

# Fast Large-Scale Reionization Simulations

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## ABSTRACT

We present an efficient method to generate large simulations of the Epoch of Reionization (EoR) without the need for a full 3-dimensional radiative transfer code. Large dark-matter-only simulations are post-processed to produce maps of the redshifted 21cm emission from neutral hydrogen. Dark matter haloes are embedded with sources of radiation whose properties are either based on semi-analytical prescriptions or derived from hydrodynamical simulations. These sources could either be stars or power-law sources with varying spectral indices. Assuming spherical symmetry, ionized bubbles are created around these sources, whose radial ionized fraction and temperature profiles are derived from a catalogue of 1-D radiative transfer experiments. In case of overlap of these spheres, photons are conserved by redistributing them around the connected ionized regions corresponding to the spheres. The efficiency with which these maps are created allows us to span the large parameter space typically encountered in reionization simulations. We compare our results with other, more accurate, 3-D radiative transfer simulations and find excellent agreement for the redshifts and the spatial scales of interest to upcoming 21cm experiments. We generate a contiguous observational cube spanning redshift 6 to 12 and use these simulations to study the differences in the reionization histories between stars and quasars. Finally, the signal is convolved with the LOFAR beam response and its effects are analyzed and quantified. Statistics performed on this mock data set shed light on possible observational strategies for LOFAR.

**Key words:** quasars: general – cosmology: theory – observation – diffuse radiation – radio lines: general.

## 1 INTRODUCTION

The history of our Universe is largely unknown between the surface of last scattering ( $z \approx 1100$ ) down to a redshift of about 6. Because of the dearth of radiating sources and the fact that we know very little about this epoch, it is often referred to as the “dark ages”. Theoretical models suggest that around redshifts 10 – 20, the first sources of radiation appeared that subsequently reionized the Universe. Two different experiments provide the bounds for this epoch of reionization (EoR); the high polarization component at large spatial scales of the temperature-electric field (TE) cross-polarization mode of the cosmic microwave background (CMB) providing the upper limit for the redshift at  $z \approx 11$  (Page et al. 2007) and the

rapid increase in the Lyman- $\alpha$  optical depth towards redshift 6, observed in the spectrum of high redshift quasars (Fan et al. 2006), the lower limit. Although the redshifted 21cm hyperfine transition of hydrogen was proposed as a probe to study this epoch decades ago (Sunyaev & Zeldovich 1975), the technological challenges to make these observations possible are only now being realised. In the meantime, theoretical understanding of the EoR has improved greatly (Hogan & Rees 1979; Scott & Rees 1990; Madau, Meiksin, & Rees 1997). Over the past few years there have been considerable efforts in simulating the 21cm signal from the Epoch of Reionization. Almost all of the methods employed in simulating the 21cm involve computer intensive full 3-D radiative transfer calculations (Gnedin & Abel 2001; Ciardi et al. 2001; Ritzerveld, Icke, & Rijkhorst 2003; Susa 2006; Razoumov & Cardall 2005; Nakamoto, Umemura, & Susa 2001; Whalen & Norman 2006; Rijkhorst et al.

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2006; Mellema et al. 2006; Zahn et al. 2007; Mesinger & Furlanetto 2007; Pawlik & Schaye 2008).

Theories predict that the process of reionization is complex and sensitively dependent on many not-so-well-known parameters. Although stars may be the most favoured of reionization sources, the role of mini-quasars (miniqsos), with the central black hole mass less than a few million solar masses, are debated (Nusser 2005; Zaroubi & Silk 2005; Kuhlen & Madau 2005; Thomas & Zaroubi 2008). Even if the nature of the sources of radiation would be relatively well constrained, there are a number of “tunable” parameters like the photon escape fraction, masses of these first sources, and so on, that are not well constrained.

In a couple of years, next generation radio telescopes like LOFAR<sup>1</sup> and MWA<sup>2</sup> will be tuned to detect the 21cm radiation from the EoR. Although the designs of these telescopes are unprecedented, the prospects for successfully detecting and mapping neutral hydrogen at the EoR critically depends on our understanding of the behaviour and response of the instrument, the effect of diffuse polarized Galactic & extra-galactic emission, point source contamination, ionospheric scintillations, radio frequency interference (RFI) and, not least, the characteristics of the desired signal. A good knowhow of the above phenomena would enable us to develop advanced signal processing/extraction algorithms, that can be efficiently and reliably implemented to extract the signal. In order to test and confirm the stability and reliability of these algorithms, it is imperative that we simulate, along with all the effects mentioned above, a large range of reionization scenarios.

Fig. 1 shows the basic building blocks of the simulation pipeline being built for the LOFAR-EoR experiment. This paper basically constitutes the first block, i.e., simulation of the cosmological 21cm EoR signal. This then passes through a sequence of blocks like the foreground simulation (Jelić et al. 2008), instrument response and extraction (Lambropoulos et al., *in prep*). The extracted signal is then compared with the original signal to quantify the performance of the extraction scheme. This process needs to be repeated for various reionization scenarios to avoid any bias the extraction scheme would have if only a subsample of all possible signal characteristics were used.

Simulating observing windows as large as the Field of View (FoV) of LOFAR ( $\sim 5^\circ \times 5^\circ$ ) and for frequencies corresponding to redshift 6 to 12 is a daunting task for conventional 3-D radiative transfer codes because of multiple reasons such as a requirement for high dynamic range in mass for the sources of reionization, their large number towards the end of reionization and the size of the box which strains the memory of even the largest computer cluster. In order to facilitate the simulation of such large mock data sets for diverse reionization scenarios, we need to implement an approximation to these radiative transfer methods that mimic the “standard” 3-D simulations to good accuracy. It was clear from the onset that the details of the ionization fronts like its complex non-spherical nature will not be reproduced by the semi-analytical approach that we propose here. But the argument towards overlooking this discrepancy is that when the outputs of our semi-analytical approach and that of a 3-D radiative transfer code are passed through the machinery of the LOFAR-EoR pipeline, they are experimentally indistinguishable. The reason being the filtering nature of the telescope’s point spread function (PSF) across the sky and the substantial bandwidth averaging along the frequency/redshift direction that

is needed to recover the signal, smoothes out the structural details captured by 3-D codes.

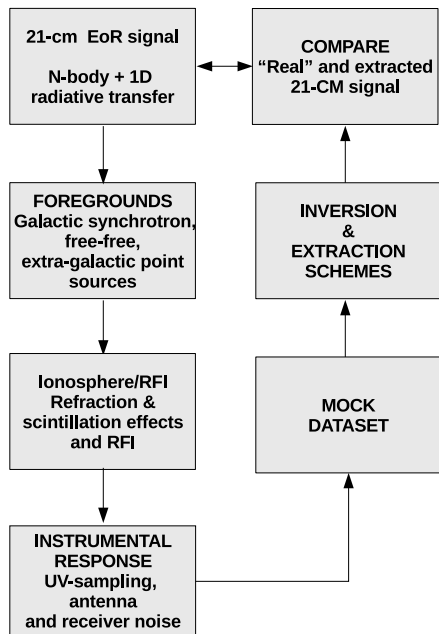
Recently, several authors (Zahn et al. 2007; Mesinger & Furlanetto 2007) have proposed schemes to reduce the computational burden of generating relatively accurate 21cm maps. These methods do fairly well, although there are some caveats, like for example the intergalactic medium (IGM) ionization being treated as binary, i.e., the IGM is either ionized or neutral (Mesinger & Furlanetto 2007). Although this might be the case for stellar-like sources, others with a power-law component could exhibit an effect on the IGM wherein the ionizing front is extended and hence this assumption need not hold (Zaroubi & Silk 2005; Thomas & Zaroubi 2008). Added to this, the schemes presented in order to compute the 21cm maps, make the assumption that the spin temperature of hydrogen,  $T_s$  is much larger than the CMB temperature. Towards the end of reionization ( $z < 8$ ) this might very well be valid. But the dawn of reionization would see a complex spatial correlation of IGM temperatures with the sources of radiation, its clustering and spectral energy distributions (Venkatesan, Giroux, & Shull 2001; Zaroubi et al. 2007; Thomas & Zaroubi 2008; Pritchard & Furlanetto 2007). In the current paper we have assumed that the spin temperature is coupled to the kinetic temperature and that they are much higher than the CMB temperature. At higher redshifts this need not be a valid assumption. The effects of heating by different types of radiative sources on the IGM and the coupling (both Ly- $\alpha$  and collisional) between the spin and kinetic temperature will be simulated accurately in a follow-up paper *Thomas et al., in prep*, using the same scheme, but now applied to heating.

In this paper we propose a method of post processing numerical simulations in order to rapidly generate realistic 21cm maps. Briefly, the algorithm consists of simulating the ionization fronts created by the “first” radiative sources for a range of parameters which include the power spectrum, source mass function and clustering. We then identify haloes in the outputs of N-body simulations and convert them to a photon count using semi-analytical prescriptions, or using the photon count derived from a Smoothed Particle Hydrodynamics (SPH) simulation. Depending on the photon count and the spectrum, we embed a sphere around the centre-of-mass (CoM) of the halo whose radial profile matches that of a profile from the table created by the 1-D radiative transfer code of Thomas & Zaroubi (2008). Appropriate operations are carried out to conserve photon number. Since, the basic idea is to expand bubbles around locations of the sources of radiation, we call this method BEARS (Bubble Expansion Around Radiative Sources). For the sake of brevity and comparison with full 3-D radiative transfer codes, we restrict ourselves to monochromatic radiative transfer with a fixed temperature. A following paper will include a full spectrum along with the temperature evolution. The results of our semi-analytic scheme will be compared to those obtained with the full 3-D Monte Carlo radiative transfer code CRASH (Ciardi et al. 2001; Maselli, Ferrara, & Ciardi 2003).

In §2 we describe the various steps involved in implementing the BEARS algorithm on the outputs of N-body simulations. We describe the specifications of the N-body simulations, the 1-D radiative transfer code used to produce the catalogue of ionization profiles, the algorithm employed to embed the sources and finally an illustrative example of the procedure to correct for the overlap of ionized bubbles. In §3 the fully 3-D cosmological radiative transfer code CRASH is summarized and the results of its qualitative and statistical comparison with BEARS are discussed. §4 describes the method of generating the cube with maps of the brightness temperature ( $\delta T_b$ ) at all the frequencies that will be observed by an EoR

<sup>1</sup> [www.lofar.org](http://www.lofar.org)

<sup>2</sup> <http://www.haystack.mit.edu/ast/arrays/mwa/>



**Figure 1.** The big picture: This simple flow diagram encapsulates the essence of the “LOFAR EoR simulation pipeline”. Starting from the generation of the cosmological EoR signal, the pipeline includes the addition of foreground contaminants like Galactic synchrotron and free-free radiation and other point sources, and the LOFAR antenna response. This “mock” data set is then used to extract the signal using various inversion algorithms and the result is then compared to the original “uncorrupted” signal in order to study the accuracy and stability of the inversion schemes employed.

experiment. In §5 we use the simulation of the cube, with maps of the sky at different frequencies, to study the difference between two popular sources of reionization, i.e., stars and quasars. These maps in the cube are then filtered through the LOFAR antenna response to output the final data cube in §6. Finally in §7 we summarize our results and outline further improvements that need to be made in our approach in order to start exploring the large parameter space involved in reionization studies.

## 2 SIMULATIONS: THE BEARS ALGORITHM

In this section the various components of the simulation that lead towards 21cm brightness temperature ( $\delta T_b$ ) maps are explained. The very first step of the entire process consists of generating a catalogue of 1-D ionization profiles for different masses/luminosities of the source, their spectra and the density profiles that surround them at different redshifts. Although we assume the density around each source to be constant, we do vary its value as detailed below. Given the locations of the centres of mass of haloes, the photon rate emanating from that region is calculated based on a semi-analytical description (discussed in section 5). Given the spectrum, luminosity and the overdensity around the source, a spherical bubble is embedded around that pixel whose radial profile is selected from the table. The justification for this simple-minded approach is that the Universe is relatively homogeneous in density at these high redshifts on the scales probed by upcoming EoR experiments. Therefore, we can assume spherical symmetry in our construction of the ionized regions.

In the following subsections we summarize the N-body simulations employed and the 1-D radiative transfer code that was used to generate the catalogue, and we describe in detail the algorithm used to embed the spherical bubbles and the method used to conserve photons in case of overlap.

### 2.1 N-body/SPH simulations

We used a modified version of the N-body/TreePM/SPH code GADGET-2 (Springel 2005) to perform a dark matter (DM) cosmological simulation containing  $512^3$  particles in a box of size  $100 h^{-1}$  comoving Mpc and a DM+SPH cosmological simulation containing  $256^3$  DM and  $256^3$  gas particles in a box of size  $12.5 h^{-1}$  comoving Mpc. The DM particle masses were  $4.9 \times 10^8 h^{-1} M_\odot$  and  $6.3 \times 10^6 h^{-1} M_\odot$ , respectively.

