Modelling the stochasticity of high-redshift halo bias

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ABSTRACT

A very large dynamic range with simultaneous capture of both large- and small-scales in the simulations of cosmic structures is required for correct modelling of many cosmological phenomena, particularly at high redshift. This is not always available, or when it is, it makes such simulations very expensive. We present a novel sub-grid method for modelling low-mass ($10^5 M_\odot \leq M_{\text{halo}} \leq 10^9 M_\odot$) haloes, which are otherwise unresolved in large-volume cosmological simulations limited in numerical resolution. In addition to the deterministic halo bias that captures the average property, we model its stochasticity that is correlated in time. We find that the instantaneous binned distribution of the number of haloes is well approximated by a log-normal distribution, with overall amplitude modulated by this “temporal correlation bias”. The robustness of our new scheme is tested against various statistical measures, and we find that temporally correlated stochasticity generates mock halo data that is significantly more reliable than that from temporally uncorrelated stochasticity. Our method can be applied for simulating processes that depend on both the small- and large-scale structures, especially for those that are sensitive to the evolution history of structure formation such as the process of cosmic reionization. As a sample application, we generate a mock distribution of medium-mass ($10^8 M_\odot \leq M_\odot \leq 10^9 M_\odot$) haloes inside a 500 Mpc grid simulation box. This mock halo catalogue bears a reasonable statistical agreement with a halo catalogue from numerically-resolved haloes in a smaller box, and therefore will allow a very self-consistent sets of cosmic reionization simulations in a box large enough to generate statistically reliable data.

Key words: haloes — cosmology: theory — dark ages, reionization, first stars — methods: numerical

1 INTRODUCTION

Cosmological haloes are the sites where most active astrophysical processes occur. Understanding the formation, evolution and spatial distribution of cosmological haloes thus allows theoretical access to many astrophysical phenomena and links to observational cosmology. The halo information is typically summarised in the form of a halo catalogue. Modelling galaxy surveys in observational cosmology and studies of the process of cosmic reionization, which generates observational features at cosmological scales, are both examples that can benefit from reliable, realistic halo catalogues.

For cosmic reionization modelling in particular, properly understanding the nature of the ionising sources responsible for the Epoch of Reionization (EoR) is an important problem which can aid in interpreting current and future detection experiments. Mini-haloes, small haloes in which gas cannot cool through atomic line cooling, are generally conceived to be the site of the first, Pop. III, stars responsible for the early stages of EoR (e.g. Barkana & Loeb 2001). At the same time, both the stellar-mass binaries and the progenitors of super-massive black holes are believed to be among the main sources of X-ray radiation, which heats the neutral intergalactic medium (IGM) unreachable by UV radiation from stars (Ricotti & Ostriker 2004; Madau et al. 2004; Knevitt et al. 2014). The later stages of re-ionisation are thought to be dominated by emission from more massive galaxies, with halo masses above about $10^8 M_\odot$, which we refer to as atomically cooling haloes (ACHs) based on their dominant gas cooling mechanism. These can in turn be split into low-mass ACH (LMACHs), with masses less than about $10^9 M_\odot$, which we can suppress by radiative feedback, and the larger, high-mass ACH (HMACHs) which are largely unaffected by such feedback (Iliev et al. 2007; Dixon et al. 2016; Ahn et al. 2015). The process of reionization is believed to be inhomogeneous and anisotropic on large scales (Iliev et al. 2014), hence a large-volume simulation box is needed to capture the extent of the processes involved. However, this also means that cosmic reionization simulations often have a relatively low resolution, resulting in the need for sub-grid mod-
elling of the low-mass haloes in which the majority of reionization sources reside.

One perspective towards modelling the sub-grid halo population is the peak-background split scheme [Bardeen et al. 1986], which provides a framework for understanding how haloes form in a way biased toward high-density environment. In this approach, a halo is associated with the linear overdensity \( \delta_{\text{lin}} \) that satisfies the halo formation criterion, \( \delta_{\text{lin}} > \delta_c \), where \( \delta_c \approx 1.636 \) is the critical overdensity. This put theoretical foundations under the well-known Press-Schechter (PS) formalism [Press & Schechter 1974], whose fudge multiplicity factor 2 was later explained rigorously by Bond et al. [1991] through their extended Press-Schechter formalism (or the excursion set formalism). The halo bias due to a large-scale density environment specified by its linear overdensity \( \Delta_{\text{linear}} \) can also be naturally accounted for in this framework, because the small-scale density fluctuation now only needs to satisfy the modified criterion \( \delta_{\text{lin}} > \delta_c - \Delta_{\text{linear}} \) [Cole & Kaiser 1989].

