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An Epoch of Reionization simulation pipeline based on BEARS

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ABSTRACT

The quest to unlock the mysteries of the Epoch of Reionization (EoR) is well poised with many experiments at diverse wavelengths beginning to gather data. Albeit these efforts, we are yet uncertain about the various factors that influence the EoR which include, the nature of the sources, their spectral characteristics (blackbody temperatures, power-law indices), clustering property, efficiency, duty cycle etc. Given these physical uncertainties that define the EoR, we need fast and efficient computational methods to model and analyze the data in order to provide confidence bounds on the parameters that influence the brightness temperature at 21-cm. Towards this goal we developed a pipeline that combines dark matter-only N-body simulations with exact 1-dimensional radiative transfer computations to approximate exact 3-dimensional radiative transfer. Because these simulations are about two to three orders of magnitude faster than the exact 3-dimensional methods, they can be used to explore the parameter space of the EoR systematically. A fast scheme like this pipeline could be incorporated into a Bayesian framework for parameter estimation. In this paper we detail the construction of the pipeline and describe how to use the software which is being made publicly available. We show the results of running the pipeline for four test cases of sources with various spectral energy distributions and compare their outputs using various statistics.

1. Introduction

During the Epoch of Reionization (EoR), between 300 and 500 million years after the Big Bang, the first sources of ionizing radiation appeared. These sources changed the thermal and chemical constitution of the Universe. From measurements of the cosmic microwave background (CMB) we obtain an integral measure of the ionized intergalactic medium via the Thomson scattering cross-section which has been measured by both the WMAP (Komatsu et al., 2011) and the Planck collaborations (Planck Collaboration et al., 2016). Along with the quasar absorption spectra and the Gunn–Peterson effect (e.g. Fan et al., 2006), these observations provide bounds within which the EoR resides ($12 < z < 6$). Although there have been recent discoveries of stellar clusters and galaxies in this range of redshifts, we are yet to directly measure the neutral hydrogen content of the Universe in this epoch.

For the last decade there have been concerted efforts towards the direct measure of the EoR using arrays of radio-telescopes such as the LOw Frequency ARray (LOFAR) in the Netherlands (e.g. van Haarlem et al., 2013; Patil et al., 2016; 2017), the Murchison Widefield Array

(MWA) in Australia (e.g. Tingay et al., 2013; Bowman et al., 2013), and the Precision Array for Probing the Epoch of Reionization (PAPER) in South Africa (e.g. Pober et al., 2015). These arrays have to overcome a number of technical challenges, that include galactic and extra-galactic foreground emission, ionospheric distortions, radio-frequency interference and other known and unknown measurement errors pertaining to the hardware of the telescopes. Additionally, the signal from the EoR (≈ 20 mK in brightness temperature) is buried under aforementioned foregrounds (≈ 200 K), which is 4–5 orders-of-magnitude larger. Our hope to detect the signal from the EoR therefore strongly depends on our ability to forward model the statistics of the EoR. In other words, theoretical simulations of the EoR provides us with a prior distribution of statistical parameters that can be improved in a Bayesian fashion, when more evidence is accumulated over the duration of the observation. These models will also enable us to interpret the data in a parsimonious manner.

Simulations of the EoR rely on a myriad different physical processes that occur in the Universe which are very often highly non-linear. These processes include, the nature and time-evolution of the ionizing sources. Do these sources have significant UV- (stars) and/or X-ray-

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(quasars) emission? What are the abundances of these sources as function of redshift? What is the escape fraction of ionizing photons from early galaxies/stellar clusters? These astrophysical uncertainties are surmounted by possible differences in the underlying cosmology, e.g., cosmologies featuring cold or warm dark matter, or different neutrino components.

To study these open problems in the most accurate way possible one can employ codes that couple gravitational, hydrodynamical and three dimensional radiative transfer calculations to evolve a simulation, such as the ART (Nakamoto et al., 2001; Yajima et al., 2009), RAMSES-RT (Rosdahl et al., 2013), or TRAPHIC (Pawlik and Schaye, 2008) codes. While this approach is the most accurate, it is also computationally very expensive to simulate large volumes, taking weeks or months for a single simulation run, and it is therefore not suitable for conducting large scale parameter studies. Hence, we need methods that are approximate and orders-of-magnitude faster than detailed cosmological simulation with exact radiative transfer calculations to feasibly simulate large fractions of this parameter space.

Alternative, faster methods have been developed and are based on the idea of post-processing N-body simulation or density fields. CRASH (Maselli et al., 2003) and C²-Ray (Mellema et al., 2006) are two codes which compute the three dimensional radiative transfer in such a manner. But even they are not fast enough to conduct large scale parameter space exploration.

Semi-analytic simulation methods are much faster. Battaglia et al. (2013) presented one such method which is based on a linear bias model derived from N-body and radiation-hydrodynamic simulations that can map a given large volume density field to a reionization redshift field to explore a limited parameter space. Other semi-analytic simulation methods, based on an excursion set approach, as employed in 21cmFast (see Mesinger et al., 2011) or SIMFAST21 (see Santos et al., 2010), take only minutes to run. These codes rely on the Zel'dovich approximation to evolve density fields which feature clustering properties of halos which match high resolution N-body simulations well on scales larger than 10 Mpc/h (White, 2014). Codes based on this approach capture the effects of non-linear processes introduced into the density field only in a limited manner and consequently the computed ionization fields will reflect that fact. This could be significant especially at lower redshifts, but generally also when correcting for redshift space distortions.

Another method to simulate the EoR was proposed by Thomas et al. (2009). The much faster scheme rests on the ansatz of using precomputed 1D radiative transfer simulations, which are then embedded into a dark-matter only N-body simulation. This procedure is further illustrated in Section 3.

The 1D radiative transfer code that is employed therein is called STARDUST,¹ whose inner workings were first described in Thomas and Zaroubi (2008). The spectral profiles that are generated by STARDUST are used by the BEARS² code which performs the actual EoR simulations. Thomas et al. (2009) demonstrated qualitatively and quantitatively that after applying the instrumental response of the LOFAR telescope simulations performed with BEARS are comparable to more sophisticated simulation codes and its approach to compute the EoR signal can be considered as valid. It should also be noted that BEARS served as the basis for the independently developed GRIZZLY code (see Ghara et al., 2015a; 2015b; 2018), which has already produced some interesting results.

Since the BEARS approach is computationally not as expensive as 3D radiative transfer codes, it is possible to study many different reionization scenarios and explore a large parameter space. To this end we created a simulation pipeline through which STARDUST, BEARS and a number of supporting codes work seamlessly together. The

Python pipeline package is called pyBEARS. A parameter file is used to instantiate a simulation and the pipeline returns a variety of useful information.

The purpose of this work is to provide a full and complete pipeline that builds upon the STARDUST and BEARS programs in order to simulate the Epoch of Reionization in a fast and reliable way. The STARDUST and BEARS programs are available on-line³ and the pyBEARS package, along with all other pipeline components will be made available as well. We have further developed a new faster algorithmic scheme to treat overlapping ionization bubbles than the one used in (Thomas and Zaroubi, 2008) and we have included this into the BEARS module.

