques such as the Monte Carlo Markov Chains, machine learning, etc. However, the details of parameter estimation such as convergence time, accuracy, etc., are beyond the scope of this work and will be addressed in future works.

Although GRIZZLY is quite fast compared to the full radiative transfer simulations and generally reproduces the results well, our comparison also shows where improvements could be made. (i) GRIZZLY shows lower accuracy at small scales. We speculate that the accuracy at small scales can be improved by optimizing the technique GRIZZLY uses to deal with overlapping ionized regions. (ii) The comparison for a single source shows that GRIZZLY underestimates the effect of recombinations. This could be improved by taking into account the cosmological evolution of the density field over the life time of the source. (iii) The halo suppression model used in GRIZZLY is currently a very simple one. It may be possible to implement the evolution of relic H\(^\text{II}\) regions better and thereby to improve the accuracy of GRIZZLY for scenarios where source can turn “off”.

Besides the neutral fraction maps, GRIZZLY can also provide the kinetic temperature and Ly\(\alpha\) flux maps. Thus, it can be used to predict signal in presence of spin-temperature fluctuations. The detailed comparison of the results in presence of \( T_\text{b} \) fluctuations with fully numerical simulations such as Ross et al. (2017) is beyond the scope of this paper and will be addressed in the future.

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