Mo & White [1996] calculated a fully nonlinear bias prescription, by combining this peak-background split scheme with the spherical top-hat collapse model.

A notable shortcoming of both the average PS halo mass function and the nonlinear halo bias model by Mo & White [1996] is that the number of haloes predicted this way does not match the numerically simulated haloes well, especially massive, rare haloes at any given epoch. The discrepancy in the average halo mass function stimulated a set of fitting functions based either on a more detailed theory in the halo formation, supported by simulation data (e.g. Sheth & Tormen 1999, ST hereafter) or empirical fits to numerical simulations (Jenkins et al. 2001; Warren et al. 2006; Reed et al. 2007; Lukic et al. 2007; Lim & Lee 2013; Watson et al. 2014). The discrepancy in the biased halo mass function seems to be resolved by a simple yet attractive solution by Barkana & Loeb [2004, BL hereafter], which is a hybrid scheme of combining the ST mass function and the bias prescription from the extended PS formalism. Ahn et al. [2015] extended this idea to combine the average mass function of simulated haloes, instead of the ST mass function, and the bias prescription from the extended PS formalism, and have found that this scheme has an excellent predictive power on the nonlinear bias of haloes in the high-redshift regime.

In order to add more naturality to the sub-grid modelling, however, the “deterministic” prescription described so far is not sufficient, and the stochasticity of halo bias also needs to be implemented. This stochasticity does not follow the pure Poisson distribution, because the correlation of haloes at the sub-grid level produces a variance in the number of haloes, in addition to the usual shot noise [Peebles 1993; Dekel & Lahav 1999]. In the presence of the sub-grid correlation, this additive variance extends the tails of the distribution function of the halo number, or “super-Poissonian” distribution, which is well fitted by functional forms by Saslaw & Hamilton [1984] and Sheth [1995].

The sub-grid modelling of haloes is naturally connected to the effort to generate mock halo catalogues under the knowledge of large-scale density field. This idea is implemented in PINOCCHIO [Monaco et al. 2002; 2013] and PTHALOES [Scoccimarro & Sheth 2002; Manera et al. 2015], which generate mock halo catalogues based on the quasi-linear density field. With an adaptive high-order perturbation theory, mock catalogues can be generated even more precisely (e.g. Patchy by Kitaura et al. [2014] in which they used the 2nd-order Lagrangian perturbation theory but at the same time improved on mitigating the problems caused by the unwanted free-streaming of particles in small scales). The feasibility to use such a prescription to study e.g. the Baryon Acoustic Oscillation (BAO) feature in density power spectrum has been presented [Kitaura et al. 2014].

We find that one key ingredient is still missing in sub-grid modelling efforts described above. This is the \emph{temporally correlated stochasticity}: stochasticities in the halo distribution at mutually nearby epochs should be correlated. This would not be crucial if one is interested only in a limited range of redshifts. For example, the study of BAO through galaxy surveys at low redshift may need to focus only on the fields of halo population that is instantaneous or mildly changing in time. However, in cases where continuous evolution is important, correlation of stochasticity in time is also crucial. For example, in the study of cosmic reionization, how haloes are generated in time and space are cumulatively imprinted in the late phase of the process in terms of the morphology of H II regions. Therefore, in this paper, we present our quantitative study on the temporally correlated stochasticity and the feasibility to use this prescription to self-consistently generating mock halo catalogues both in time and space. Previously we have implemented the deterministic bias only, without stochasticity, as sub-grid treatment. Nevertheless, through this method, we have found that small-mass haloes impact the physics of reionization quite substantially: minihaloes yield extended and self-regulated reionization epoch [Ahn et al. 2012] even found favoured by the CMB polarization data by Planck: Heinrich et al. [2017], the observed 3-dimensional (3D) imaging and 21-cm power spectrum depends on the minimum halo mass [Dixon et al. 2016; Giri et al. 2018], and statistics of neutral gas islands in the late phase of islands will be affected by LMACHs [Giri et al. 2019], to give a few examples. Application of a self-consistently calculated stochasticity is therefore expected to provide a more reliable picture on the physics of cosmic reionization.