This paper is structured as follows: In Section 2, we briefly cover some theoretical basics and in Section 3 we introduce the BEARS pipeline and its individual components in more detail and present some example runs. Section 4 includes our conclusions and we give an outlook of future work. Throughout this work we are employing the following cosmological parameters $\Omega_\Lambda = 0.6911$, $\Omega_m = 0.3089$, $\Omega_b = 0.0486$, $h = 0.6774$, and $\sigma_8 = 0.8159$.

2. Theoretical background

The hyperfine transition of a neutral hydrogen atom emits a photon with a wavelength of 21 cm, which is detectable in the radio regime. The intensity of the emission, naturally, depends on the amount of neutral hydrogen, which makes this emission line an important tracer of the ionization state of the intergalactic medium (IGM). To quantify the ionization state of the hydrogen component of the IGM, one makes use of the spin temperature T_{spin} , which can be defined via $n_1/n_0 = 3 \exp(T_*/T_{\text{spin}})$, where n_1 and n_0 are the number densities of neutral hydrogen in triplet and singlet states and $T_* = hc/k_B \lambda_{21\text{cm}}$. The spin temperature is influenced by collisional coupling (hydrogen-hydrogen and hydrogen-free electrons) and gas-radiation interactions, e.g. the coupling of neutral hydrogen to CMB photons via Thomson scattering or Ly α coupling via the Wouthuysen-Field effect. First formulated by Field (1958, 1959), T_{spin} can be expressed as follows

$$T_{\text{spin}}^{-1} = \frac{T_{\text{CMB}}^{-1} + x_\alpha T_\alpha^{-1} + x_c T_{\text{kin}}^{-1}}{1 + x_\alpha + x_c}. \quad (1)$$

Therein, x_α and x_c are the Ly α and collisional coupling coefficients respectively, T_{CMB} is the CMB temperature, T_{kin} is the kinetic gas temperature and T_α is the temperature which corresponds to the coupled Ly α photons, however, it is usually set to $T_\alpha = T_{\text{kin}}$. Following Field (1958) we note that the coupling coefficient x_α can be written as

$$x_\alpha = \frac{16\pi^2 T_* e^2 f_{12} J_0}{27 A_{10} T_{\text{kin}} m_e c} \quad (2)$$

where e is the electron charge, f_{12} oscillator strength of the Lyman- α transition, J_0 is the Lyman- α background flux, A_{10} denotes the Einstein coefficient for spontaneous emission of the 21 cm transition, m_e is the electron mass, and c is the speed of light.

The quantity that is measured by radio telescopes is the offset between spin temperature T_{spin} and background CMB temperature T_{CMB} , called the brightness temperature contrast δT_b , shown here as presented by Madau et al. (1997)

$$\begin{aligned} \delta T_b \approx & 28 \text{ mK} (1 + \delta_m) x_{\text{HI}} \left(1 - \frac{T_{\text{CMB}}}{T_{\text{spin}}} \right) \left(\frac{\Omega_b h^2}{0.023} \right) \\ & \times \left(\frac{dv_r/dr}{H(z)} + 1 \right)^{-1} \left[\left(\frac{1+z}{10} \right) \left(\frac{0.15}{\Omega_m h^2} \right) \right]^{\frac{1}{2}} \end{aligned} \quad (3)$$

The equation shows that the signal 21 cm experiments try to measure depends on a number of quantities related to astrophysical as well as

¹ Spectrum Transport Around RaDiating Universal Source Type.

² Bubbles Expanding Around Radiative Sources.

³ See <https://github.com/EoR/>.

and cosmological processes. The temperatures term, $\left(1 - \frac{T_{\text{CMB}}}{T_{\text{Spin}}}\right)$, and the neutral fraction term, $x_{\text{H I}}$ fall into the first category, while the terms that involve the cosmological parameters Ω_{i} , the matter overdensity field δ_{m} , the co-moving gradient of the gas velocity dv_r/dr , the redshift z , and the Hubble parameter $H(z)$ fall into the latter. To evaluate the spatial fluctuations of the brightness temperature contrast, we normalize δT_{b} so that the $\delta_{21}(\mathbf{x})$ distribution has a mean of zero and a variance of one

$$\delta_{21}(\mathbf{x}) = \frac{\delta T_{\text{b}}(\mathbf{x}) - \langle \delta T_{\text{b}} \rangle}{\langle \delta T_{\text{b}}^2 \rangle}. \quad (4)$$

To find δT_{b} the first generation EoR experiments measure the spherically averaged power spectrum $P(k)$, which is related to $\delta_{21}(\mathbf{x})$ via

$$\langle \hat{\delta}_{21}(\mathbf{k}) \hat{\delta}_{21}^*(\mathbf{k}') \rangle = (2\pi)^3 \delta(\mathbf{k} - \mathbf{k}') P(k). \quad (5)$$

Here, $\hat{\delta}_{21}(\mathbf{k})$ is the Fourier transformation of $\delta_{21}(\mathbf{x})$ and δ is the Dirac delta function. The dimensionless power spectrum is

$$\Delta^2(k) = k^3 P(k) / 2\pi^3. \quad (6)$$

3. The BEARS pipeline

To simulate the temperature brightness contrast δT_{b} , one has to simulate the different components of Eq. (3). In this section we introduce the simulation pipeline and give an overview of its individual components which can be grouped in three main categories: N-body simulations, radiative transfer codes and components related to the generation of the mock EoR signal. An organizational chart of the pipeline is depicted in Fig. 1.

Fig. 1. Current schematic of the simulation pipeline. It consists of three major parts: Components related to radiative transfer (RT) calculations, components related to setting up, running and post-processing N-body simulations, and lastly the actual EoR component. Red lines denote necessary inputs for the EoR simulations, solid lines show individual codes, while dashed lines represent components which are handled by the pipeline itself. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 2. Example slice plot of a density field and locations of the halo centers super-imposed (green stars). The density field stems from an N-body simulation employing 1024^3 dark matter particles and a box size of $100 \text{ cMpc } h^{-1}$. The snapshot is from redshift $z = 6.000$ and the triangular shaped cloud (TSC) method was used to grid the density field. The halos were found with the AMIGA halofinder (AHF). Density peaks without stars in this picture are associated with halos in adjacent slices (or did not fulfill the halofinder's search criteria). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

3.1. N-body simulations

We perform dark matter only N-body simulations to find the locations of the sources of ionizing radiation driving the EoR and to extract density fields of the simulation boxes. Both serve as inputs for the radiative transfer simulations.

The pipeline employs the freely available cosmological N-body code GADGET-2⁴ (Springel, 2005) and uses its accompanying initial conditions generator N-GenIC. The pipeline features different gridding algorithms to extract the density fields: the nearest grid point (NGP), the cloud in cell (CIC) and the triangular shaped cloud (TSC) methods. The AMIGA Halo Finder (AHF), presented in Knollmann and Knebe (2009), is used to find halos which are contained in the simulation, specifically their masses, position of centers, and peculiar velocities. The latter are used to account for redshift space distortions. As a visual aid, we present in Fig. 2 an example density slice plot obtained from the pipeline superimposed with the halo centers associated with the slice.