Initial particle positions and velocities were obtained from glass-like initial conditions using CMBFAST (version 4.1; Seljak & Zaldarriaga 1996) and employing the Zeldovich approximation to linearly evolve the particles down to redshift  $z = 127$ . We assumed a flat  $\Lambda$ CDM universe and employed the set of cosmological parameters  $\Omega_m = 0.238$ ,  $\Omega_b = 0.0418$ ,  $\Omega_\Lambda = 0.762$ ,  $\sigma_8 = 0.74$ ,  $n_s = 0.951$  and  $h = 0.73$ , in agreement with the WMAP 3-year observations (Spergel et al. 2007). Data was generated at 50 equally spaced redshifts between  $z = 20$  and  $z = 6$ . Halos were identified using the Friends-of-Friends algorithm (Davis et al. 1985), with linking length  $b = 0.2$ .

The gas in the DM+SPH simulation is of primordial composition, with a hydrogen mass fraction  $X = 0.752$  and a helium mass fraction  $Y = 1 - X$ . Radiative cooling and heating are included assuming ionisation equilibrium, using tables<sup>3</sup> generated with the publicly available package CLOUDY (version 05.07 of the code last described by Ferland et al. 1998). The gas is allowed to cool by collisional ionisation and excitation, emission of free-free and recombination radiation and Compton cooling off the cosmic microwave background. Molecular cooling (by hydrogen and deuterium) is prevented by the inclusion of a soft (i.e. cut off at the Lyman-limit) UV background. We employed the star formation recipe of Schaye & Dalla Vecchia (2008), using a Chabrier (2003) initial mass function (IMF) with mass range  $[0.1, 100] M_\odot$ .

For further analysis, SPH particle masses were assigned to uniform meshes of size  $64^3$ ,  $128^3$  and  $256^3$  cells using TSC (Hockney & Eastwood 1988) and the gas densities were calculated. The density field was smoothed on the mesh with a Gaussian kernel with standard deviation  $\sigma_G = 12.5/512$  comoving Mpc/h. Each cell was further assigned a hydrogen-ionizing luminosity according to the stellar mass it contained. Star particles were treated as simple stellar populations and their luminosity was calculated with the population synthesis code of Bruzual & Charlot (2003). We used stellar masses and ages as determined by the simulation, a Chabrier IMF consistent with the star formation recipe and assumed a fiducial metal mass fraction  $Z = 0.0004$ .

### 2.2 1-D radiative transfer (RT) code.

The catalogue of ionization profiles for different redshifts (which also translates to different densities at a given redshift), spectral energy distributions (SED), times of evolution and

<sup>3</sup> For a detailed description of the implementation of radiative cooling see Wiersma, Schaye & Smith (2008).

masses/luminosities, was created using the 1-D radiative transfer code developed by Thomas & Zaroubi (2008).

Following Fukugita & Kawasaki (1994), a set of rate equations are solved at every cell as a function of time. The equations follow the time-evolution of  $H_I$ ,  $H_{II}$ ,  $He_I$ ,  $He_{II}$ ,  $He_{III}$  and temperature at every grid cell. The ionization rates are integrals over the spectrum and the cross sections of the various species. These were pre-computed and stored in a table to facilitate faster execution. Case-B recombination coefficients are used to calculate the rate at which hydrogen recombines.

The 1-D radiative transfer code starts the simulation at  $R_{start}$ , typically 0.1 physical kpc from the location of the source. All hydrogen and helium is assumed to be completely ionized inside this radius,  $R_{start}$ . Each cell is then updated for time  $\Delta t$ . This  $\Delta t$  is not the intrinsic time-step used to solve the differential equation itself because that is adaptive in nature and varies according to the tolerance limit set in the ordinary differential equation (ODE) solver. On the other hand, the  $\Delta t$  here decides for how long a particular cell should evolve before moving on to the next. The code is causal in the sense that cell  $i+1$  is updated after cell  $i$ . The light travel time is not taken into consideration explicitly since the ionization front (I-front) is typically very subluminal. Hence, all cells are updated to time  $n\Delta t$  at the  $n^{th}$  time-step.

After all cells except the last cell  $i_{Rmax}$  have been updated to time  $\Delta t$ , the resulting values are stored and then passed on as initial conditions for the evolution of the cell in the next interval of time. The update of all  $n_{cell}$  cells is repeated  $n$  times such that  $n\Delta t = t_{source}$ , where  $t_{source}$  is the life time of the radiating source. The various quantities of interest can be stored in a file at intervals of choice.

A radial coverage of  $R_{max}$  is chosen *a priori* which, depending on the problem, can be set to any value. Typically we do not need to solve the radiative transfer beyond ten comoving megaparsecs. We use an equally spaced grid in radius with a resolution of  $\Delta r$  which, like the time resolution, is decreased to half its value until it meets a given convergence criterion, which here is that the final position of the I-front converges to within 0.5%.

The implementation of the code is modular. Hence it is straightforward to include different spectra corresponding to different ionizing sources. Our 1-D code can handle X-ray photons and the secondary ionization and heating it causes and therefore performs well for both high (quasars) and low energy (stars) photons. Further details of the code can be found in Thomas & Zaroubi (2008).

### 2.3 Embedding the 1-D radiative code into the simulation box

In the following section we discuss the algorithm employed to expand reionization bubbles around the locations of radiative sources. The numerical simulation provides us with the density field at every grid point, the centres of mass of the haloes identified by the FoF algorithm, the velocities of these particles and, if the simulation also contains gas, the ionizing luminosity associated with the halo.

Equipped with this information about the simulation box at a given redshift, we follow the steps enumerated below to embed the ionized bubbles around the source locations:

(i) Given the redshift, ionizing luminosity and the time for which the ionization front should evolve (this depends on the type

of source), select a corresponding file from the catalogue of ionization profiles generated earlier.

(ii) The sources are usually in an overdense region and the density around the source follows a profile. Since the profiles vary from source to source we use the following approximation: we calculate the overdensity around the source for a radius  $R_{od}$  (where the subscript “od” stands for overdensity). We then assume that the source is embedded in a uniform density whose value is the average overdensity within the radius  $R_{od}$ . This naturally translates in selecting the same ionization profile but now from the table at a higher redshift. This radius is estimated as described in §2.3.1.

(iii) At lower redshifts there is considerable overlap between bubbles. Thus, in order to conserve the number of photons, we need to redistribute the photons that ionize the overlapped regions to other regions which are still neutral. The details of this correction process are given below (see §2.3.2).

(iv) When computing the reionization history, ionized regions are mapped one-to-one from the current simulation snapshot onto the next. Note that ionization due to recombination radiation has not been included.

#### 2.3.1 Estimating the averaging radius

The radius  $R_{od}$  is calculated as follows:

- For any given source (we choose the largest) in the box we perform the radiative transfer and compute the ionization profile using the (exact) spherically averaged radial density profile of the surrounding gas;

- The density within a radius  $R_{od}$ , which we initially choose to be very small, is spherically averaged around the source and the ionization profile corresponding to this mean density is selected from the catalogue. This step is repeated for increasing values of  $R_{od}$  until the extent of the ionization profile matches that of the “exact” radiative transfer calculation done in the previous step. We will refer to the resulting radius as the calibrated  $R_{od}(cal)$ ;

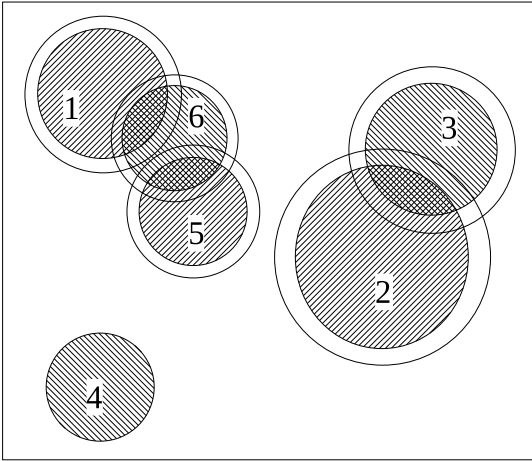
- $R_{od}$  for all the other sources are calculated by scaling them with the luminosity of the source according to  $R_{od} = R_{od}(cal) \left( \frac{L_{source}}{L_{cal}} \right)^{1/3}$ , where  $L_{source}$  and  $L_{cal}$  are the luminosities of the source under consideration and the calibration source respectively.

A comment to be made here is that because the dynamic range in the halo masses derived from the simulation is not very high the value of  $R_{od}$  does not vary considerably between sources.

#### 2.3.2 Correction for overlap

At lower redshifts the sources become more massive and more numerous. This causes considerable overlap between spheres of close-by sources. The regions of overlap correspond to some number of unused photons (depending on the density). The relative simplicity of the implementation of the algorithm arises due to the fact that the ionization fronts created by most sources are “sharp”, at least for the resolutions we are able to simulate. If the ionization front is extended, we can modify the procedure below to accommodate it. The procedure for correction is illustrated with the help of a simple example shown in Fig. 2:

- Create an analogue to an incidence/admittance matrix  $\mathbf{A}$  (ref equation 1 for the connection between ionized regions of sources): The matrix  $\mathbf{A}$  is a square matrix of size  $N_{source} \times N_{source}$ , whose



**Figure 2.** A cartoon depicting the distribution and overlap of bubbles in the simulation. The number within each circle is just an associated identity of the circle. In the above figure circles (1:6:5), (2:3) and (4) form three different “connected” regions. Each circle of the region is expanded just enough that the size of the region expanded corresponds to the area of overlap. In this manner we hard-wire the conservation of photons into the algorithm.

elements are set to 1 if two sources overlap and 0 otherwise. Here  $N_{\text{source}}$  is the total number of sources in the box.

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 \end{pmatrix} \quad (1)$$

- Segment the simulation box into regions that are connected. This is done by identifying rows that are identical in the matrix  $\mathbf{A}$ . Thus, for the example shown in Fig. 2 there are three different “connected regions”, Reg1:(1,6,5), Reg2:(2,3) and Reg3:(4).

- Calculate the total volume of the overlap zones in each of the connected regions. For example for Reg1, we have  $\text{Overlap}(1,6) + \text{Overlap}(5,6)$ .

- The sizes of all the bubbles in a particular connected region is increased so as to entail a volume that corresponds to the average overlapped region, i.e., total overlapped region divided by the number of bubbles in that connected region.

- The sizes of the bubbles are iteratively increased until the volume of the regions that are “newly ionized”, i.e., excluding the regions ionized by the sources before the correction, equals the total overlapped volume. This ensures a homogeneous redistribution of unused photons all around the region. The unshaded bubbles in Reg1:(1,6,5) and Reg2:(2,3) in Fig. 2 depict the expansion of the bubbles.

### 3 COMPARISON WITH A FULL 3-D RADIATIVE TRANSFER CODE.

The BEARS algorithm is used to generate a series of cubes of ionized fractions at different redshifts and resolutions for the case in which the radiative sources are stars. In this section these cubes are

compared with those obtained from the full 3-D radiative transfer code CRASH using the same source list i.e., source locations, luminosities and spectra. In all comparisons made below we make use of ionizing luminosities derived from the N-Body/SPH simulation (refer §2.1). We have assumed the spectra to be monochromatic at 13.6 eV. We first summarize the essentials of the 3-D radiative transfer code CRASH and then discuss a set of visual and statistical comparisons between the results generated using these two approaches.

All comparisons except for the case of  $12.5 h^{-1}$  comoving Mpc,  $128^3$  box, in this section is done on boxes where we have not included the reionization history. One of the major reasons for this is that a full 3-D radiative transfer code like CRASH would require enormous computational resources to achieve this task. And on the other hand, it is easier to judge the performance of BEARS when there a large number of sources overlapping at lower redshifts, whereas if the reionization history is included, the lower redshifts would be completely ionized and most of the interesting characteristics of the comparison would be wiped out.

#### 3.1 CRASH: An overview

CRASH is a 3-D ray-tracing radiative transfer code based on Monte Carlo (MC) techniques that are used to sample the probability distribution functions (PDFs) of several quantities involved in the calculation, e.g. spectrum of the sources, emission direction and optical depth. The MC approach and the code architecture enables applicability over a wide range of astrophysical problems and allows for additional physics to be incorporated with minimum effort. The propagation of the ionizing radiation can be followed through any given H/He static density field sampled on a uniform mesh. At every grid point and time step the algorithm computes the variations in temperature and ionization state of the gas. The code allows for the possibility of the addition of multiple point sources at any specified point in the box, and also diffuse radiation (e.g. the ultraviolet background or the radiation produced by H/He recombinations) can be self-consistently incorporated.