This paper is organized as follows. We describe our method to generate halo bias that can assimilate the N-body simulation data in \S 2. We present mock realizations of haloes in those boxes that resolve haloes of given mass range, and compare the resulting statistical measures of the actual N-body data and the mock data in \S 3.1 An application of our method to a large, \( 500 \, h^{-1} \, \text{Mpc} \) box with a test on its validity is described in \S 3.2 We summarise our results and discuss relevant issues in \S 4.

2 METHODOLOGY

2.1 The N-body simulation data

Halo bias is composed of the deterministic bias and the stochastic bias. The former represents the average conditional probability that cells with given overdensity \( \delta \) will host haloes of given mass range. The latter represents the unavoidable stochasticity, due to dependencies beyond local density, in the number (or collapsed fraction) of haloes across cells with given \( \delta \). These two components can be expressed in a single probability distribution function in terms of the average quantity \( \mu \) and at the least the standard deviation \( \sigma \) (that of the approximately log-normal distribution in our case as in Equation 3.1), respectively.

Motivated by the physics of the radiation sources during the Cosmic Dawn and EoR, we split the dark matter haloes into three physically-motivated mass ranges (see e.g. Iliev et al. 2007): high-mass atomically-cooling haloes (HMACHs), defined by \( M_{\text{halo}} > 10^7 \, M_\odot \); low-mass atomically-cooling haloes (LMACHs), with \( 10^5 \, M_\odot < M_{\text{halo}} < 10^7 \, M_\odot \), and minihaloes (MHs), with \( M_{\text{halo}} < 10^5 \, M_\odot \). We focus on implementing the stochasticity of...
Figure 1. PDF of the number of MHs, $N_{5.8}$, contained within cells of given overdensity $\delta$ on our $14^3$-grid 6.3$h^{-1}$ Mpc-box. $\delta$ is shown on top of each subplot while redshifts are shown on the left. The PDF of the N-body halo data (black solid) is fit by a log-normal distribution (red dashed).

Figure 2. Same as in Fig. 1 but with the number of haloes sampled on a $44^3$ grid.
Figure 3. PDF of the LMACH collapsed fraction, $f_{\text{col},8:9}$, contained within cells of given overdensity $\delta$ on our $64^3$-grid $114\, h^{-1}$ Mpc-box. Plotting convention is the same as in Figure 1.

Figure 4. Same as in Fig. 3 but with the collapsed fraction sampled on a $128^3$ grid.
the latter two types in large-scale simulations, since HMACHs are relatively more easily resolved and thus sub-grid modelling is usually unnecessary, although our model is easily extensible to such haloes as well. By definition, ACHs form stars efficiently by cooling the gas through atomic line radiation, and the star formation is expected to be roughly proportional to the total amount of gas available, which in turn is proportional to the collapsed fraction in such haloes. In contrast, gas in MHs is easily disrupted and photo-evaporated by the first star(s) to form within each halo, or in nearby haloes, thus we expect that each MH forms just one, or at most a few stars, irrespective to its actual total gas mass. Therefore, in our modelling for LMACHs we consider the local collapsed fraction, while for MHs we consider the local number of haloes. Our model is applicable to either quantity.

The simulation data used throughout this work is based on a suite of N-body simulations using the CubeM code (Hamann et al. 2013). The MH data is based on a high-resolution simulation in a box of $6.3 \times 10^{-3}$ Mpc per side, with $1728^3$ particles, force resolution of $182 h^{-1}$ pc and minimum halo mass resolved (with 20 particles or more) of $\sim 10^8 M_\odot$. This roughly corresponds to the halo 'filtering mass' (Gnedin 2000) below which haloes struggle to keep their gas content even before reionization. The LMACHs data is based on a simulation in a box of $114 h^{-1}$ Mpc per side, with $3072^3$ particles, force resolution of $1.8 h^{-1}$ kpc and minimum resolved halo mass of $\sim 10^5 M_\odot$. The density field is smoothed onto a uniform grid of $14^3$ or $44^3$ cells when sampling MHs (hereafter $N_{5.8}$), and into $64^3$ and $128^3$ cells when sampling the local collapsed fraction of LMACHs ($f_{\text{coll}, 8.9}$), given by

$$f_{\text{coll}, 8.9} = \frac{M_{8.9}}{M}, \quad (1)$$

where $M_{8.9}$ is the mass of haloes between $10^8$ and $10^9 M_\odot$, and $M$ is the mass of a cell. The local overdensity, $\delta$, of each cell is defined by

$$\delta = \frac{\rho}{\bar{\rho}} - 1, \quad (2)$$

where $\rho$ is the average density of a cell and $\bar{\rho}$ is the mean density of the universe.