The halo positions found by the halofinder are updated to correspond with the nearest grid point of the BEARS computing grid. Due to the finite nature of the computing grid, it is possible for more than one halo to occupy the same grid-point. We combine these halos into one by summing over their masses and assign a new velocity, which is the mass-weighted sum of the original velocities. This correction can yield a reduced halo number of approximately 15% at redshift $z \sim 6$ for a simulation box of $100 \text{ cMpc } h^{-1}$ with spatial resolution of $\sim 200 \text{ kpc}$.

We test this section of the pipeline by comparing the halo catalogs obtained from simulations of different mass and spatial resolutions to a theoretical halo mass function (HMF) from Sheth et al. (2001), see Fig. 3. For all test runs we set the minimum number of dark matter particles that constitute a halo to 200. We find that the fiducial HMFs contain too much mass in almost all mass bins in case of the 256^3 run, contain too much mass in lower mass bins in case of the 512^3 run, and are comparable to the theoretical prediction in the 1024^3 case. We therefore use the N-body simulation employing 1024^3 dark matter

⁴ <http://www.mpa-garching.mpg.de/gadget/>.

Fig. 3. Plot of the distribution of halos found in simulations of varying resolution at redshift $z = 7$. The simulations were run in a box of size 100 cMpc with 256^3 , 512^3 , and 1024^3 dark-matter particles. For comparison we plot the theoretical halo mass function (HMF) from Sheth et al. (2001). The relatively low mass resolution of the 256 and 512 runs cannot adequately reproduce halos at the low-mass end. The halos we do find in those runs are thus too massive compared to the theoretical result. We therefore decided to employ results from the 1024 run for our BEARS simulations.

Table 1
Overview of our SED test models and the chosen parameters.

ID	Description
PL 1.5	SED model (a) with $\alpha = -1.5$
PL 1.0	SED model (a) with $\alpha = -1.0$
BB 8	SED model (b) with $M_{\text{star}} = 8M_{\odot}$ and $f_{\text{esc}} = 0.10$
IMF 10	SED model (c) with $f_{\text{esc}} = 0.10$
IMF 05	SED model (c) with $f_{\text{esc}} = 0.05$
CE 1.5	SED model (d) with $\alpha = -1.5$
CE 1.0	SED model (d) with $\alpha = -1.0$
	power-law contribution only for $z < 8.5$
	both: $\epsilon_{\text{QSO}} = 0.1$, $f_{\text{esc}} = 0.10$, and $5 < M_{\text{star}}/M_{\odot} < 100$

particles as the basis for the EoR test simulations shown in this work.

It should be noted that it is possible to use a completely different N-body simulation software stack if the halo catalogs and density fields are provided in a pipeline-compatible format. An interesting way to make use of this would be to forgo the time consuming N-body simulations all together and instead use a semi-analytic approach such as the PINOCCHIO code (Monaco et al., 2002). To limit the scope of this work we do not yet account for sub-resolution halos and will include an approach, e.g. as proposed by Kohler et al. (2007), in the future.

We provide the list of all pipeline parameters related to running and post-processing the N-body simulations, e.g. finding halos or gridding of the density fields, as well as the parameters for the STARDUST and BEARS parts of the pipeline with the code itself.

Fig. 4. Comparison of our seven spectral energy distribution models for a host halo of mass $M = 10^{10} M_{\odot}$ at redshift $z = 8$. The model parameters are shown in Table 1.

3.2. 1D Radiative transfer

The 1D radiative transfer code STARDUST is used to generate catalogs of radiative profiles at different redshifts (IGM densities) and for different source types. It is essentially an implementation of the radiative transfer calculations in an expanding IGM detailed in Fukugita and Kawasaki (1994). Results from previous versions of the code were presented and used in Thomas and Zaroubi (2008, 2011) and Thomas et al. (2009).

Provided with a source's spectral energy distribution (SED), STARDUST performs the radiative transfer computation along a grid whose extent and resolution are user defined. The code produces profiles at user defined time intervals of hydrogen and helium ionization fractions as well as the kinetic temperature of the IGM. These quantities are coupled by a system of stiff ordinary differential equations (see Section A.1) for whose solution STARDUST offers the following solvers: Dormand-Prince 5, Fehlberg 78, Bulirsch-Stoer, and Rosenbrock 4, all of which are provided by the ODEINT package, which is part of the peer-reviewed boost library collection⁵ (see Ahnert and Mulansky, 2011). Furthermore, we employ the GNU Scientific Library⁶ for interpolation and integration routines.

The code is made faster by using precomputed look up tables to obtain ionization rates at a given radius. It is for example possible to evolve a source's profile for 10^7 yr along a 10^3 kpc grid at a resolution of 0.1 kpc in under 10 minutes on a laptop.

The pipeline features a number of simple models to generate SEDs for sources embedded in halos of a given mass and redshift:

- A model for power-law like sources, such as quasars, with a given spectral index α which assumes that the central black hole's mass is computed as $M_{\text{bh}} = 10^{-4} (\Omega_b / \Omega_m) M_{\text{halo}}$ (Thomas and Zaroubi, 2011) and that the source emits radiation at given fraction of the Eddington luminosity, ϵ_{QSO} .
- A single blackbody model, which assumes the halo is populated by stars of only one type. We make use of the population III model put forward in Schaerer (2002).
- A model that populates a halo with stars following the Salpeter

⁵ <https://www.boost.org/>.

⁶ <https://www.gnu.org/software/gsl/>.

Fig. 5. To illustrate the time evolution of profiles, we chose the single star model BB 8. For a dark matter host halo of $M_{\text{halo}} = 10^{10} M_{\odot}$ at redshift $z = 8.0$, the outputs of STARDUST are plotted after 1, 3, 5, 7 and 9 Myr, starting from left to right in every sub-panel.

initial mass function (IMF). Here, we also make use of the population III model used in the previous model.

(d) A co-evolution model which combines (a) and (c).

Populating a given halo of mass M_{halo} with stars is done in the following manner: First we find the halo's total stellar mass with the fitting formula provided in Behroozi et al. (2013) and extrapolate from it for higher redshifts $z > 8$. In case of the single blackbody model we then pick a population III stellar mass M_{star} , interpolate the effective temperature T_{eff} and luminosity L from table 3 provided in Schaerer (2002), and compute a corresponding SED via the Planck law. We then scale up the SED with a factor of $f = M_{\text{star, total}}/M_{\text{star}}$ to arrive at the final SED. In the case of the IMF model we divide up the total stellar mass into different mass bins, apply the procedure for each bin, and add

up the resulting SEDs. In BEARS, we use profiles that were evolved in STARDUST for a fixed time t . We set this time to $t = 10 \text{ Myr}$ in order to roughly correspond to the duty cycle of quasars. We therefore have to account for the fact that some stars are not alive for the whole duration for which we evolve the SED in STARDUST. We equate a star's time on the main sequence (t_{MS}) to its' life time. If we find a $t_{\text{MS}} < t$ for a given star or stellar mass bin in the IMF case, we simply assume that the halos' stars burn consecutively and re-normalize the SED accordingly.