The energy emitted by point sources in ionizing radiation is discretized into photon packets, beams of ionizing photons, emitted at regularly spaced time intervals. More specifically, the total energy radiated by a single source of luminosity  $L_s$ , during the total simulation time,  $t_{\text{sim}}$ , is  $E_s = \int_0^{t_{\text{sim}}} L_s(t_s) dt_s$ . For each source,  $E_s$  is distributed in  $N_p$  photon packets, emitted at the source location at regularly spaced time intervals,  $dt = t_{\text{sim}}/N_p$ . The time resolution of a given run is thus fixed by  $N_p$  and the time evolution is marked by the packets’ emission: the  $j$ -th packet is emitted at time  $t_{\text{em},c}^j = j \times dt$ , with  $j = 0, \dots, (N_p - 1)$ . Thus, the total number of emissions of continuum photon packets is  $N_{\text{em},c} = N_p$ . The emission direction of each photon packet is assigned by MC sampling the angular PDF characteristic of the source. The propagation of the packet through the given density field is then followed and the impact of radiation-matter interaction on the gas properties is computed on the fly. Each time the packet pierces a cell  $i$ , the cell optical depth for ionizing continuum radiation,  $\tau_c^i$ , is estimated summing up the contribution of the different absorbers (H I, He I, He II). The probability for a single photon to be absorbed in the  $i$ th cell is:

$$P(\tau_c^i) = 1 - e^{-\tau_c^i}. \quad (2)$$

The trajectory of the packet is followed until its photon content is extinguished or, if open boundary conditions are assumed, until it

exits the simulation volume. The time evolution of the gas physical properties (ionization fractions and temperature) is computed solving in each cell the appropriate discretized differential equations each time the cell is crossed by a packet. The reader is referred to Maselli, Ferrara, & Ciardi (2003); Ciardi et al. (2001) for details of the code.

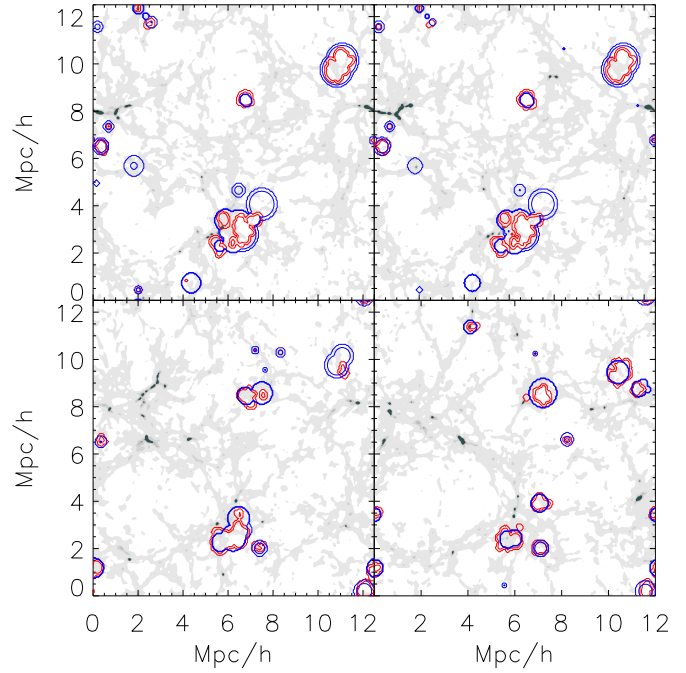
### 3.2 “Visual” comparison

Figure 3 shows a 3-D view of the ionized fraction of hydrogen calculated using CRASH (left panel) and BEARS (right panel), with isosurfaces shaded dark. The box shown here is a  $256^3$ -simulation at a redshift of six for a box with a comoving length of  $12.5 h^{-1}$  comoving Mpc on each side. Globally the two boxes do look very similar. Statistics on these cases and others are presented later. Also bear in mind that this case, i.e., redshift six, is the one for which we should expect maximum discrepancy between the two methods. Reasons being: one, the universe is much less homogeneous at redshift six than at higher redshifts which is contrary to the basic assumption in BEARS that the IGM is predominantly uniform, two, the bubbles from these ionizing sources become larger (because the sources grow more massive and because the gas density decreases) and they invariably overlap with several others which in our case is dealt with in an approximate manner as explained before.

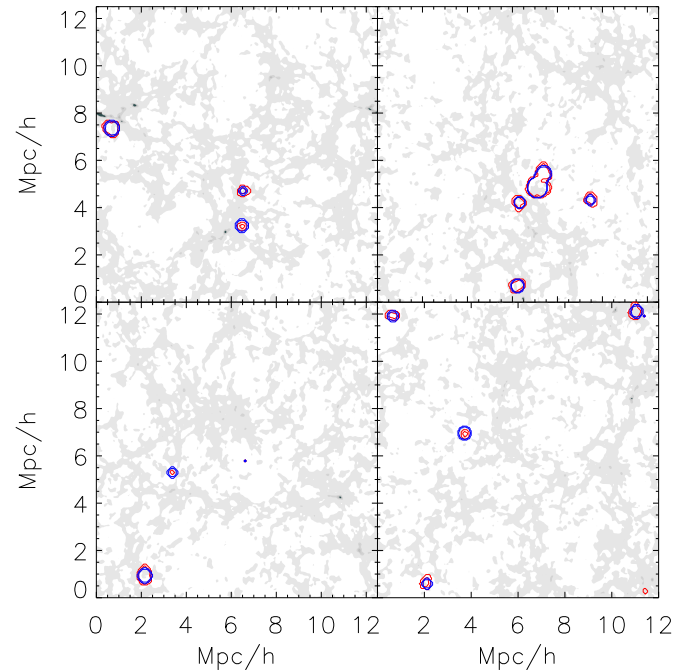
In Figs. 4 & 5 we compare the ionization isocontours from BEARS (blue contours) and CRASH (red contours) for redshifts 6 and 9, respectively. The images refer to the simulations in a  $256^3$  box with side of length  $12.5 h^{-1}$  comoving Mpc. As expected, redshift 6 is structurally the most complex with many more sources and multiple overlaps. In all these images we see a distinct feature of the BEARS algorithm, i.e., that the ionized regions are perfectly spherical when there is no overlap. Also, in case of overlap, the shapes of ionized regions are much more regular than those of CRASH. The reason for this discrepancy is the local inhomogeneity of the underlying density field. As explained in §2.3, the BEARS algorithm averages over a radius of  $R_{od}$  and uses the same density in all directions, whereas CRASH follows the local density separately in each direction. With higher resolution the agreement between the two simulations is expected to decrease because the density field is not as isotropic, and in situations like this the 3-D codes are better at following the non-spherical nature of the ionizing front.

In Figs. 6 and 7, we compare BEARS and CRASH for a lower resolution simulation, i.e.,  $64^3$  in a  $12.5 h^{-1}$  comoving Mpc box for redshifts 6 to 9. These figures indeed show a much better agreement because the detailed structure of the ionization front traced by CRASH at a higher resolution has been smoothed out.

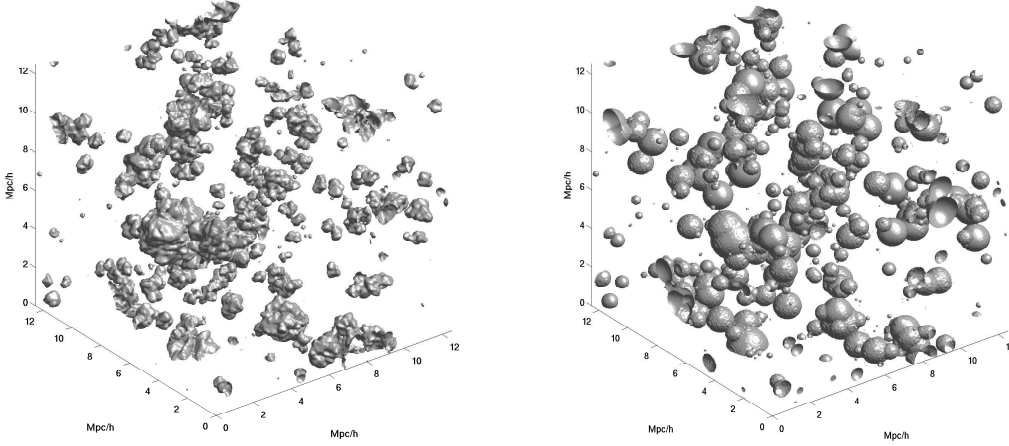
All the previous figures of comparison of CRASH and BEARS were performed without taking into account the history of reionization, i.e., radiative transfer was performed on each snapshot assuming that it had not been previously ionized. In Figure 8 and the top panel of Figure 9 we plot four slices of the  $12.5 h^{-1}$  comoving Mpc,  $128^3$  box at redshifts of 6.2 and 9 respectively, which do include the memory of ionization from previous redshifts. We observe that the agreement in this case is not as good as in the case without the history of reionization, but given that this comparison is made at the lowest redshift of interest and for a high resolution ( $12.5 h^{-1}$  comoving Mpc) simulation, the results are acceptable. The bottom panel of Figure 8 shows the mean (solid line) and variance (dashed line) of the mass-weighted ionized fraction as a function of redshift for a  $12.5 h^{-1}$  comoving Mpc,  $128^3$  box. The



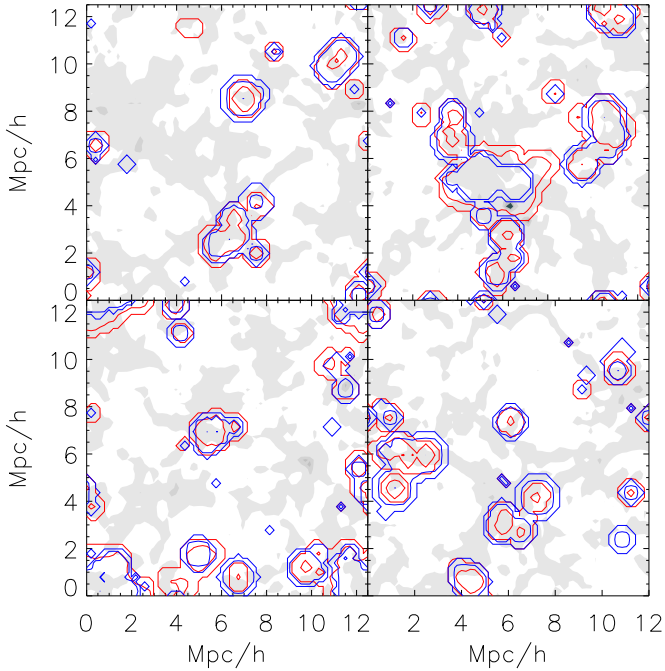
**Figure 4.** Four slices (thickness  $\approx 0.05 h^{-1}$  comoving Mpc), randomly selected along a direction in the  $12.5 h^{-1}$  comoving Mpc,  $256^3$  box, are plotted that displays the contours (three levels [0, 0.5, 1]) of the neutral fraction of CRASH (red) and BEARS (cyan) at  $z \approx 6$ . The underlying “light gray” contours represent the dark matter overdensities.



**Figure 5.** Same as Fig. 4 but for redshift  $z \approx 9$ .



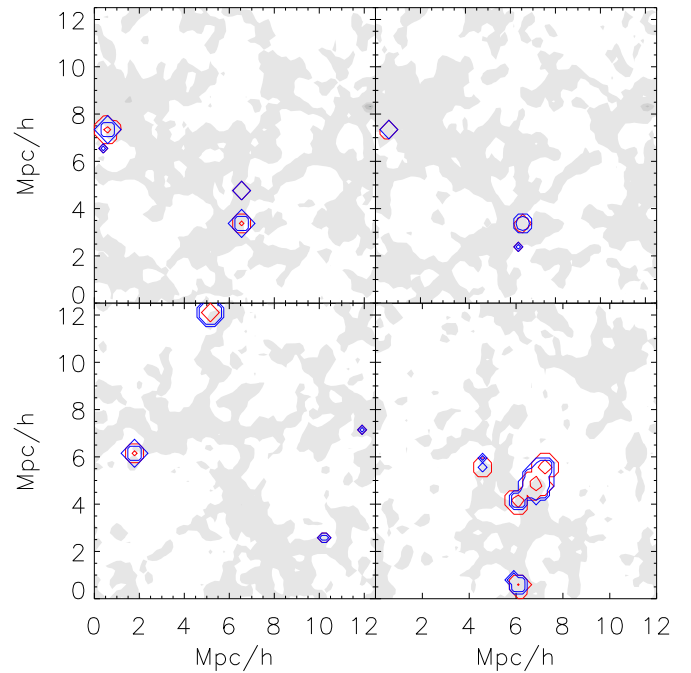
**Figure 3.** A 3-D visualization of the ionized box from CRASH (left) and BEARS (right) at redshift  $z \approx 6$  for a boxsize of  $12.5 h^{-1}$  comoving Mpc at a resolution of  $256^3$ . As we see, although this is the redshift for which we expect a large discrepancy, the figures seem to be morphologically comparable.



**Figure 6.** Four slices (thickness  $\approx 0.2 h^{-1}$  comoving Mpc), randomly selected along a direction in the  $12.5 h^{-1}$  comoving Mpc,  $64^3$  box, are plotted that displays the contours (three levels [0, 0.5, 1]) of the neutral fraction of CRASH (red) and BEARS (cyan) at  $z \approx 6$ . The underlying “light gray” contours represent the dark matter overdensities.

reason why the statistics of mass-weighted ionized fraction agree so well whereas the contour plots have some discrepancy is that when the underlying density is high, BEARS estimates the extent of the ionization correctly, whereas in case of under-dense regions, BEARS overestimates the size of the bubble.