### 2.2 Instantaneous halo bias in N-body simulation

We empirically quantify the instantaneous halo bias ("instantaneous bias" hereafter) from N-body simulation data. For now we ignore any possible temporal correlation but just consider the local cell overdensity $\delta$ and redshift $z$. First, we sample $\delta$’s of cells with the bin width $\Delta \delta = 0.1$. This guarantees a reasonable amount of sampling of grid cells for any $\delta < 10$. Only for the highest-$\delta$ cells which are rare, we enlarge the bin size substantially: cells of $\delta > 10$ are grouped into two coarse bins – $10 \leq \delta < 15$ and $\delta > 15$. Second, for each $\delta$ bin, we measure the empirical Probability Density Function (PDF) of $N_{5.8}$ or $f_{\text{coll}, 8.9}$ by visiting all cells of the given $\delta$.

Any conditional parameters hereafter denote parameters measured in appropriate bins; e.g. $\mu(z|\delta = 0.5)$ is the average value of all $\mu(z|\delta)$’s when $\delta \in [0.5 - \Delta \delta/2, 0.5 + \Delta \delta/2] = [0.45, 0.55]$. The following terminology and parameters are useful in describing the empirical, instantaneous stochasticity:

- $x$: the value of either $N_{5.8}$ or $f_{\text{coll}, 8.9}$.
- $x_{\text{min}}(z|\delta), x_{\text{max}}(z|\delta)$: the minimum and maximum, respectively, of $x$ found in cells of overdensity $\delta$ at redshift $z$.
- $\mu(z|\delta)$: the average of $\ln(x)$, given cells of $\delta$ at $z$.
- $\sigma(z|\delta)$: the standard deviation of $\ln(x)$, given cells of $\delta$ at $z$.
- $N_+(z|\delta)$: the total number of non-empty cells at $z$.
- $N_0(z|\delta)$: the total number of empty cells at $z$.
- $N_{\text{coll}}(z|\delta)$: the number of cells of $\delta$ which are non-empty at redshift $z$.
- $N_0(z|\delta)$: the number of cells of $\delta$ which are empty at $z$.

The empirical results for PDFs of $N_{5.8}$ are shown in Figures 1 and 2 and those for PDFs of $f_{\text{coll}, 8.9}$ are shown in Figures 3 and 4. The PDFs are roughly Gaussian close to its peak, but have considerable skewness away from it, and are thus overall not well represented by a Gaussian. This "super-Poissonian" distribution is caused by the non-zero auto-correlation of halo population in the sub-cell scale (Peebles 1980; Ahn et al. 2015), which can be well-fit by distribution functions suggested by Saslaw & Hamilton (1984) and Sheth (1995). Instead, we employ a lognormal distribution, with which the skewness is easily realized with just two parameters – the average and the standard deviation of the logarithmic – to fit the empirical data:

$$f(x, z|\delta) = \frac{1}{x \sigma \sqrt{2 \pi}} \exp\left(-\frac{\ln x - \mu(z|\delta)}{\sigma(z|\delta)}\right), \quad (3)$$

where $\mu = \mu(z|\delta)$ and $\sigma = \sigma(z|\delta)$. We use this lognormal PDF to represent the PDF of non-empty cells only, since empty cells are not of interest here and including them would distort distribution. Note that we do not take ($\mu$, $\sigma$) as free parameters to find the best fit to the empirical data, but instead use the empirical values of ($\mu(z|\delta)$, $\sigma(z|\delta)$) and consider the goodness of the fit later.

The lognormal fits (red dashed lines in Figs. 1, 2, 3, 4) largely match the empirical distributions well. In both cases of MHs and LMACHs, the lognormal fit works better for the larger cell size: $N_{\text{grid}} = 14$ case (Fig. 1) is better than $N_{\text{grid}} = 44$ case (Fig. 2) for MHs, and $N_{\text{grid}} = 64$ case (Fig. 3) is better than $N_{\text{grid}} = 128$ case (Fig. 4) for LMACHs. The mismatch occurs in many cases, but only in the tails of PDFs where the fractional contribution becomes relatively unimportant. Only at high-redshift ($z \geq 15$), small cell-size cases for LMACHs show the biggest mismatch (Fig. 4), even in its amplitude. Overall, we expect that any resulting statistical measures from this lognormal fitting will be only slightly different from those of the N-body data.