Note that we excluded population II stars here to limit the scope of this work and to allow for comparison with works which employed previous versions of the here presented software (see Thomas and Zaroubi, 2008; Thomas et al., 2009; Thomas and Zaroubi, 2011). Future EoR parameter studies will include these types of stars.

If converted to a pipeline compatible format, it is also possible to use

Fig. 6. Output of STARDUST for the spectra from Fig. 4. These results pertain to a dark matter halo of $M_{\text{halo}} = 10^{10} M_{\odot}$ at redshift $z = 8.0$. All the spectra have been evolved until $t = 10.0$ Myr.

spectral energy distributions generated by other means to explore additional parameters. In any case, the provided SED models can be used to build profile catalogs for different model parameters, dark matter halo masses, or redshifts. The latter translate directly to different background IGM densities.

To illustrate STARDUST's outputs, in Fig. 5 we show the time-evolution of the ionization of the various species of hydrogen and helium, along with the spin, kinetic and differential brightness temperatures profiles around a source embedded in a dark matter host halo of $M_{\text{halo}} = 10^{10} M_{\odot}$. The source features an SED of the BB 8 model and we plot profiles in intervals of 2 Myr after the source was switched on, starting from 1 and ending at 9 Myr. We can see how after an initial

phase of rapid expansion the ionization fronts slow down to eventually converge to a quasi-equilibrium state. In Fig. 6 we present a comparison of STARDUST outputs for all our different model SEDs as shown in Fig. 4 for the same dark matter host halo. All spectra were evolved for 10 Myr.

The different recipes to convert a dark matter halo to SEDs corresponding to different sources produce vastly different ionization and heating patterns around the source. As the PL 1.5 model produces the ionization front with the largest radius as measured from the source, one could conclude that this source model will most likely re-ionize the Universe the quickest. However, when looking at larger host halo masses we find that other models, notably the IMF 10 and CE 1.0

Fig. 7. Graphical representation of BEARS' improved overlap scheme. The smoothing filter we apply to the excess ionization fields is realized via a Gauß kernel with a smoothing scale σ of the order of the smallest bubble diameter.

Fig. 8. Required number of iterations to achieve a maximum ionization excess, ϵ , for different redshifts at two grid resolutions. Here we employ the CE 1.0 model in a 100 cMpc/h simulation box. The smoothing scale was set to $\sigma = 200$ kpc.

models produce larger ionization bubbles. It should be noted that both PL models assume an efficiency of $\epsilon_{\text{QSO}} = 1.0$, which means the quasars luminosity is equal to the Eddington limit and therefore very likely too high. Power law sources, especially with low spectral indices, generally

Fig. 9. Comparison of the power spectrum for two simulations (CE 1.0 model at $z = 9.0$) which only differed in the value of ϵ . Both curves are almost identical.

do not ionize as much as stellar sources because most of the produced photons are of higher energy and thus they escape being captured by neutral hydrogen. However, this type of source features an extended heating profile, which can be seen nicely when comparing the IMF 10 and CE 1.0 models. Both share the same stellar component but the latter features a QSO contribution. While both models have very similar hydrogen and helium I profiles (see solid red and blue dashed line in Fig. 6) their kinetic temperature profiles differ considerably.

We also observe the formation of helium II shells at different distances from the sources featuring different ionization fractions. The significant differences in the shown examples in Fig. 6 illustrate one of the reasons why we need fast reionization simulations. STARDUST can be used to study a wide range of possible sources and the produced profiles can be used to investigate different EoR scenarios by embedding them into N-body simulation outputs – the next step of the BEARS pipeline.

3.3. The BEARS code

BEARS (see Thomas et al., 2009) embeds the one dimensional radiative profiles generated with STARDUST into a three dimensional computing grid assuming spherical symmetry for the ionization profile. The density around the source is assumed to be the mean density of the Universe at that redshift. Although an approximation, simulations carried out using a more realistic Navarro-Frenk-White profile (see, Navarro et al., 1997) lead to minor changes for radii below ~ 50 kpc but overall provided similar results. It is assumed that the source profiles' origins correspond to the halo centers, i.e. we assume an inside out reionization scenario. It should be noted that in these simulations the clumping factor around a halo is not considered and thus the ionization bubbles are symmetric and no "shadowing effects" caused by density clumps are observed.

Despite these drawbacks in Thomas et al. (2009) it was shown that a comparison with CRASH, a full 3-D radiative transfer code, yielded results that we qualitatively and quantitatively shown to be much alike. Furthermore, when the images obtained from the simulation were smoothed using a Gaussian kernel with the same resolution as future EoR experiments ($\sim 3'$), the results were almost identical.

The BEARS pipeline typically requires, at a given redshift, (i) the list of all the halo masses and their corresponding positions, (ii) a catalog of precomputed profiles of ionization under the assumption of mean density at that redshift, (iii) the density at every grid point computed using one of the gridding algorithm. The outputs consists of hydrogen

Fig. 10. The improved BEARS overlap scheme: Here we present three simulation slices of the hydrogen ionization fraction during the iteration process of the overlap scheme. The middle row corresponds to a slice located in the middle of the box. The rows above and below represent two slices located 15 pixels apart from the central slice. Pixels with an ionization fraction that does not exceed a value of 1 are represented in gray-scale, while pixels with excess ionization, i.e. $x_{\text{HII}} \geq 1$, are shown in color. The simulation used here is a $100 \text{ cMpc } h^{-1}$ box with a 512^3 grid at redshift $z = 7.858$ and the sources are power-law like. The panels on the left hand side show the state of the simulation after the source profiles were embedded and before any smoothing was applied. The middle column of panels show the simulation after 20 iterations of the overlap algorithm and the third column of panels shows the simulation after 506 iterations after which the desired maximum excess of $\varepsilon = 10^{-7}$ was reached. The size of the smoothing kernel used here was $\sigma \approx 100 \text{ kpc}$ – the size of the smallest ionization bubble. It should be noted that the mean hydrogen ionization fraction remains constant throughout the smoothing process.

and helium fractions ionization fractions, the kinetic and spin temperatures, and the brightness temperature contrast.

3.4. Overlap of ionized bubbles

Since BEARS does not track individual photons through the simulation box, but rather embeds these ionizing bubbles around sources, it is necessary to account for overlapping bubbles. The overlapping regions are those that are ionized more than one bubble. In order to properly account for the photon budget, the code originally employed a correction algorithm (see Thomas et al., 2009) whose run-time scaled as $O(N_{\text{halo}}^3)$ after parallelizing, where N_{halo} denotes the number of halo centers. For simulations with $N_{\text{halo}} \gtrsim 10^5$ most of the computation time of a BEARS run is thus spend on the overlap correction.

In this paper, we have devised a new algorithm to deal with the overlapping problem in BEARS so that run time is minimized. The new algorithm scales as the time it takes to Fourier transform a box, i.e.

$N_{\text{pix}} \log(N_{\text{pix}})$. When embedding the three-dimensional source profiles, or bubbles, in the computing box we initially allow for ionization fractions $x_i > 1$ and distribute the excess ionization in the following way: we compute a separate box with the excess ionized fractions and convolve that with a Gaussian filter (we note that the choice of filter can be changed provided that the kernel is small enough) by performing two Fourier transforms. We then redistribute this excess ionization to the original box. This will diffuse regions on high ionization to locations close by in the box which are not fully ionized, which is what we would expect in regions where bubbles overlap. We perform this step until a convergence criterion is achieved. The smoothing filter is chosen to be a Gaussian with σ of the order of small bubble diameter. For a graphical representation of the algorithm, see Fig. 7.