Although there are still differences in the images at lower redshifts due to the overlap, we expect that convolving the image with

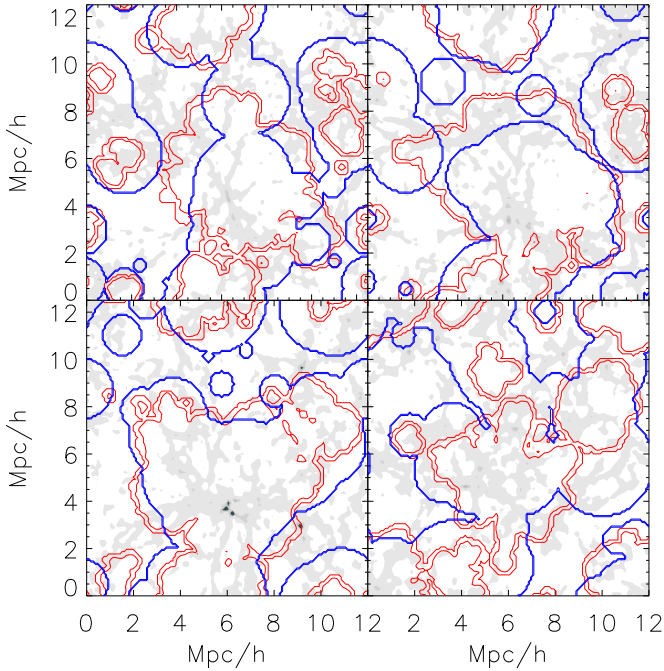


**Figure 7.** Same as Fig. 6 but for redshift  $z \approx 9$ .

the beam response of the antenna will result in very similar images. This is indeed what we see in Fig. 10. The slice used in the figure was obtained from a  $256^3$ -box at redshift 6. The beam response (see §6) eliminates the detailed structures of the ionizing front tracked by the 3-D radiative transfer code.

### 3.3 Statistical comparison

In this section we describe several statistical comparisons between the results obtained by CRASH and BEARS. The bottom panel of Fig. 9 shows the difference between the mass-weighted mean and



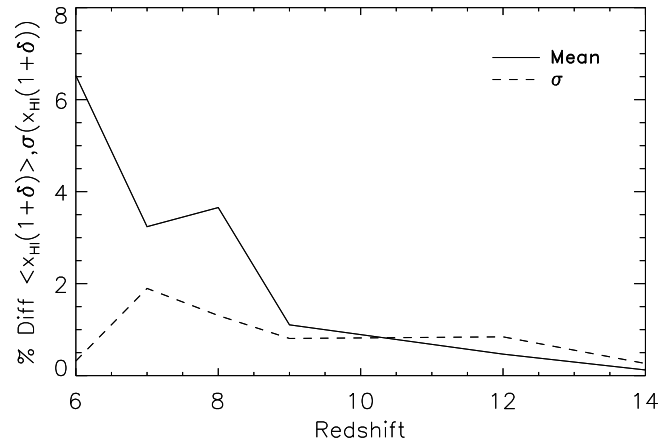
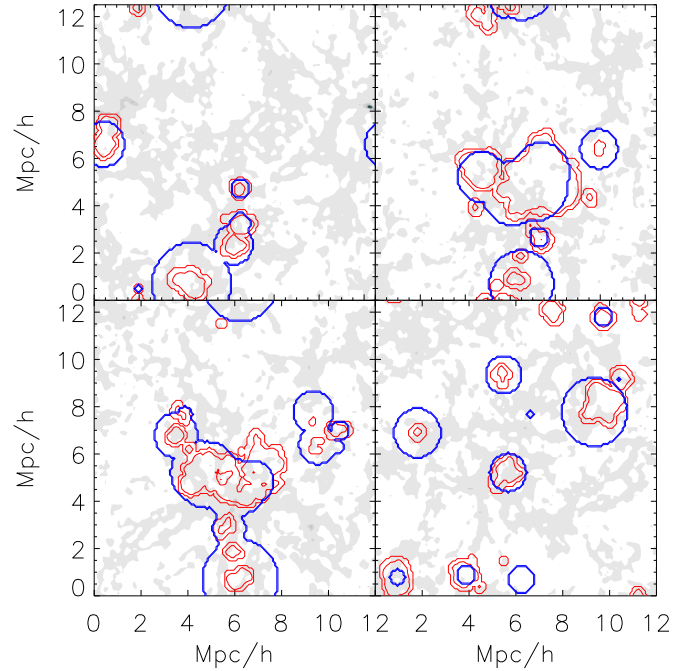
**Figure 8.** Four slices (thickness  $\approx 0.1 h^{-1}$  comoving Mpc) from a  $12.5 h^{-1}$  comoving Mpc,  $128^3$  box are randomly selected and contours (three levels [0, 0.5, 1]) of the neutral fraction of CRASH (red) and BEARS (blue) at  $z \approx 6$  are plotted. The underlying “light gray” contours represent the dark matter overdensities. In this figure we have taken into account the ionization history, i.e., the radiative transfer is performed on the box which had been partially ionized at earlier redshifts.

variance of the neutral fraction in the  $12.5 h^{-1}$  comoving Mpc,  $128^3$  box as a function of redshift including the reionization history. The difference is within 2% for high redshifts ( $z > 9$ ), and even at redshift six it is around 5%.

As a second probe, Fig. 11 shows a histogram of the fractional volume in a  $12.5 h^{-1}$  comoving Mpc,  $128^3$  box occupied by different neutral fractions. This plot reveals details of the discrepancy in the two approaches. At higher redshifts the volume is predominantly neutral, whereas at lower redshifts, as reionization proceeds, radiation (partially) ionizes parts of the volume. We see that the black solid line in the figure, which corresponds to BEARS agrees very well with the histogram of CRASH (red-dashed) at very low ( $X_{HI} < 10^{-3.5}$ ) and at very high ionization levels ( $X_{HI} \approx 1$ ), but during the intermediate ionization levels they do not compare very well. The reason for this is that the ionized bubbles in BEARS have sharp transitions from neutral to a fixed ionized fraction at the ionization front whereas in CRASH, depending on the density distribution, the ionized fraction across the ionization front falls off slowly.

A final diagnostic is presented in Fig. 12. The neutral fraction in each voxel<sup>4</sup> is plotted against the overdensity in that pixel. As in the previous diagnostic there is overlap between the two methods at high and very low neutral fractions. But we see that CRASH (red) spans the entire range of neutral fractions whereas the points corresponding to BEARS (black) are clustered. This again can be

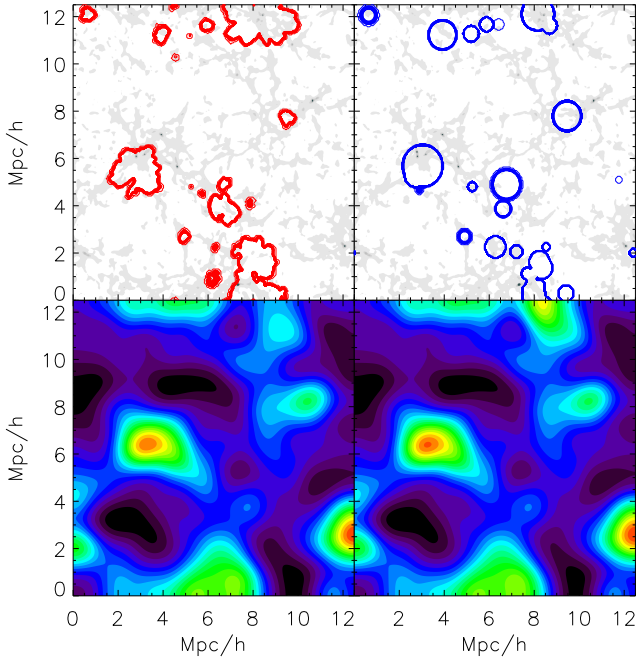
<sup>4</sup> *voxels* is a short-hand to denote a 3-dimensional pixel. It is a portmanteau of words, *volumetric* and *pixels*.



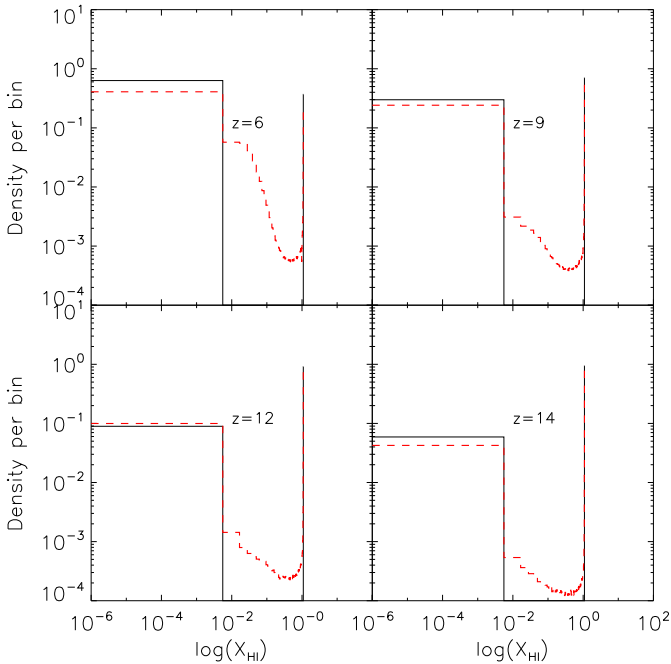
**Figure 9.** The top panel is same as Fig. 8 but for redshift  $z \approx 9$ . The bottom panel shows the percentage difference between CRASH and BEARS in the mean (solid line) and variance (dashed line) of the mass-weighted ionized fraction (ionized fraction  $> 0.95$ ) in the  $128^3$  box as a function of redshift when the history of reionization is included.

attributed to the sudden transition in the neutral fraction around radiative sources used by BEARS. Also, most higher density environments are ionized by BEARS because in most cases a source is centred on the high density pixels of the box. Another aspect of the implementation of the BEARS scheme is apparent in this plot, i.e., at higher densities ( $\frac{\rho}{\langle \rho \rangle} > 2.0$ ) the agreement between CRASH and BEARS is extremely good. This is because sources are usually located at overdense location and BEARS uses the density around the source location to estimate the radius of ionized sphere. Thus, around the source and consequently in high dense regions, BEARS correctly estimates the radius of the ionized spheres but fails to do so in the low density environment.

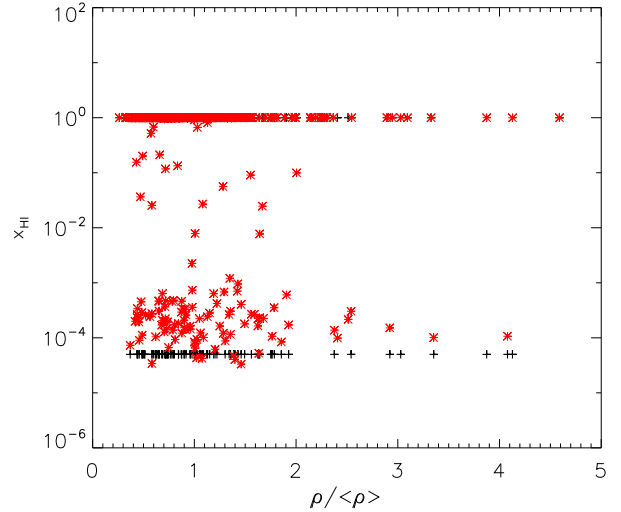




**Figure 10.** *The effect of convolution:* The ionization fronts of CRASH (red contours, top left) and BEARS (blue contours, top right) are overlotted on the underlying density field shown in light grey. This slice is extracted from a  $256^3$  box at redshift six. The corresponding figures below show the images after being smoothed by the beam response of the antenna. Details of the instrument are given in §6. As expected, the images look almost identical after the convolution operation.



**Figure 11.** Histogram of the fractional volume at various average neutral fractions of hydrogen in a  $12.5 h^{-1}$  comoving Mpc,  $128^3$  box at four different redshifts as indicated. The black solid line corresponds to BEARS and the dashed red line to CRASH.



**Figure 12.** The above diagram depicts the neutral fraction at a given voxel in the simulation box as a function of the overdensity at that pixel (only a randomly chosen subsample of all the voxels are shown). In the above figure points corresponding to CRASH (red) span a larger range of ionizations compared to BEARS (black) which are more clustered. Results plotted are for a  $12.5 h^{-1}$  comoving Mpc,  $128^3$  box at redshift 6, including the entire reionization history.

#### 4 CREATING THE “FREQUENCY CUBE”

Outputs from different frequency channels of an interferometer/LOFAR measure the radiation (in our case the 21cm emission) from varying redshifts. Thus, the spectral resolution of the telescope dictates the scales over which structures in the Universe are smoothed or averaged along the redshift direction. The shape of the power spectrum and the characteristics of the line of sight signal are influenced by this operation. In order to study its effect on the “true” underlying signal it is therefore imperative to create, from outputs of different individual redshifts, a contiguous data set of maps on the sky at different frequencies. This section explains how we create just such a frequency cube (FC). For the purpose of the LOFAR-EoR experiment we create a cube spanning the observing window of the experiment, i.e., from redshift 6 ( $\approx 200$  MHz) to 11.5 ( $\approx 115$  MHz).