### 2.3 Implementing instantaneous halo bias

We now describe our scheme to realize instantaneous bias for generating mock halo catalogues using the empirical parameters, described in section 2.2 as the basis. A fluctuating 3D density field should be provided at a target redshift, ideally by numerical simulations that resolve the nonlinear density environment for a given filtering scale (Eulerian cell size).

Our algorithm is described by the sequence below. Any quantity with a prime symbol denotes a value related to the mock data.

1. Once the N-body particle density field is interpolated onto a uniform grid, group the grid cells according to discrete bins of $\delta$.
2. Among the cells of given $\delta$, randomly choose a fraction $P_+(z|\delta)$ of these cells that will host haloes, with the "conditional occupation probability":

$$P_+(z|\delta) = \frac{N_+(z|\delta)}{N_+(z|\delta) + N_0(z|\delta)}, \quad (4)$$

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and leave the remaining cells devoid of any haloes. The number of non-empty cells of \( \delta \) in the given density field found this way, \( N_i(z) \), may differ from \( N_{i}^\prime(z) \) in general, because \( N_{i}^\prime(z) = P_{i}(z) N_i(z) \), where \( N_i(z) \) is the number of grid cells of \( \delta \) in the given density field. The total of \( N_{i}^\prime(z) \), \( (N_{i}^\prime(z)) \) however, should follow
\[
N_{i}^\prime(z) = \frac{N_{i}(z)}{N_{g}d} \times N_{g}d.
\]

(iii) Use Monte Carlo sampling of \( x \) based on Equation (3) to populate these non-empty cells with haloes. Sample \( x \) from the bounded range \( x = [x_{\min}(z) \delta, x_{\max}(z) \delta] \).

(iv) When \( N_{i}^\prime(z) \leq 10 \) it is inappropriate to use the Monte Carlo sampling due to rarity of such cells; in such cases the empirical data shows convergence of \( x \) to \( \mu(z) \delta \). If this happens, only use the deterministic bias, by setting \( x = e^{\mu(z) \delta} \) in those cells.

This scheme only considers the instantaneous information, and thus can be easily applied once the empirical parameters described in \( \S2.2 \) are available. Note that when the range of \( \delta \) in the given density field extends the range of the empirical values due to e.g. the increased size of a simulation box, one needs to extrapolate the empirical parameters for those outliers of \( \delta \).

### 2.4 Temporal halo bias in N-body simulation

Just as in the case of the instantaneous bias, we first find an empirical model for the temporal stochastic halo bias ("temporal bias" hereafter) from N-body halo data, and then develop a method to generate mock halo catalogues based on this model. Ideally, it would be best to find e.g. a universal relation between the redshift \( z \) and the degree of stochasticity for any given Eulerian or Lagrangian cell. Unfortunately we could not find such a clean relation yet, but instead found a model that reflects temporal stochasticity of N-body halo catalogues to a significant extent. We will show how well this method mimics the actual N-body halo catalogues in \( \S3 \) through various statistical measures.

Our empirical model for temporal stochasticity can be described by the following parameters, where appropriate binning is assumed for conditional values:

- \( \Delta z_{i} ; t \): the redshift interval during which an Eulerian cell \( i \) is not empty.
- \( \Delta z \): the full duration of our N-body simulation, under the assumption that haloes of interest start to emerge in the simulation volume from the starting redshift.
- \( \delta \): the average overdensity of the cell \( i \) over \( \Delta z \).
- \( f_{x,i} \equiv \Delta z_{i}/\Delta z \): the fraction of time during which the cell \( i \) is not empty.
- \( f_{x,i}(\delta) \): the time fraction that an Eulerian cell with mean overdensity \( \delta \) is not empty. Here, the average of \( f_{x,i} \) of cells having \( f_{x,i} = f_{x,i}(\delta) \), and thus this function relates \( f_{x,i} \) and \( \delta \) in an averaged, deterministic way.
- \( N_{i}(z|x_{\text{prev}},+) \): the total number of non-empty cells at \( z \), among those cells which had \( x = x_{\text{prev}} \equiv x(z_{\text{prev}}) > 0 \). Here, \( z_{\text{prev}} \) is the redshift of the N-body data recorded just before the redshift \( z \).
- \( N_{0}(z|x_{\text{prev}},+) \): the total number of empty cells at \( z \), among those cells which had \( x = x_{\text{prev}} > 0 \).