We can achieve orders of magnitude improvement on the implementation of this method given that it is FFT-based as opposed to the original scheme implemented in Thomas and Zaroubi (2008). The actual runtimes of the overlap algorithm depend on the number of CPU

Fig. 11. Density weighted hydrogen neutral fraction for our test models. Models featuring stars, especially those with escape fractions of 10%, seem to yield the most realistic EoR scenarios. Changes in the escape fraction have a more pronounced effect on the re-ionization history than the contribution of quasar-like sources.

cores, the smoothing scale σ , maximum ionization excess ϵ , redshift, and resolution of the simulation. To illustrate the effect of the latter three quantities we run tests employing the CE 1.0 source model in a $100 \text{ cMpc}/h$ sized box with a smoothing kernel of fixed $\sigma = 200 \text{ kpc}$. The results of these performance runs are shown in Fig. 8. We find that the algorithm requires more iterations to reach lower ionization excess threshold for lower redshifts, which is a consequence of the emergence of more sources and thus more overlapping ionization bubbles. The increase in resolution, which, in the context of our simulation pipeline, results in finding more halos and thus sources, has a similar effect, albeit on a lesser scale. We used 64 CPU cores⁷ to conduct the test and measured 8.5 s/iteration in the 1024^3 grid case and 0.95 s/iteration in the 512^3 grid case.

Since the computational cost of the improved overlap scheme is largely determined by the maximum ionization excess ϵ , we explored its effect on an observable statistics, namely the 21cm power spectrum, and found that an $\epsilon = 0.1$ ensures sufficient convergence with more prudent choices for this parameter. An example comparison for a simulation at redshift 9 is shown in Fig. 9.

Fig. 10 illustrates the smoothing process for the ionization fraction. We show the central slice of the box, along with two slices offset by 15 pixels, and how the bubbles therein grow in locations with an excess of ionization fraction, i.e. multiple overlapping sources. The offset slices are shown to illustrate the 3D nature of the problem. This scheme for dealing with overlap of halos does indeed have drawbacks, one of which is that we can in principle move photons in the box in an arbitrary way and one could be worried about moving them in unphysical ways such as superluminally, however, the way that the bubbles grow is very slow compared to the speed of light and therefore this should not be a problem for us. However this scheme could in principle disrupt the recombination that happens in the center of galaxies and cores of overdensities, where the density is high and it is therefore more likely for us to have recombination and self shielding. It is beyond the scope of this

paper to deal properly with the cores of galaxies where recombination happens and in future work, one would have to consider the physical effect of this overlap to recombination regions.

3.5. Light cones & mock observations

The LOFAR-EoR experiment spans frequencies from about 100–200 MHz. These frequencies correspond to redshifts around 12 to 6, respectively. To reproduce such an observation, the BEARS pipeline is designed to produce the “cube” of observation in these frequencies. We call these mock simulations frequency-cubes or light cones. A brief summary of the process is as follows. First, we determine the number of slices that would go into the frequency cube. We assume a spectral resolution of 0.1 MHz between 100 and 200 MHz, giving us ≈ 1000 slices. For each of these slices, we calculate the corresponding redshift. Given that we output on the order of 25 simulations (instead of 1000) we use an interpolation scheme to estimate the brightness temperatures in the slices. The procedure is as follows; for a given slice we select the output boxes from BEARS that bracket the given redshift. From one of these boxes (usually the one with the lower redshift) we traverse a cosmological distance corresponding to the change in redshift required to reach the slice. We then average a few slices around this slice corresponding to the a resolution of 1KHz (this is the resolution of the LOFAR filter banks). Subsequently, we average the corresponding slices in the other box. The final estimate is obtained as a weighted average of the slices from the lower and higher redshift boxes with the weight being a function of their distances from the redshift of interest. A thorough description along with the equations for the implementation of the light cone can be found in Thomas and Zaroubi (2008), Section 4.

3.6. Results and statistics

3.6.1. Neutral fraction

The mean (mass-weighted) neutral fraction of our test models is shown in Fig. 11. We find that the models which fully ionize the box in accordance with observational constraints, i.e. $z < 7$ e.g. from the Gunn-Peterson effect, are BB 8, CE 1.0, and IMF 10. They all feature a stellar source component and the escape fraction was set to 10%. The contribution of the power-law, or QSO-like, source component in the CE 1.0 model does little to affect the model’s ionization history. The stand-alone effect of this component can be seen in the PL 1.0 run where 35% of hydrogen remains neutral at redshift $z = 6$. This does not come as a big surprise as most of the photons produced by sources featuring power-law like SEDs are too energetic to ionize hydrogen, whose ionization cross section scales with ν^{-3} for photon-energies larger than 13.6 eV. In light of this it makes sense that the PL 1.5 model with its steeper SED achieves a lower neutral fraction: Its sources produce far more photons near the hydrogen ionization edge compared to the PL 1.0 model. The IMF 05 and the CE 1.5 models are very similar as they share the same stellar SED component. The latter model ionizes the box slightly more due to its QSO contribution. The fact that the PL 1.5 model overtakes the CE 1.5 model at low redshift is probably due to the emergence of more low mass halos and the more efficient mass to light conversion of the PL model (see also Fig. 6 and related discussion). We note that when comparing stellar, quasar, and co-evolution models it becomes clear that stars are the driving force in our EoR scenarios.

3.6.2. Slice plots from BEARS outputs

To visualize differences in morphology we present slice plots of our simulations for selected models at redshift $z = 8$ in Fig. 12. Here we chose one power law, one IMF, and one co-evolution model: PL 1.5, IMF 10, and CE 1.5, respectively. The panels in the first four rows of the plot are the BEARS simulation products: the hydrogen neutral fraction x_{HI} , kinetic as well as spin temperature and lastly the brightness temperature contrast. The three neutral fraction slice plots reflect the results of the mean neutral fraction plot discussed above. The IMF 10 model

⁷ The machine used for these tests is equipped with Intel Xeon E7-8850 CPUs running at 2.00 GHz.

Fig. 12. Slice plots of selected BEARS outputs for the PL 1.5, IMF 10, and CE 1.5 models at redshift $z = 8$ are shown in the first four rows: The neutral fraction of hydrogen, the kinetic and the spin temperatures as well as the brightness temperature contrast. Assuming that $T_{\text{spin}} > T_{\text{CMB}}$, we re-computed the brightness temperature contrast, which is displayed in row five.

exhibits the largest continuous ionized regions, followed by the CE 1.5 and the PL 1.5 models. The spin and kinetic temperature maps look similar across all three models, though it is possible to discern the different temperature profiles for individual halos.