The following steps were employed to obtain maps of the 21cm EoR signal at different redshifts, given a number of snapshots from a cosmological simulation between the redshifts of interest:

- Inputs: Start and End frequencies,  $\nu_{\text{start}}$  &  $\nu_{\text{end}}$  (corresponding to redshifts bounded by 6 & 12); the resolution in frequency  $\delta\nu$ , at which the maps are created. We typically choose a value  $\delta\nu$  smaller than the bandwidth of the experiment, because once this data set has been created, we can always smooth along frequency to any desired bandwidth.
- Create an array of frequencies and redshifts at which the maps are to be created,

$$\nu_i = \nu_{\text{start}} + i\delta\nu, \quad (3)$$

where  $i = 0, 1, \dots, (\nu_{\text{end}} - \nu_{\text{start}})/\delta\nu$ , and convert each of these frequencies into a redshift array,

$$z_i = \frac{\nu_{21}}{\nu_i} - 1, \quad (4)$$

where  $\nu_{21} = 1420$  [MHz], the rest frequency of the 21cm hyperfine hydrogen line.

- Now, for each of these redshifts  $z_i$ , we identify a pair of simulation snapshots whose redshifts bracket  $z_i$ . Let us call these snapshots  $z_L$  and  $z_H$ , such that  $z_L < z_i < z_H$ .

- Although all voxels in the output of a simulation are at the same redshift ( $z_L$  in this case), we assume that the voxels of the central slice (along the redshift or frequency direction) correspond to the redshift of the simulation box. We then move to a slice,  $S_L$  (we wrap around the box if necessary, since the simulations are performed with periodic boundary conditions) at a distance corresponding to the radial comoving distance between  $z_L$  and  $z_i$  given by;

$$D_{z_L \rightarrow z_i} = \frac{c}{H_0} \int_{z_L}^{z_i} \frac{dz}{(1+z)\sqrt{X(z)}}, \quad (5)$$

with  $X$  defined as;

$$X(z) = \Omega_m(1+z) + \Omega_r(1+z)^2 + \Omega_l/(1+z)^2 + (1 - \Omega_{tot}). \quad (6)$$

We use parameters obtained from *WMAP3* (Spergel et al. 2007).

- With slice  $S_L$  as the centre, we average all the slices within  $\pm \Delta z/2$ , where  $\Delta z$  is the redshift interval corresponding to a frequency width of  $\Delta \nu$  at redshift  $z_L$ . Lets call this average  $SL_{avg}$ .

- All the steps performed above do not account for the time-evolution of the slice between the two outputs and thus it is important to interpolate between two corresponding slices (to preserve the phase information of the underlying density field). Therefore, we identify the corresponding slice,  $S_H$  (in position w.r.t the central slice) in the snapshot  $z_H$ . Again, we average slices within  $\pm \Delta z/2$  with slice  $S_H$  as the centre and call it  $SH_{avg}$ . Note, however, that the number of slices in the previous step need not be the same as in this step, owing to the fact that the  $\Delta z$  corresponding to  $\Delta \nu$  is a function of  $z$ .

- The final step in the generation of the slice  $S_{z_i}$ , at  $z_i$ , involves the interpolation of  $SL_{avg}$  and  $SH_{avg}$ :

$$S(z_i) = \frac{(z_i - z_L)SH_{avg} + (z_H - z_i)SL_{avg}}{z_H - z_L}. \quad (7)$$

Fig. 13 shows an example of a slice through the box for the the ionization history due to stars constructed using the algorithm above. Because the size of the box used is  $100 h^{-1}$  Mpc in comoving coordinates and the comoving radial distance between redshifts of 6 and 12 is  $\approx 1600 h^{-1}$  Mpc, we would expect there to be repetition of structures along the frequency/redshift direction. In plotting the above figure this has been reduced by a factor  $\sqrt{3}$  since the slice has been extracted along the diagonal of the FC. In the following sections we will do all our analysis and comparisons on the box generated in the above manner.

Although the radiative transfer is performed on each box with the underlying density in real space, we produce the FC for the brightness temperature with densities estimated in redshift space to account for the redshift distortions introduced by the peculiar velocities.

## 5 STARS VERSUS QUASARS: EXPLORING DIFFERENT SOURCE-SCENARIOS

Although the general consensus is that the dominant sources of reionization are stellar in nature, there is also evidence to support quasars as additional sources of reionization (Kuhlen & Madau 2005; Thomas & Zaroubi 2008; Zaroubi et al. 2007). One of the

main differences between stars and quasars, apart from the extent of reionization caused by individual sources, is the heating due to quasars. We simulate only the reionization history for the cases involving either stars or quasars and leave simulating the effect of heating for future work. We use a  $512^3$  particle,  $100 h^{-1}$  Mpc ( $L_{box}$ ) dark-matter-only simulation for this purpose. For details on the N-body simulation see Section 2.1. About 75 simulation snapshots between redshifts 12 and 6 were used to create the FC. The entire operation of doing the radiative transfer on each of these snapshots and converting them into the FC takes approximately 12 hours on an 8-dual-core AMD processor machine with 32GB of memory.

In the sections below we describe the prescriptions used to embed the dark matter haloes with quasars and stars. Following that we discuss some of the statistical differences in the ionization fractions and contrast the statistical nature of the  $\delta T_b$  for these different scenarios, as a function of frequency. We caution that the scenarios described here are mostly meant to illustrate the potential of the techniques being developed here. For example, although the quasar model described below seems to ionize the Universe effectively, care has not been taken to constrain the quasar population based on the soft X-ray background excess between 0.5 and 2 KeV (Dijkstra, Haiman, & Loeb 2004).

### 5.1 Prescription for quasar type sources

From the output of the N-body simulation, dark-matter haloes were identified using the friends-of-friends algorithm and a linking length  $b = 0.2$ . Black holes embedded in them were assigned a mass according to Zaroubi et al. (2007),

$$M_{BH} = 10^{-4} \times \frac{\Omega_b}{\Omega_m} M_{halo}, \quad (8)$$

where the factor  $10^{-4}$  reflects the Magorrian relation between the halo mass ( $M_{halo}$ ) and black hole mass ( $M_{BH}$ ), and  $\frac{\Omega_b}{\Omega_m}$  gives the baryon ratio (Ferrarese 2002).

The template spectrum we assumed for the quasars is a power law of the form,

$$F(E) = \mathcal{A} E^{-\alpha} \quad 10.4\text{eV} < E < 10 \text{ keV}, \quad (9)$$

where  $\alpha$  is the power-law index which is set to unity. A quasar of mass  $M$  shines at  $\epsilon_{rad}$  times the Eddington luminosity,

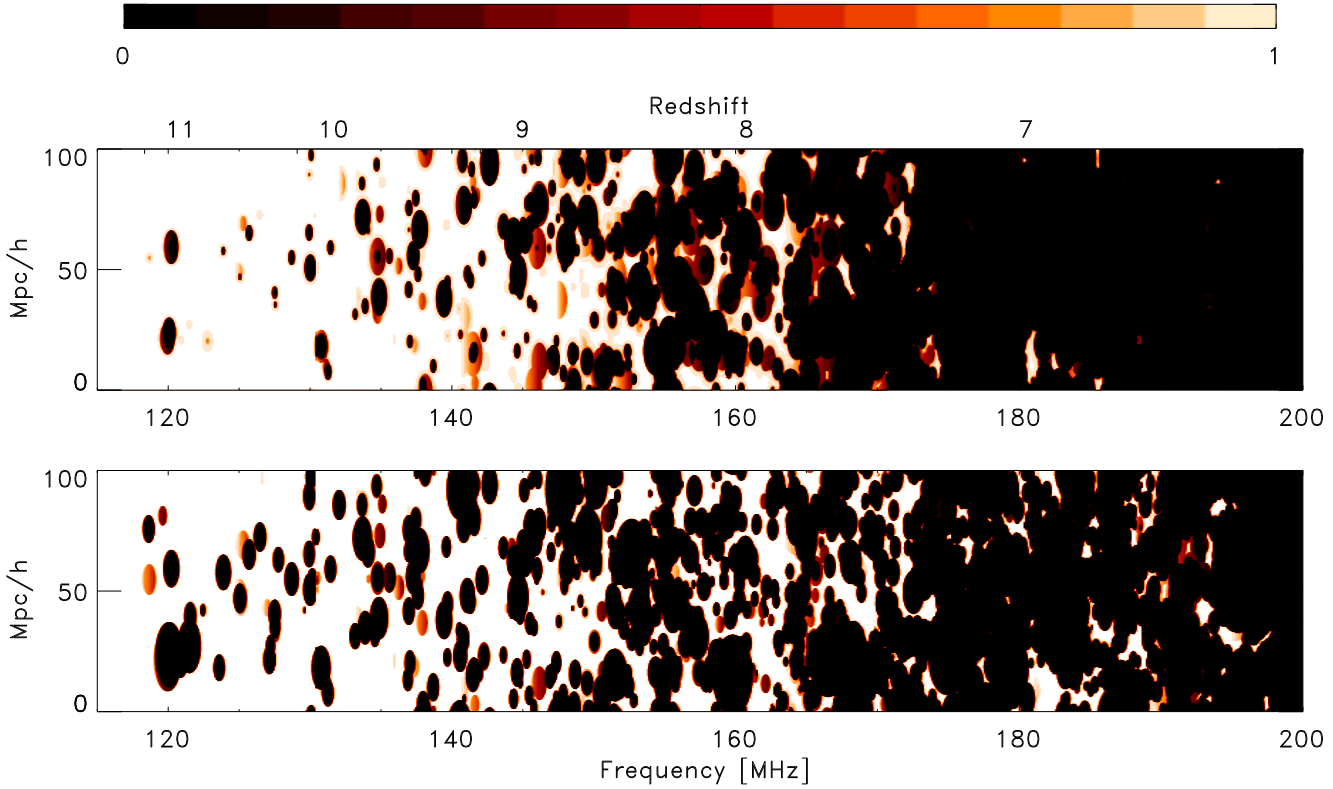
$$L_{Edd}(M_{BH}) = 1.38 \times 10^{38} \left( \frac{M_{BH}}{M_{\odot}} \right) [\text{erg s}^{-1}]. \quad (10)$$

Therefore  $\mathcal{A}$  is given by:

$$\mathcal{A}(M_{BH}) = \frac{\epsilon_{rad} L_{Edd}(M_{BH})}{\int_{E_{range}} E^{-\alpha} dE \times 4\pi r^2} [\text{ergs}^{-1} \text{cm}^{-2}], \quad (11)$$

where  $E_{range} = 10.4\text{eV} - 10 \text{ keV}$ .

In the above model, we have assumed that the spectral energy distribution (SED) of the quasar extends well above the ionization energy of hydrogen. This ensures that copious amounts of photons are available to ionize the hydrogen in the IGM while at the same time reducing the number of hard X-ray photons that could potentially heat the IGM. Because we concentrate on the ionization history in this paper, we postpone a detailed study of the effect of cutoff in the SED at the higher and lower end of the energies.



**Figure 13.** A slice along the frequency direction for the neutral fraction for two different scenarios. One with quasars (top panel) and the other with stars (bottom panel). The repetition along the frequency direction, which is expected due to the finite size of the box, is reduced by a factor  $\sqrt{3}$  because the slice is obtained diagonally across the box. We see from the figure that although the stars do start ionizing earlier, for the models we have developed (details in the text, section 5), quasars are far more efficient at ionizing the IGM.

## 5.2 Prescription for stellar sources

We associate stellar spectra with dark matter halos using the following procedure. The global star formation rate was calculated using;

$$\dot{\rho}_*(z) = \dot{\rho}_m \frac{\beta \exp[\alpha(z - z_m)]}{\beta - \alpha + \alpha \exp[\beta(z - z_m)]} [\text{M}_\odot \text{yr}^{-1} \text{Mpc}^{-3}], \quad (12)$$

where  $\alpha = 3/5$ ,  $\beta = 14/15$ ,  $z_m = 5.4$  marks a break redshift, and  $\dot{\rho}_m = 0.15 \text{M}_\odot \text{yr}^{-1} \text{Mpc}^{-3}$  fixes the overall normalisation (Springel & Hernquist 2003). Now, if  $\delta t$  is the time interval between two outputs in years, the total mass density of stars formed is

$$\rho_*(z) \approx \dot{\rho}_*(z) \delta t [\text{M}_\odot \text{Mpc}^{-3}]. \quad (13)$$

Notice that this approximation is valid only if the typical lifetime of the star is much smaller than  $\delta t$ , which is the case in our model because we assume  $100 \text{M}_\odot$  stars as the source that have a lifetime of about few Myrs (Schaerer 2002).