### 2.5 Implementing temporal halo bias

We now describe our method to generate mock halo catalogues with temporal bias, based on the empirical parameters described in Sections 2.2 and 2.4. Again, a fluctuating 3D density field should be provided at target redshifts and the uniform Eulerian grid is used, while any quantity with a prime symbol denotes a value related to the mock data.

(i) Set \( \Delta z \) of the density field identical to \( \Delta z \) of the N-body simulation that were used to set parameters in \( \S2.4 \).

(ii) At starting redshift, which should also be identical to that of the N-body simulation, apply the scheme for instantaneous bias (\( \S2.3 \)) but using \( f_{x,i}(\delta) \) instead of \( P_{i}(z) \) to choose the cells.

(iii) Presume that mock haloes were generated at \( z_{\text{prev}} \). Among the cells of given \( x' = x_{\text{prev}} > 0 \) at \( z_{\text{prev}} \), randomly choose a fraction \( P_{0}(z|x_{\text{prev}},+) \) of these cells that will become empty at \( z \), with the "conditional de-occupation probability"
\[
P_{0}(z|x_{\text{prev}},+) = \frac{N_{0}(z|x_{\text{prev}},+)}{N_{0}(z|x_{\text{prev}},+) + N_{i}(z|x_{\text{prev}},+)}
\]

and let the remaining cells host haloes again at \( z \). The number of these empty cells at \( z \) given they were non-empty at \( z_{\text{prev}} \) chosen this way, \( N_{0}(z|x_{\text{prev}},+) \), may differ from \( N_{0}(z|x_{\text{prev}},+) \) in general, so similarly, \( N_{i}(z|x_{\text{prev}},+) \), may also differ from \( N_{i}(z|x_{\text{prev}},+) \). Let \( \text{Group}(++) \) denote the group of these cells which will still host haloes.

(iv) Get the total number of cells in \( \text{Group}(++) \) from step (iii), \( N_{i}(z) = \sum \text{bin of } x_{\text{prev}} N_{i}(z|x_{\text{prev}},+) \).

(v) Exclude \( \text{Group}(++) \) from the whole set of grid cells at \( z \). Let \( \text{Group}(0) \) denote this group of cells. Note that \( \text{Group}(0) \) also includes cells that have been de-occupied of halos at this redshift.

(vi) Obtain \( N_{i}(z) \) using Equation 5 of \( \S2.3 \).

(vii) Inside \( \text{Group}(0) \), try selecting \( N_{i}(z) - N_{i}(z|+) \) cells through the following procedure. For each and every cell inside \( \text{Group}(0) \), identify \( f_{x,i}(\delta) \) as the probability for the cell to host haloes, where \( \delta \) is the average overdensity of the cell over \( \Delta z \). Perform Monte Carlo sampling cell by cell to mark non-empty cells, and count their number \( N_{i}(A|0) \). Check if \( N_{i}(A|0) \) is within preset tolerance of the target number \( N_{i}(z) - N_{i}(z|+) \). If not, then iterate the Monte Carlo procedure until convergence. Let \( \text{Group}(++|0) \) denote the resulting group of non-empty cells.

(viii) Finally, apply steps (iii) and (iv) in \( \S2.3 \) on all cells of both \( \text{Group}(++) \) and \( \text{Group}(+|0) \).

(ix) Steps (iii) \( \text{--} \) (viii) are done over all redshifts, taking the results from step (ii) as the first case of \( z_{\text{prev}} \).

We note that the target number of non-empty cells at \( z \) is \( N_{i}(z) \) (step vi) is also the number of non-empty cells in the case of instantaneous bias following Equation 3. This is because the temporal bias prescription should of course satisfy the instantaneous statistics at the least. We also note that the smaller \( x_{\text{prev}} \) is, the larger \( P_{0}(z|x_{\text{prev}},+) \) becomes, implying that cells containing a small number or mass of haloes are relatively likely to become devoid of haloes in the near future.