BEARS does not yet compute δT_B in a completely self-consistent manner, heating via Lyman- α flux is included in the simulation by using a constant Ly- α Flux J_0 , taken from Table 1 from Latif et al. (2011) (model 8). However, to obtain more realistic results, we assume full Ly- α coupling and furthermore assume that $T_{\text{spin}} > T_{\text{CMB}}$, which is likely to be true for redshifts $z < 11$ (see, e.g., Zaroubi, 2013). We re-calculate the brightness temperature contrast and plot the results in the fifth row of panels in Fig. 12. Seeing that the slice plots show mainly the effects of sources placed into relatively massive halos it becomes once more apparent that we are limited to inside out EoR scenarios with

BEARS and that the lack of low mass halos makes it difficult to study EoR scenarios driven by faint galaxies. Implementing a prescription for low mass halos to remedy this shortcoming goes beyond this work but we hope to include an adequate treatment in the future. Note that slice plots of the remainder of our models can be seen in the appendix in Fig. B.23.

3.6.3. Power spectra

We present power spectra of three models at three different redshifts in Fig. 13. They are based on the modified δT_B outputs discussed above. At high redshift the highest power spectra amplitudes feature at high k , or on small scales, and as the EoR process sets in and ionizes more and larger regions, we see a loss in power at larger k and an increase at smaller values. Let us examine the different length scales in more detail:

Fig. 13. Power spectra for selected models at three redshifts. As more and larger regions are ionized, the power at high k , or small scales, is reduced and the amplitudes at lower k increase. The strong features at $k \lesssim 0.4$ are likely due to the small box size while the features in the $0.4 \lesssim k \lesssim 1$ range correspond to the emerging and growing ionization bubbles.

At large scales, i.e. $k \lesssim 0.4$, we can see strong features, even at high redshift when only few small ionization bubbles have started to appear. Small scale structures should not have such a strong influence on power spectrum amplitudes at large scales and we therefore conclude that these features are very likely a result of a relatively small box size (for EoR simulations). Within this limited box volume one will find only few large scale modes, leading to higher uncertainties in the power spectrum results for low k . At intermediary scales, i.e. $0.4 \lesssim k \lesssim 1$, we can see fluctuations in the power spectrum amplitude which we ascribe to the emerging bubbles, as those k values correspond to the characteristic sizes of our ionization bubbles. Higher amplitudes can be seen for the IMF 10 model (blue line) because the reionization progresses more rapidly in this model. For the same reason we can also see a stark decrease in signal over the whole spectrum for this model at redshift $z = 7$, which one would expect towards the end of the reionization

Fig. 14. Redshift evolution of the mean (top panel) and skewness (bottom panel) of the brightness temperature contrast for our different source models.

process. We included power spectra for the remaining four models in the appendix, see Fig. B.21.

3.6.4. Further statistical analysis

To study the differential brightness temperatures in more detail, we compute the distribution's mean and to characterize the shape of the distribution, we look at the skewness. The evolution of both quantities is shown in top and bottom panels of Fig. 14 respectively. The evolution of the mean, $\langle \delta T_B \rangle$, largely mirrors the results of the mean neutral fraction comparison (see Fig. 11). The models, which fully ionize the box reach $\langle \delta T_B \rangle = 0$, whereas the other models do not. The skewness of a given (continuous) distribution, usually defined as a non-dimensional number, can be expressed as the fraction of the third moment about the distribution's mean, $\langle \delta T_B \rangle_3$, and its standard deviation σ :

$$\text{Skew} = \frac{\langle \delta T_B \rangle_3}{\sigma^3} = \frac{1}{N} \sum_{i=1}^N \left[\frac{\delta T_{B,i} - \langle \delta T_B \rangle}{\sigma} \right]^3, \quad (7)$$

where $i = 1 \dots N$ denote the individual pixels of our 3 dimensional computing grid. The skewness has a positive value if the distribution features an asymmetric tail extending towards positive values, which is what we see to varying degrees in our results. The three models, which fully ionize their boxes see a moderate increase in skewness first (when compared to the other models) and then a very strong increase from redshift $z < 8$ onwards, hinting at a much more efficient mass to light conversion and subsequent increase in ionization at those redshifts.

In order to visualize the δT_B distributions, we plot probability distribution functions (PDF) of three models and their respective redshift evolutions in Fig. 15. We can see how the distributions in all three models become more skewed towards lower redshifts as more pixel are

Fig. 15. We plot the fraction of pixels per δT_B bin for our three models at different redshifts. The distributions become more strongly (positively) skewed for lower redshifts – the IMF 10 model more notably so compared to the two others.

ionized and move into the first bin. By redshift $z = 7$ approximately 90% of pixels reside in the first bin in the IMF 10 model. For the CE 1.5 and PL 1.5 model, this only applies to 55% and 45% of the pixels, respectively. Plots for the remaining models can be found in appendix in Fig. B.22.

To show that pixels associated with different over-dense regions are ionized at different rates, we show the fraction of ionized hydrogen pixel in different over-density bins for the CE 1.0 model in Fig. 16. We deem a pixel to be ionized if it features a 99% ionization fraction. It does not come as a surprise that we see pixels associated with high density regions ionized first, which is expected as those are host to our sources or at least close to them. At redshift $z = 10$ only $\sim 5\%$ of the pixels in the lowest over-density bin are ionized. This figure grows to $\sim 51\%$ at redshift $z = 8$.

3.6.5. Visualization of instrumental response

EoR simulation pipelines ultimately aim to produce simulation end products which are comparable to data obtained from telescopes. One

Fig. 16. Fraction of ionized pixel for different over-densities at three redshifts for the CE 1.0 model. High density regions are on average ionized first, in accordance with the (BEARS intrinsic) inside out reionization scenario.

important step is thus to include a prescription into our pipeline to model the instrumental response of a first generation EoR instrument on our simulation outputs. Note that at this point we do not add galactic or ionospheric foregrounds to our fiducial signal and limit ourselves to creating images that were convolved with the instrument's point spread function (PSF), the so called dirty images. The PSF, also called the dirty beam, can be thought of as the Fourier transform of the combined aperture of the telescope. EoR observations with LOFAR are performed primarily with the array's dense core of antennas. Combining observations from many nights the synthesized beam approaches a two dimensional Gaussian in the beam center (see, e.g. van Haarlem et al., 2013; Patil et al., 2016; 2017). To mimic LOFAR's PSF we assume it to be a Gaussian function with a full width half maximum (FWHM) of approximately $4'$ and convolve simulation slices at a given redshift, i.e. frequency, to produce a dirty image as it can be obtained from the visibilities that the telescope registers. The thus produced images also rely on the assumptions that our mock observation has good coverage of the uv -plane and that calibration as well as image plane errors were minimized. We apply our simplified version of LOFAR's point spread function to simulation outputs of three of our models and show the results in Fig. 17. The three models produce three easily distinguishable maps. However, we note that in order to (statistically) differentiate between more similar models larger simulation volumes will be required. Our current simulation box size of $100 h^{-1}\text{cMpc}$ corresponds to a field of view of approximately $50' \times 50'$ (at $z \sim 8.5$), which presents only a small part of LOFAR's field of view of $5^\circ \times 5^\circ$. To simulate such a

Fig. 17. Maps of the brightness temperature contrast for three models at redshift $z = 7.75$ as obtained from our simulations (left) and as seen by LOFAR (not considering foregrounds or noise). The simulation snapshots slices were convolved with a Gaussian smoothing kernel with a FWHM of $4'$.

field of view one would need box sizes in excess of approximately $600 h^{-1}\text{cMpc}$, which is not out of reach for the new version of the BEARS pipeline.