Therefore, the total mass in stars in the box is  $M_*(box) \approx L_{box}^3 \rho_*$  [ $\text{M}_\odot$ ]. This mass in stars is then distributed among the halos according to the mass of the halo as,

$$m_*(halo) = \frac{m_{halo}}{M_{halo}(tot)} M_*(box), \quad (14)$$

where  $m_*(halo)$  is the mass of stars in “halo”,  $m_{halo}$  the mass of the halo and  $M_{halo}(tot)$  the total mass of halos in the box.

We then assume that all of the mass in stars is distributed in stars of 100 solar masses, which implies that the number of stars in

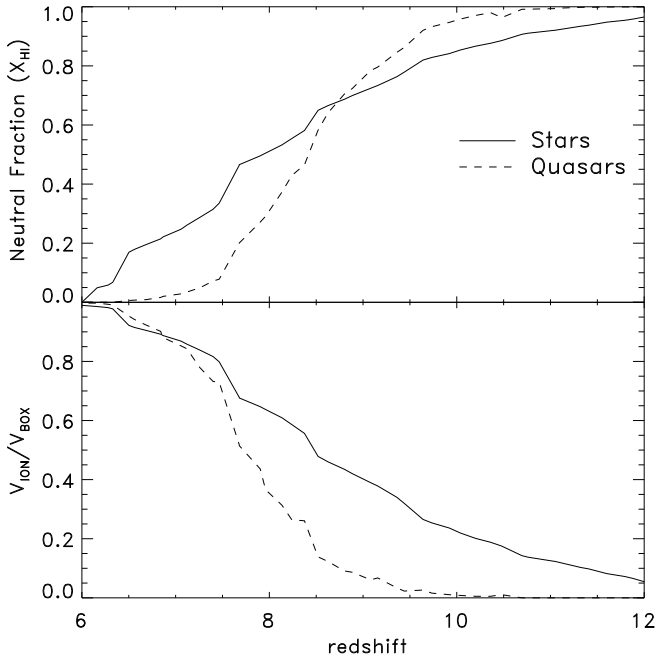
the halo is  $N_{100} = 10^{-2} \times m_*(halo)$ . The number of ionizing photons from a  $100 \text{M}_\odot$  star is taken from Table 3 of Schaerer (2002) and multiplied by  $N_{100}$  to get the total number of ionizing photons emanating from the “halo” and the radiative transfer is done assuming these photons are at  $13.6 \text{eV}$ . The escape fractions of ionizing photons from early galaxies is assumed to be 10%.

## 5.3 Statistical differences in the history of reionization

Using the models of ionizing sources and the algorithm to generate the FC described above, we plot a slice along the frequency direction of the ionization histories in Fig. 13. We see from the figure that the stars start ionizing much earlier than the quasars, but the rate at which they ionize is low. Therefore, even though the effect of quasars on the ionization is seen later, they manage to ionize the IGM earlier than stars. This is mainly due to the efficiency (per unit baryon) of the quasar to ionize the medium and to the fact that in the model we have constructed the miniqso population is not constrained based on the excess of soft X-ray background radiation and therefore the miniqso number density is higher than it would be in reality. It should be noted that if the escape fractions are allowed to change the ionization histories due to stars can be altered significantly.

This can be seen more clearly and quantitatively in Fig. 14, which shows the volume averaged mean neutral fraction as a function of redshift (top panel) and the volume fraction that is ionized ( $X_{HI} < 0.05$ ) in the box (bottom panel).

Fig. 15 shows a slice through the FC of  $\delta T_{bs}$  for the case of



**Figure 14.** The figure shows the volume averaged mean neutral fraction (top panel) in the box as a function of redshift for stars (solid) and quasar (dashed) populations. Although both the populations ionize the entire box by redshift 6, the ionization history follows very different paths. Within the models used for the simulation the quasars seem to ionize earlier than the stars. A similar diagnostic is the volume fraction of the box that is ionized as a function of redshift.

quasars (first panel from the top) and stars (second panel) which was calculated following Madau, Meiksin, & Rees (1997):

$$\delta T_b = (20 \text{ mK}) \left( \frac{X_{HI}}{h} \right) \left( 1 - \frac{T_{CMB}}{T_{spin}} \right) \times \left( \frac{\Omega_b h^2}{0.0223} \right) \left[ \left( \frac{1+z}{10} \right) \left( \frac{0.24}{\Omega_m} \right) \right]^{1/2}, \quad (15)$$

where  $h$  is the Hubble constant in units of  $100 \text{ km s}^{-1} \text{ Mpc}^{-1}$ ,  $\delta$  is the mass density contrast, and  $\Omega_m$  and  $\Omega_b$  are the mass and baryon densities in units of the critical density.  $T_{CMB}(z)$  is the temperature of the cosmic microwave background at redshift  $z$  and  $T_{spin}$  the spin temperature. In all our calculations we have assumed  $T_{spin} \gg T_{CMB}$ .

The third panel in Fig. 15 shows the variance of  $\delta T_b$  as a function of frequency for stars (red dashed line) and quasars (black solid lines). Since quasars start ionizing late and completely ionize the Universe by redshift 6, the variance stays below that for stars at the beginning and end of reionization but peaks at around 160 MHz corresponding to a redshift of 7.8. Interestingly, for stars the peak of the variance occurs around the same frequency. This is a welcome coincidence from an observation point of view. LOFAR will initially observe using instantaneous bandwidths of 32 MHz (Lamproulous et al., *in prep*). Thus, it becomes important to make an educated guess of the frequency around which the observation has to be made, to be sure that we capture reionization activity at its peak. And because the variance of these two very different scenarios peak around the same redshift, this frequency ( $\approx 160$  [MHz]) is a reasonable guess. It is worth emphasizing that these are predictions based on the simple-minded models prescribed above. Never-

theless this exercise illustrates the capability of our algorithm to implement diverse scenarios and help guide the observational strategies of LOFAR.

Finally, in the fourth panel we plot the image (slice) entropy as a function of redshift. Image entropy is a measure of randomness in the image and in our case it reflects the inhomogeneity of reionization as a function of redshift. The entropy of an image is calculated as follows: first, a histogram of the intensities in the image, which in our case correspond to  $\delta T_b$  values, is made and normalized. If there are  $N_{bins}$  bins and each bin  $i$  has a normalized value  $\rho_i$ , then the entropy is given by,

$$\text{Entropy} = \sum_{N_{bins}} \rho_i \log \rho_i. \quad (16)$$

The meaning of image entropy is illustrated with an example in section §6, aided with Fig. 21. In the context of our study the image entropy has the following meaning:

(i) *Before convolution with the LOFAR beam (ref. Fig. 15):*

At low frequencies ( $< 145$  MHz) the universe is still mostly neutral and homogeneous. Thus a histogram of  $\delta T_b$  at a given frequency less than 145 MHz would be very narrow and hence have lower entropy (ref. Eq 16). But as the sources start ionizing the IGM, it introduces fluctuations in  $\delta T_b$  and the histogram spreads out thus increasing the entropy. Similarly, at much higher frequencies ( $> 180$  MHz) the entropy drops down because the Universe is largely ionized and the histogram of  $\delta T_b$  is narrow but now centred at 0.

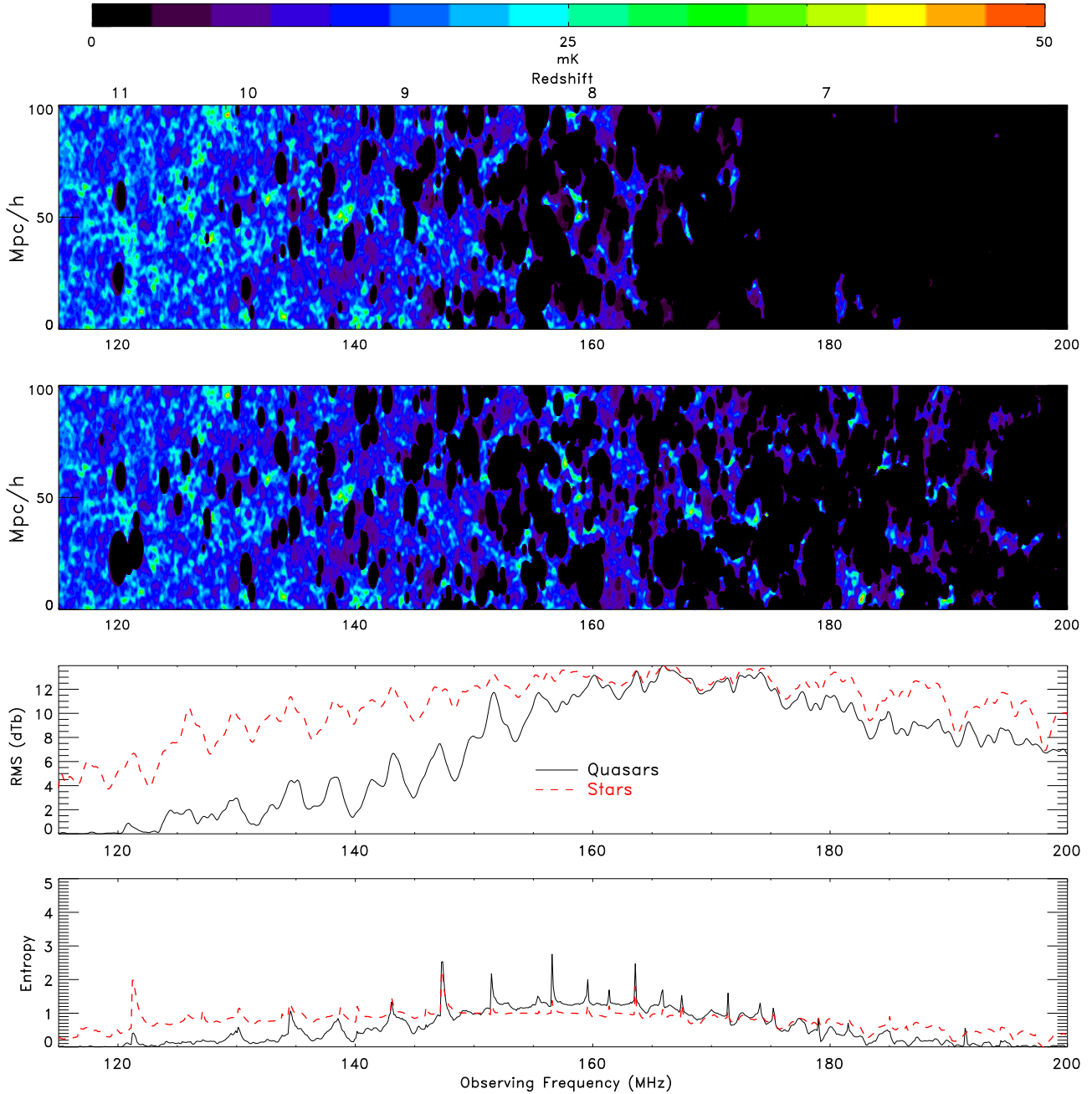
(ii) *After convolution with the LOFAR beam (ref. Fig. 20):*

In this case, although the overall behaviour is similar to that of the previous case before convolution, the effect is enhanced. This can be understood with the aid of Fig. 21. Lower frequencies ( $120 < \nu < 145$  MHz) is analogous to case (a) & (c) and its corresponding histogram in (Ha) & (Hc). Because, at these frequencies the Universe is still largely neutral with just a few sources and the effect of smearing  $\delta T_b$  with the observing beam spreads the histogram thus increasing the entropy. At intermediate frequencies ( $120 < \nu < 180$  MHz), the effect of decreasing entropy is analogous to case (b) & (d) with its corresponding histogram in (Hb) & (Hd). Although the entropy increased from (b) to (d) and also in case of  $\delta T_b$  after the convolution, the increase is relatively less. This is because the smearing action was on scales larger than the fluctuations in  $\delta T_b$  hence narrowing the histogram to a few values. At higher frequencies of course  $\delta T_b$  is zero and hence the entropy drops to 0 as well.

A final statistic that was calculated was the probability distribution function (PDF) of the  $\delta T_b$  at four different redshifts for stars and quasars. If the IGM is not ionized and if the neutral hydrogen is measurable (i.e. the signal-to-noise ratio is high enough), the distribution of  $\delta T_b$  reflects the underlying density field (eq. 15). But as reionization proceeds, larger and larger regions become ionized and the PDF of  $\delta T_b$  skews because of the excess of  $\delta T_b$  close to zero. This fact can be made use of as a tool for the statistical detection of the EoR signal as will be explored in an upcoming paper by Harker et al., *in prep*. The features of the PDF seem to vary dramatically between the two scenarios.