### 3 RESULTS

Based on the methodology presented in \( \S2 \) we can create mock realizations of halo spatial distributions based on an input cosmological density field for a given spatial resolution (cell size) and simulation volume. Our immediate aim and first application for this method is to create such mocks as input for large-volume radiative
Figure 5. Number of MHs, $N_{5.8}$, per cell vs cell overdensity $\delta$ at $z = 17.215$ (upper panel) and $z = 10.110$ (lower panel) for 6.3 Mpc/h box and $14^3$ grid (cell size $450 \, h^{-1} \, \text{kpc}$). Shown are the N-body halo data (left panels), the instantaneous mock halo (middle panels), and temporal mock halo (right panels).

Figure 6. Same as Fig. 5 but for $44^3$ grid (cell size $143 \, h^{-1} \, \text{kpc}$).
transfer simulations of cosmic reionization for cases where low-mass galaxies driving reionization cannot be resolved numerically. This is discussed in §3.2 below.

However, before discussing the large-scale mocks in §3.2, we first demonstrate in §3.1 our methodology on the density fields derived from the same high-resolution N-body simulations that provided the fitting parameters in the first place, both with and without the temporal bias. Since in this case we directly resolve the low-mass haloes of interest, we can evaluate the fidelity of our mocks against the actual known halo numbers and spatial distribution.

Furthermore, the direct comparison of the cases with and without temporal bias helps us understand the importance of its inclusion in modelling the stochasticity. We start sampling the data from $z = 30$, but only start implementing the stochasticity from $z \leq 25$ to ensure that there is sufficient data to determine the parameters that are truly reflective of the distribution.

### 3.1 Testing the method

In Figures 5 and 6, we show the relation between the number of MHs per cell, $N_{3,h}$, and the density of a cell, $\delta$, at $z = 17.215$ (upper panels) and $z = 10.110$ (lower panels) based on data from our 6.3 Mpc$^{-1}$ box simulation with cell sizes $450 h^{-1}$kpc and $143 h^{-1}$kpc, respectively. Shown are the N-body simulation data (left panels), the instantaneous mock haloes (middle panels), and temporal mock haloes (right panels). The colours indicate the density of haloes and the solid black lines correspond to the mean (deterministic) bias relation based on Ahn et al. (2015). The particular redshifts shown are chosen as representative of the early and late stages of the epoch during which the MHs are expected to be an important component of and a regulating factor to early star formation (Ahn et al. 2012). For consistency, we will use the same colour scheme throughout this paper to represent the different types of data.

Similarly, Figures 7 and 8 show plots of the LMACH collapsed fraction, $f_{\text{coll,3.9}}$, vs. $\delta$ at redshift $z = 12.603$ (upper panels) and $z = 7.570$ (lower panels). Data is based on the 114 Mpc$^{-1}$ volume with $64^3$ and $128^3$ grid cells per each dimension (cell sizes of $1.781 h^{-1}$Mpc and $0.891 h^{-1}$Mpc, respectively). We again show the N-body simulation data (left panels), the instantaneous mock haloes (middle panels), and temporal mock haloes (right panels). The illustrative redshifts shown roughly correspond to the beginning and the peak of the reionization process in certain classes of EoR models.

Figures 5 and 6 show that the relation between $N_{3,h}$ and $\delta$, including stochastically, closely replicates that of N-body MHs once the bias is sampled from the lognormal distribution described in the previous section. This is true for both the instantaneous and the temporal case with only minor differences. In all cases the agreement with the mean bias trend (black curve) is excellent.

The stochasticities in the mock halo data have a good agreement with those of the N-body halo data, but with some modest difference in the low-$\delta$ regime as seen in Figures 7 and 8. We attribute this difference to the Poisson noise and our specific scheme of smoothing $\mu(\delta)$ in the low-$\delta$ regime, whose empirical values have a rather strong fluctuation for varying $\delta$. The Poisson noise in these cells having a small number of haloes seems to bias $\mu(\delta)$ toward relatively large values, and as a result a smooth fitting function of $\mu(\delta)$ we tend to push the overall dispersion of mock data points upward in Figures 7 and 8. Nevertheless, these cells take only a minor fraction and thus the overall agreement seems excellent.

Credibility of the generated mock halo catalogues can be tested in terms of statistical measures, and we investigate (1) overall normalisations (either number of haloes or total collapsed fraction) for the deterministic bias, (2) the temporal correlation coefficient for the cell-wise evolution, and (3) the power spectrum for the spatial clustering of haloes.