3.6.6. Light-cone

Following the prescription we presented in Section 3.5, we created frequency cubes, or light-cones, from individual simulation outputs for our test models and show three of them in Fig. 18 and, including LOFAR's response, in Fig. 19 (The remaining models are shown in the appendix, see Figs. B.24 and B.25). The plots span over a redshift range of $6 < z < 12$, which corresponds to LOFAR's EoR observation window, and can therefore be seen as a tomography of each model's reionization history. The IMF 10 model can be seen as creating large ionized bubbles, which grow to larger patches and finally to full ionization at redshift $z \sim 6$. The other two models show much smaller patches of ionized regions and a few small neutral regions at low redshift resulting in a not fully ionized IGM at redshift $z = 6$ leaving approximately 5% of the simulated hydrogen neutral. Comparing The raw light cone with the PSF-applied versions, see Figs. 18 and 19, only highlights the need for larger simulation volumes as the visibly smoothed, and more realistic data will thus gain in expressiveness in a statistical sense. As we aim to create meaningful priors to analyze and compare future observation

data with, here, bigger is better.

4. Conclusion & outlook

In this paper we presented a new simulation pipeline based on the codes STARDUST and BEARS, which can be used to simulate the Epoch of Reionization in a fast way. BEARS was first introduced in Thomas et al. (2009) and we have extended and improved upon their work – notably a new, more generalized subsystem to model sources and a new algorithm to compute the effects of overlapping ionization bubbles. The resulting pipeline is now faster, more flexible, more efficient, and more physically motivated. It consists of the BEARS and STARDUST codes as well as a light-cone code, a density gridding code, a module to generate SEDs, analysis routines, and a Python package for pipeline-related purposes. The pipeline's key properties and capabilities are summarized below:

- The package offers the user the possibility to simulate the EoR faster than simulations that make use of full 3D radiative transfer codes.
- The pipeline successively runs dark matter only N-body simulations and a halo finder to locate halos, which are assumed to have hosted the sources of Reionization and extracts density as well as velocity fields. These data serve as input for the radiative transfer calculations. Pre-existing simulations or simulations performed with different codes can also be used if provided in a BEARS compatible format.
- The 1D radiative transfer code STARDUST is used to build catalogs of ionizing profiles based on user-provided spectral energy distributions for the EoR sources or SEDs generated with the pipeline's SED generator, which allows for the modeling of a wide range of radiative sources.
- BEARS embeds the source profiles in the simulation box and accounts for overlaps of ionized bubbles in a much faster way than before.
- The pipeline features a number of visualization and analysis routines.
- We have improved the runtime of all pipeline components by parallelizing and optimizing existing implementations where possible. STARDUST can evolve a single SED in minutes and BEARS can process an individual simulation snapshots in ~ 10 min and is considerably faster at high redshift. Overall run times strongly depend on the user-defined resolutions and accuracy requirements. The 1D profile catalogs used in this work featured a relatively high spatial and temporal resolution and were each generated within ~ 30 min using 40 CPU cores. The individual BEARS runs took ~ 15 h to simulate using 64 CPU cores each. The majority of computation time was spent on the overlap treatment and could have been reduced drastically had the principal author not opted for a maximum ionization threshold of $\epsilon = 10^{-7}$, see Figs. 8 and 9. The frequency cubes were computed each in ~ 15 min employing 64 CPU cores.

We highlighted the individual pipeline components and data products by running seven different source models and discussing the results. The takeaway message from this simple model comparison is that our stellar source model featuring a 10% UV escape fraction seems to provide the most realistic reionization scenario. The power law only models seem to re-ionize the Universe only when featuring a very steep spectral index of $\alpha > 1.5$ and while emitting ionizing photons at the Eddington limit. The power law contribution in our co-evolution models did not have much effect on the overall hydrogen reionization history. However, we do acknowledge that more systematic large-scale parameter studies are in order to draw more meaningful conclusions.

Future parameter studies could explore our existing parameter

Fig. 18. Frequency cubes of three selected source models, spanning LOFAR’s frequency range. Light-cone plots for the remaining models are shown in Fig. B.24 .

space but could also expand on it, for example by introducing a UV background into STARDUST’s source catalog generation. In the course of this work we tested the effect of a NFW background density profile on the 1D RT computations and found that its inclusion lead only to slight variations of the radiative profiles at small radii. It might, however, be interesting to study a wider range of background density profiles or even inhomogeneous density profiles, i.e. to mimic the statistical properties of a clumpy IGM.

Other components of the pipeline could be improved too of course. The N-body module of the pipeline could for example be extended to feature a sub-grid prescription for low mass halos. BEARS could be upgraded so that it models clumping factor effects, the Ly- α flux and self-consistently computes δT_B . Redshift space distortions will be added to the light-cone code. To produce even more realistic mock observations one could also add foregrounds.

STARDUST and BEARS have been made publicly available and the

remaining pipeline components will be published as well in the near future along with the python pipeline package itself. A lot of work remains on the pipeline but we feel that the BEARS pipeline in its present form already presents a good foundation for future projects.

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Fig. 19. Frequency cubes of three selected source models, spanning LOFAR’s frequency range and featuring the instrument’s response and a frequency resolution of 1 MHz. Equivalent light-cone plots for the remaining models are shown in Fig. B.25 .

Appendix A. Additional notes on STARDUST

A1. Rate equations

Assuming spherical symmetry, the STARDUST code solves a set of rate equation along a 1-dimensional grid for every time step until the maximum age of the source is reached. The code can make use of different background density profile to track the different hydrogen and helium species (either a flat density profile in which the density is equal to the critical density at the redshift of the simulation or the NFW profile (see below). At source age t and at distance r away from the source one can compute the optical depth (as *perceived* by a photon of energy E)

$$\tau(E, r, t) = \sum_i \int_r \sigma_i(E) n_i(r, t) dr \quad (\text{A.1})$$

where $i = \text{H i}, \text{He i}, \text{He ii}$, the n_i denote the respective number densities, and σ_i the respective cross-sections. Knowing the spectral energy distribution $I(E)$ of our source, we can now calculate the source flux:

$$N(E, r, t) \propto e^{-\tau(E, r, t)} I(E) \quad (\text{A.2})$$

We note that in the provided version of STARDUST the SEDs to be used should be appropriately normalized to take into account the flux of photons provided by the central source.