## 6 LOFAR RESPONSE AND ITS EFFECTS

The rationale behind producing these simulations is to test the effect of the interferometric response on the signal and other contributors with the same frequency band. This section gives an overview

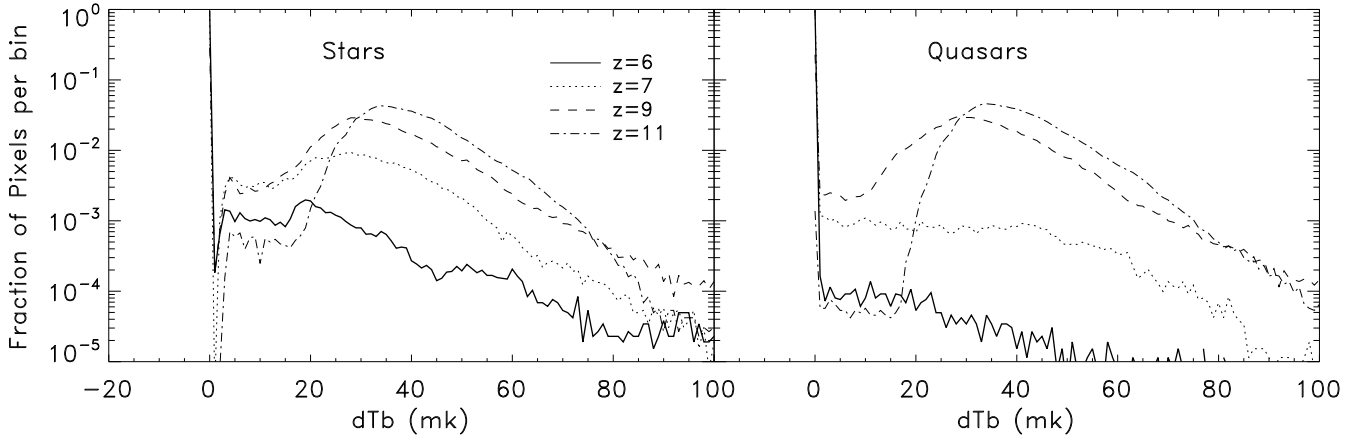


**Figure 15.** Starting from the top, *panel 1* shows the  $\delta T_b$  distribution of quasars, *panel 2* shows the same for stars, *panels 3 and 4* show the variance and entropy of slices at different frequencies for stars (red dashed) and quasars (black solid). The figure clearly shows that the nature of the reionization history differs significantly between stars and black holes. In the case of stars reionization seems to be much more extended than for the case of stars.

of simulations of the LOFAR response and shows how the signal will be seen by LOFAR in the absence of noise or other calibration errors. A more detailed discussion of the LOFAR response and the data model for the LOFAR-EoR experiment will be provided in Lambropoulos et al., *in prep*. For the EoR experiment we plan to use the LOFAR core which will consist of about 24 dual stations of tiles. Each dual station will have a diameter of approximately 35 meters and the maximum baseline between stations will be about 2 km.

For the simulations in this paper we make some simplifying assumptions regarding the telescope response. We assume the nar-

row bandwidth condition and we also assume that the image-plane-effects have been calibrated to a satisfactory level. This includes a stable primary beam and adequate compensation for the ionospheric effects such as the ionospheric phase introduced during the propagation of electromagnetic waves in the ionosphere and the ionospheric Faraday rotation. In an interferometric observation, the measured correlation of the electric fields between two sensors  $i$  and  $j$  is called visibility and is given by Perley, Schwab, & Bridle (1989):



**Figure 16.** The probability distribution functions (PDF) of  $\delta T_b$  at redshifts 6, 7, 9 and 11, as indicated by the line styles, for stars (left) and quasars (right). The PDF should reflect the underlying density distribution if the IGM is neutral, but ionization of the IGM causes a peak at a brightness temperature of zero skewing the distribution.

$$V(u, v, w) = \int A(l, m, n) I(l, m, n) e^{-2\pi i(ul+vm+wn)} dl dm dn, \quad (17)$$

where  $A$  is the primary beam,  $I$  the sky brightness,  $l, m, n$  are the direction cosines and  $u, v, w$  are the coordinates of the baseline (in units of observing wavelength) as seen from the source.

We further assume that simulated maps are a collection of point sources: each pixel corresponds to a point source with the relevant intensity. Note that the equation above takes into account the sky curvature. The visibilities are sampled for all station pairs, but also at different pair positions as the Earth rotates.

For every baseline and frequency the  $uv^5$  track points sample different scales of the Fourier transform of the sky at that frequency. We compute the  $uv$  tracks for each interferometer pair for 6 hours of synthesis with an averaging interval of 100 sec and we grid them onto a regular grid in the  $uv$  plane. Using the gridded tracks as a sampling function, we sample the Fourier transform of our model sky, which in our case is the 21cm EoR signal, at the corresponding grid cells. This gives us the time series of the visibilities for every station pair.

The Fourier (or Inverse Fourier) transform of the sampled visibilities is called the “dirty” map. It is actually the sky map convolved with the Fourier transform of the sampling function, which is called the “dirty” beam or the PSF. This is a simple-minded approach in estimating the sky brightness as it uses linear operations.

With the LOFAR core we expect to reach a sensitivity of 350 mK in one night of observations at 150 MHz. After 100 nights the final sensitivity will drop to 35mK. For total intensity observations we expect Gaussian noise with zero average and the above mentioned rms to drop to 35 mK. We assume that calibration errors, after 100 nights of integration accumulate in such a way that they follow a Gaussian distribution obeying the central limit theorem.

The effect of the “original” image passing through the response of the LOFAR antenna at a frequency of 130 MHz is shown in Fig. 17. The figure shows the brightness temperature in both cases normalized to the largest value in the corresponding figure. Note that the simulation is  $100 h^{-1}$  comoving Mpc across which is only about  $1/8^{th}$  of the total ( $5^\circ \times 5^\circ$ ) field of view of LOFAR.

<sup>5</sup> The  $uv$  plane is the Fourier-pair of the sky brightness, where  $u$  and  $v$  are the distances between antenna pairs on an interferometer measured in terms of the wavelength of observation.

Therefore we are missing the very large scale Fourier modes. We are planning to run larger simulations to overcome this problem.

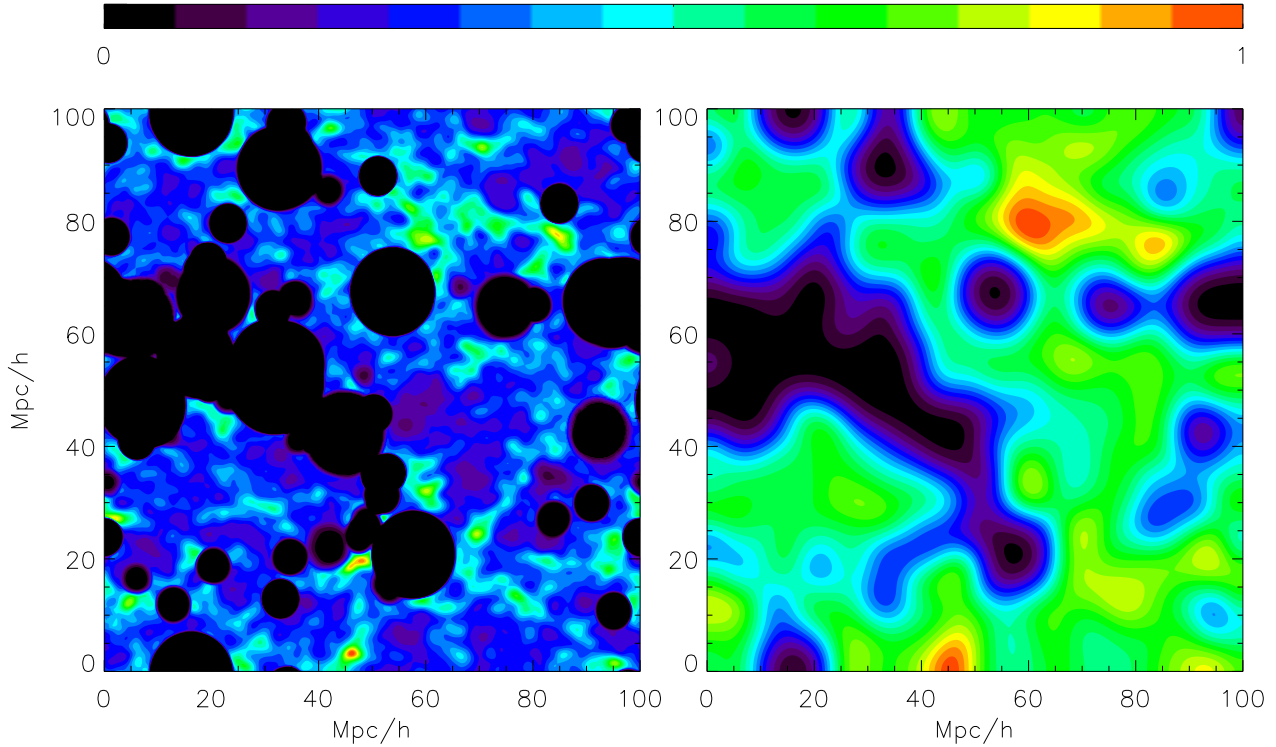
Along with the effect of the spatial resolution of LOFAR on the sky, we also studied the effect of its spectral resolution. The maps produced by LOFAR will have a bandwidth of about 1 MHz. This is essential to beat the noise level down. Figs. 18 and 19 show  $\delta T_b$  along five different lines of sight. The black solid lines indicate the signal before convolution and spectral smoothing, whereas the over-plotted blue dashed lines include the effect of LOFAR’s spatial and spectral response.

The entire FC was convolved with the antenna response of LOFAR calculated separately for each frequency. This “convolved cube” is then used to plot Fig. 20. This figure is identical in structure to Fig. 15. As expected, due to the smoothing action of the antenna beam pattern, the variance of the signal in the “convolved cube” drops by approximately 30% relative to that of the FC while conserving the overall behaviour across all frequencies. The entropy in each of these slices on the other hand shows a dramatically different behaviour. The rise and fall of the entropy in the case of quasars is much more pronounced for the “convolved cube” and the entropy for stars shows a steady increase. It is interesting that the slice-entropies for stars and quasars are very different. This could be used as a discriminant for different scenarios of reionization.

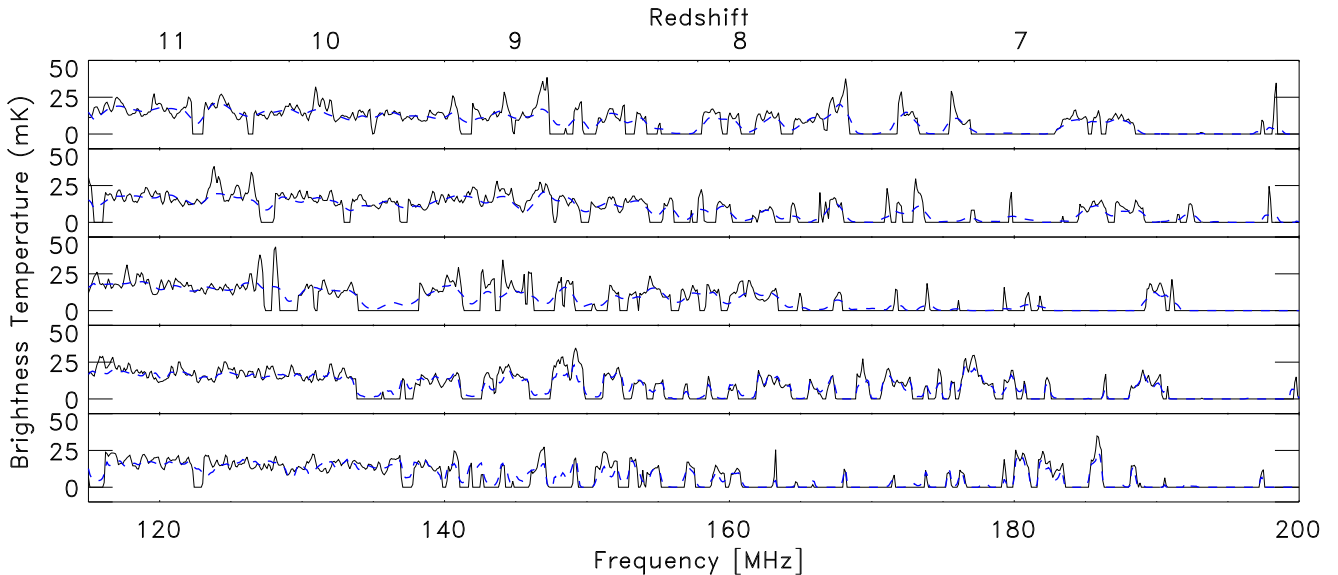
Fig. 21 is a simple example to illustrate the fact that smoothing increases the entropy in the figure. In essence, the averaging along the frequency direction introduces correlations between pixels of adjacent slices. For the simulations considered here it corresponds to 10 adjacent slices (since the resolution of the simulation is 0.1 MHz and that of LOFAR is 1 MHz). This effect is enhanced in the case of quasars because of the rapid rate of ionization and we see that the entropy peaks around 150 MHz where the transition from a neutral to an ionized Universe accelerates.