The system of stiff differential equations which STARDUST solves are based on equations (26), (29), (30), and (36) in Fukugita and Kawasaki (1994):

$$\frac{d}{dt} x_{\text{H ii}} = \Gamma_{\text{H i}} x_{\text{H i}} - \alpha_{\text{H ii}} n_e^2 / n_{\text{H}} \quad (\text{A.3})$$

Fig. A1. Results of the Strömgren sphere test, using the initial conditions of test I in Iliev et al. (2006). The code accumulates an error lower than 1% per $t_{\text{rec}} = 122.4\text{Myr}$ timescale, which we deem acceptable.

$$\begin{aligned} \frac{d}{dt}x_{\text{He ii}} &= \Gamma_{\text{He i}}x_{\text{He i}} + \beta_{\text{He i}}n_{\text{e}}x_{\text{He i}} \\ &\quad - \beta_{\text{He ii}}n_{\text{e}}x_{\text{He ii}} - \alpha_{\text{He ii}}n_{\text{e}}x_{\text{He ii}} \\ &\quad + \alpha_{\text{He iii}}n_{\text{e}}x_{\text{He iii}} - \xi_{\text{He ii}}n_{\text{e}}x_{\text{He ii}} \end{aligned} \quad (\text{A.4})$$

$$\begin{aligned} \frac{d}{dt}x_{\text{He iii}} &= \Gamma_{\text{He ii}}x_{\text{He ii}} + \beta_{\text{He ii}}n_{\text{e}}x_{\text{He ii}} \\ &\quad - \alpha_{\text{He iii}}n_{\text{e}}x_{\text{He iii}} \end{aligned} \quad (\text{A.5})$$

Here, α_i denote the respective recombination, β_i the collisional ionization, ξ_i the dielectronic recombination coefficients, and the Γ_i are the respective ionization rates. Moreover, n_{B} stands for the total baryon number density, n_{e} is the electron number density, n_{H} represents the total hydrogen number density, and n_{He} is total helium number density. The ionization rates are computed as follows:

$$\Gamma_{\text{H i}} = \beta_{\text{H i}}n_{\text{e}} + \int_{E_{\text{H i}}}^{\infty} \sigma_{\text{H i}}N(E, r, t) \frac{dE}{E} \quad (\text{A.6})$$

$$\Gamma_{\text{He i}} = \int_{E_{\text{He i}}}^{\infty} \sigma_{\text{He i}}N(E, r, t) \frac{dE}{E} \quad (\text{A.7})$$

$$\Gamma_{\text{He ii}} = \int_{E_{\text{He ii}}}^{\infty} \sigma_{\text{He ii}}N(E, r, t) \frac{dE}{E} \quad (\text{A.8})$$

The fourth equation of the ODE system, which tracks the heating rate, can be written as follows

$$\begin{aligned} \frac{3}{2} \frac{d}{dt} \left(\frac{k_{\text{B}} T_{\text{e}} n_{\text{B}}}{\mu} \right) &= \sum_i n(i)c \int \sigma_i(E - E_i)N(E, r, t) \frac{dE}{E} \\ &\quad - \sum_i n_{\text{e}}n_i(\zeta_i + \eta_i + \psi_i) \\ &\quad - \omega_{\text{He ii}}n_{\text{e}}n_{\text{He iii}} \\ &\quad - \theta_{\text{ff}}(n_{\text{H ii}} + n_{\text{He ii}} + 4n_{\text{He iii}})n_{\text{e}} \\ &\quad - \frac{15}{2} \frac{a}{a} \left(\frac{k_{\text{B}} T_{\text{e}} n_{\text{B}}}{\mu} \right) \end{aligned} \quad (\text{A.9})$$

Therein, the index $i = \text{H i}, \text{He i}, \text{He ii}$ is again a placeholder for the ion species. The n_i denote the respective ion number densities, E_i are the ionization thresholds, and σ_i the photo ionization cross sections. Furthermore, ζ_i, η_i, ψ_i are cooling coefficients for collisional ionization, recombination, and collisional excitation, respectively, while $\omega_{\text{He ii}}$ is the helium II dielectronic recombination cooling coefficient and θ_{ff} is the free-free cooling coefficient. n_{B} and n_{e} are the baryon and electron number densities, respectively. The last term, which includes the Hubble parameter $\frac{a}{a} = H$, accounts for cooling due to expansion of the Universe. Note that we do not include Compton heating for now, which becomes relevant only at higher energies.

A2. Strömgren sphere test

To gauge the results of a RT code and hence its reliability, it is ideal to have it solve a problem that has a known analytical solution – such as the Strömgren sphere test. Here, one assumes that a radiation source emits photons of energy $E = 13.6\text{eV}$ at a given rate of $\dot{N}_{\gamma}$ into a hydrogen gas of density n_{H} and constant temperature T . Assuming spherical symmetry, one can then compute the distance from the source at which the ionization

and recombination rates are in equilibrium (see e.g. [Strömgren, 1939](#)). The radius of the expanding ionization front can be written as

$$r_I = r_S \left(1 - \exp\left(-\frac{t}{t_{\text{rec}}}\right) \right)^{1/3}. \quad (\text{A.10})$$

Here,

$$r_S = \left(\frac{3\dot{N}_\gamma}{4\pi\alpha_B(T)Cn_{\text{H}}^2} \right)^{1/3}$$

is the Strömgren radius, $t_{\text{rec}} = (\alpha_B(T)Cn_{\text{H}})^{-1}$ is the recombination timescale, $\alpha_B = 2.59 \cdot 10^{-13} (T/10^4 \text{K})^{-0.85} \text{cm}^3 \text{s}^{-1}$ is the case B recombination coefficient, and C is the clumping factor. We perform this test by adopting the parameters from test I in [Iliev et al. \(2006\)](#): The source emits $\dot{N}_\gamma = 10^{48}$ photons per second, the clumping factor is set to $C = 1$, the temperature to $T = 10^4 \text{K}$, and the hydrogen density to $n_{\text{H}} = 10^{-3} \text{cm}^{-3}$. We measure the position of the I-front as the distance from the source where the ionization fraction is $x_{\text{H I}} = 0.5$. Our results, which are shown in [Fig. A.20](#), agree quantitatively and qualitatively with the majority of codes tested in ([Iliev et al., 2006](#)). The slowly but steadily increasing error reflects the fact that the analytical solution assumes a fully ionized medium within the bubble, i.e. $x_{\text{H I}} = 0$, whereas the numerically-obtained ionization fractions within the bubble are on the order of $x_{\text{H I}} \approx 10^{-7} - 10^{-5}$. For a further discussion of this point we refer the reader to Section 5.3 of [Pawlik and Schaye \(2008\)](#).

Appendix B. Additional plots

Fig. B1. Same as [Fig. 13](#) – Power spectra for remaining models. Bubbles emerge earlier in the BB 8 and co-evolution models, then in the IMF 05 and very late in the power-law model.

Fig. B2. Same as Fig. 15 – Fraction of pixels per δT_B bin for the four remaining models at different redshifts. The distributions become more strongly (positively) skewed for lower redshifts.

Fig. B3. Same as Fig. 12 – Slice plots of BEARS outputs for the remaining models at redshift $z = 8$ are shown in the first four rows: The neutral fraction of hydrogen, the kinetic and the spin temperatures as well as the brightness temperature contrast. Assuming that $T_{\text{spin}} > T_{\text{CMB}}$, we re-computed the brightness temperature contrast, which is displayed in row five.

Fig. B4. Same as Fig. 18 – Light-cone plots of the remaining models spanning LOFAR's frequency range without instrumental response .

Fig. B5. Same as Fig. 19 – Frequency cubes of the four remaining source models, spanning LOFAR’s frequency range and featuring the instrument’s response and a frequency resolution of 1 MHz.

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