## 7 SUMMARY AND OUTLOOK

We emphasized the need to expand the scenarios that need to be explored for reionization and their role in building a reliable and robust pipeline, thus necessitating fast realizations of different scenarios. We built a scheme in which a range of 1-D ionization profiles were catalogued for a number of luminosities, redshifts, den-



**Figure 17.** A comparison of the brightness temperature (normalized to the largest value) between the “original” image (left) and the same image after convolving with the LOFAR PSF (right) at a frequency corresponding to redshift 10. Since the PSF of LOFAR essentially performs as a low-pass filter the convolved image is smoother.

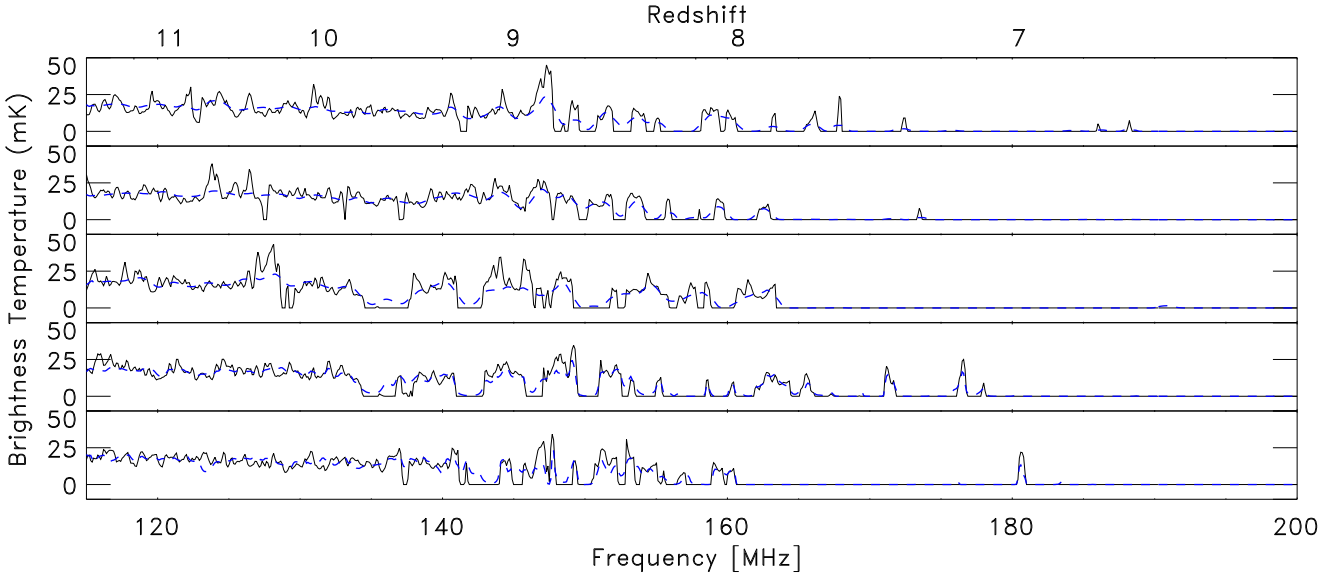


**Figure 18.** Examples of five lines of sight through the frequency direction for  $\delta T_b$  for the case of ionization by stars. Over-plotted in blue are the lines of sight as observed through the LOFAR telescope with a spectral resolution of 1 MHz

sities and source spectra and which were subsequently coupled to an  $N$ -body simulation to obtain an approximation of a “standard” 3-D radiative transfer code. The results obtained were validated using CRASH, a full 3-D radiative transfer code with ray tracing. The agreement between the two methods was excellent for early redshifts ( $z > 8$ ), but as expected, the discrepancy grew towards

lower redshifts. Several visual comparisons of the slices of different boxes were made along with three different statistical measures of the similarity between the simulations.

Many snapshots ( $\approx 75$ ) were used between a redshift of 15 and 6 and the radiative transfer done on them as described in the preceding sections. These snapshots were then used to make a con-



**Figure 19.** Same as Fig. 18 but for the case of ionization by quasars.

tiguous cube running from redshift 6 to 12. In terms of the observing frequency, the cube spans 115 MHz to 200 MHz with a frequency resolution matching that of LOFAR, about one MHz. Cubes were generated for scenarios involving only stars or quasars and some diagnostics are provided to quantitatively differentiate between them. For both models the variance in  $\delta T_b$  peaked at around 160 MHz. Although neither may reflect reality, these scenarios demonstrate the use of the techniques we have developed to span large parameter spaces of variables. The PDF of  $\delta T_b$  (see Fig. 16) provides a statistical discriminant between the different source scenarios and could be used in the future to look for the statistical detection of the signal.

The cubes generated provide  $\delta T_b$  as a function of frequency. The cube was then averaged over a bandwidth of 1 MHz and convolved with the beam pattern of LOFAR to understand the distortions caused by incomplete sampling by an interferometer. Even if the images were blurred by the operation, the overall characteristics of the signal remain detectable. Although the behaviour of the variance of the signal before and after the convolution remained the same (except that the latter had lower values on average), the image/slice entropy showed a very different behaviour. In the former case, i.e., before the convolution, the image entropy remained almost flat throughout the frequency range whereas in the latter the entropy steeply rises at around 160 MHz.

As a note, it is important to mention that although in principle the ionized bubbles do move with a peculiar velocity  $v_r(z) = v_r(0)(1+z)^{-1/2}$ , where  $v_r(0)$  is the typical peculiar velocity of galaxies at redshift zero, assuming  $v_r(0) \approx 600$  km/s, a redshift 10 object would have a peculiar velocity of 200 km/s. For a typical lifetime of the source considered, i.e., 10 Myr, this corresponds to motion of about a couple of kpc. This is an order of magnitude less than the resolution of the simulation box at that redshift. Therefore we ignore this effect. On the other hand we have taken into account the effect of redshift distortions whose effects are relatively more important.

The simulations and comparisons in this paper have focused on purely stellar or quasars sources, but it is plausible that the early sources of reionization were a mixture of stars and quasars or other yet unknown sources. It is therefore important to simulate reionization by a mixture of these sources, taking into account their

clustering properties. The simulations presented in this paper did not take into account the constraints on the population of ionizing sources imposed by various measurements like the infrared excess in the case of stars and the soft X-ray excess for quasars. Apart from the ionization patterns induced by these sources, the  $\delta T_b$  maps will also depend on the kinetic temperature which is coupled to the spin temperature via collisions or Ly- $\alpha$  pumping. Hence, it is imperative that we include these temperature effects on the IGM. We will incorporate the mixture of sources and the effect of the temperature in an upcoming paper (Thomas et al., *in prep*).

One of the main astrophysical hurdles for the detection of the EoR signal is the existence of prominent Galactic and extragalactic foregrounds. Typically, the difference between the mean amplitude of the EoR signal and the foregrounds is expected to be 4 to 5 orders of magnitude, but an interferometer like LOFAR measures only the fluctuations which in this case are expected to be different by ‘only’ three orders of magnitude (Jelić et al. 2008). In subsequent papers we will explore the effects of foregrounds and their removal strategies.

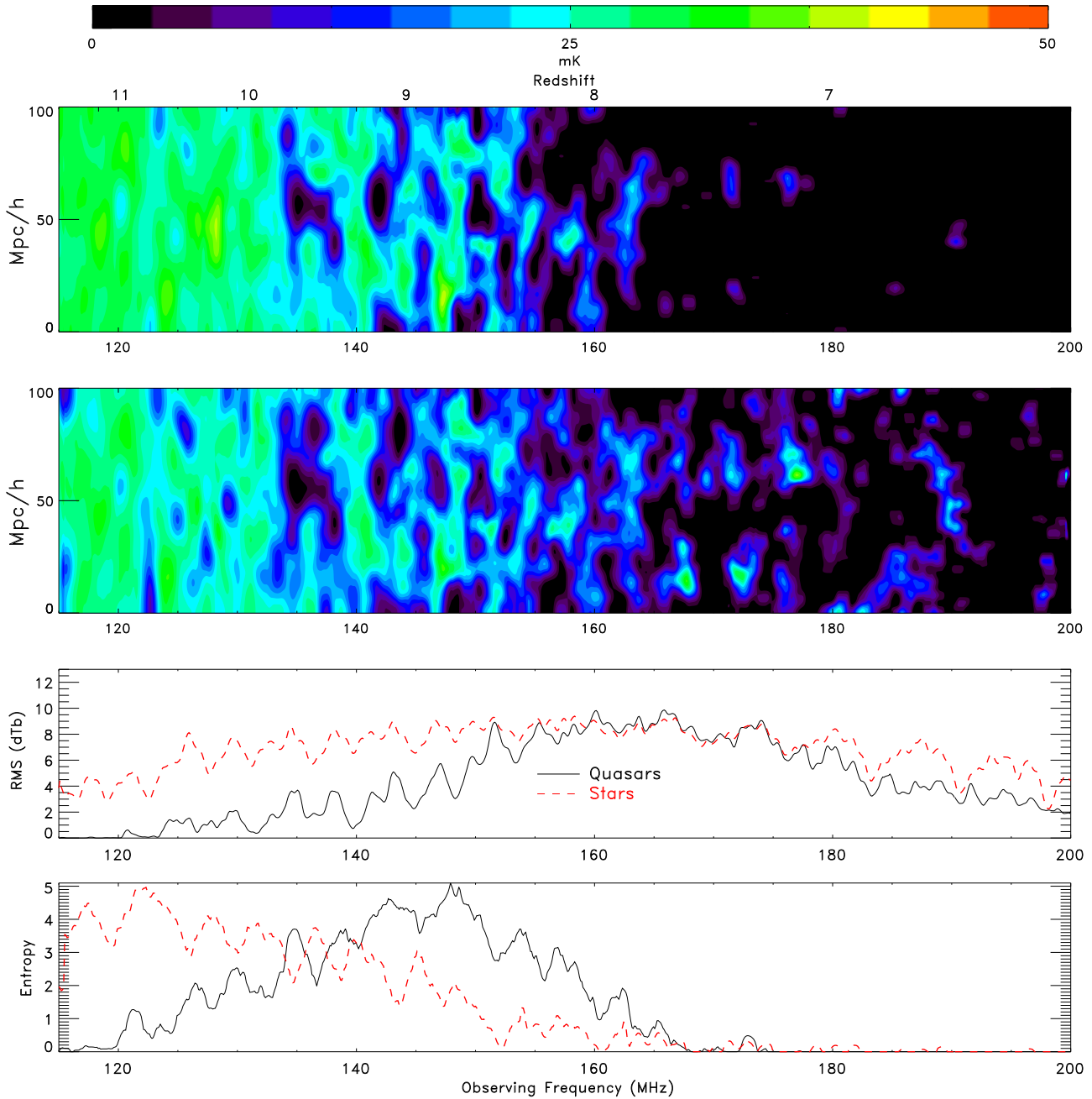
## 8 ACKNOWLEDGMENT

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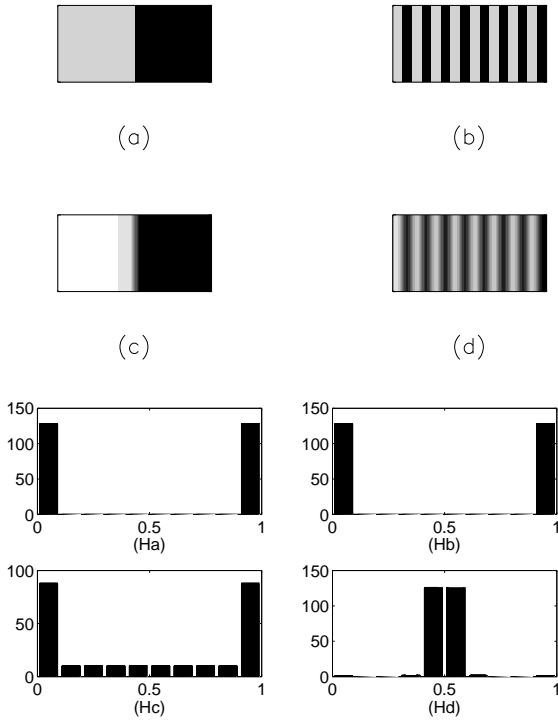




**Figure 20.** Same as in Fig. 15 but after the signal has been passed through the LOFAR response.

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**Figure 21.** Illustration of image entropy: In the above example, images (a) and (b) have the same image entropy with a value of one according to equation 16. Images (c) and (d) are the convolutions of (a) and (b) with a square top hat function with side of length  $1/4$  of the side of the image. The entropies of these images are 4.1 and 2.2, which is larger than the entropies we started with. Therefore, when we introduced correlations between pixels by smoothing them, their entropies increased. Images (Ha) to (Hd) are the histograms corresponding to images (a) to (d) respectively. As we can see, the histograms of images (a) and (b) have the same distribution, whereas image (Hc) has a histogram that has a large spread compared to (Hd). From an information theory point of view this large spread corresponds to higher information content and hence higher entropy. Similarly, when we smooth/average along the frequency direction in the FC, we introduce correlations between pixels, hence increasing the entropies considerably when the scale of smoothing is smaller than the typical correlation length of the pixels in the original image.

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