We show the overall normalisations and their evolution with redshift in Figure 2. In all cases, difference between the mock data and the N-body halo data are modest, within $\sim 15\%$, and often substantially better, particularly at lower redshifts. The mocks with temporal bias consistently match the simulations more closely than those with instantaneous bias, within $\sim 2%$ below $z = 10$ and otherwise within $5\%$ or less except for the highest redshifts, where the rarity of haloes make the correlation with the underlying density field weak. The mocks follow the N-body halo data better for the lower-resolution grids for each volume, and the temporal bias yields little difference for the number of MHs in that case. The instantaneous bias is considerably worse than the temporal bias in normalisations by up to a factor of 2-4, especially for higher grid resolutions.

Next we compare the Pearson correlation coefficient between consecutive time-slices of the simulation data and the respective generated stochastic realisations. The correlation coefficient is as usual defined as

\[
r_{X,Y} = \frac{\text{cov}(X,Y)}{\sigma_X \sigma_Y}
\]

where $X$ and $Y$ are the fields being correlated, $\text{cov}$ is the covariance matrix, and $\sigma_X$ and $\sigma_Y$ are the standard deviations of $X$ and $Y$, respectively. The value of $r_{X,Y}$ is 1 if $X$ and $Y$ are completely correlated, 0 if they are uncorrelated and $-1$ if they are completely anti-correlated. Results are shown in Fig. 10. For the simulation data, the late-time correlation is fairly tight in all cases. At early times the correlation coefficient is considerably lower than unity due to the increasing rarity of haloes, and the related significant Poisson noise. At that epoch, the halo population, which form stochastically in high-density regions, grows exponentially, thereby resulting in the lower correlation with the previous time-slice. This effect is larger for more massive haloes, as could be expected, as they are more strongly biased.

Randomly-sampled mocks without the temporal correlation bias significantly underestimate the correlations compared to the simulation data, and yield almost no correlation for LMACHs at high redshift (independent of the grid resolution). As could be expected, in all cases the agreement is significantly improved by including the temporal bias, although the correlation remains somewhat lower than the simulated one. This agreement could potentially be improved further by modifying our model to take into account the tight empirical time correlation found in the simulation data, but at the expense of a more complex model.

Finally, we consider the halo spatial clustering in each case, as represented by the spherically-averaged power spectrum $P(k)$ which is shown in Figures 11 for $z = 12.903$ and 12 for $z = 8.283$. In these figures, the lower panels show $P(k)$, and upper panels show the percentage differences between the mocks and the N-body halo data, for all cases as labelled. The halo clustering of the mock realizations with temporal bias generally matches the simulated one very well, within a few to 10 per cent. The only exceptions are at small scales ($k \gtrsim 10 h^{-1}$Mpc$^{-1}$) and at very high redshift ($z \geq 20$ for MHs and $z > 15$ for LMACHs), due to the aforementioned rarity of haloes at high redshift and the consequent Poisson noise, in which cases the discrepancy can reach $\sim 50\%$. The agreement
Figure 7. LMACHs collapsed fraction, $f_{\text{coll,8.9}}$, per cell vs cell overdensity $\delta$ at $z = 12.603$ (upper panel) and $z = 7.570$ (lower panel) for 114 Mpc h$^{-1}$ box and 64$^3$ grid (cell size 1.781 h$^{-1}$ Mpc). Shown are the N-body halo data (left panels), the instantaneous mock haloes (middle), and the temporal mock haloes (right).

Figure 8. Same as in Fig. 7 but for 128$^3$ grid (cell size 0.891 Mpc h$^{-1}$).
Figure 9. Evolution of the absolute value of the percentage difference between the N-body data and the total number of MHs, \( N_{\text{grid}} \), (upper panels) and the LMACH collapsed fraction, \( f_{\text{coll,8.9}} \), summed over the grid (lower panels) vs. redshift, \( z \), for the 6.3 Mpc \( h^{-1} \) and 114 Mpc \( h^{-1} \) box respectively. Plotted are the difference between the N-body data and the instantaneous mock haloes (triangles) and the temporal mock haloes (squares) for the \( 14^3 \), \( 44^3 \), \( 128^3 \) and \( 64^3 \) grid, as labelled.

Figure 10. Pearson correlation coefficient between consecutive time slices vs redshift \( z \) for: (top) 6.3 Mpc \( h^{-1} \) box with (left) grids of \( 14^3 \), and (right) \( 44^3 \), for the simulation data, and realisations of instantaneous mock and temporal mock haloes as labelled; (bottom) same as the top panels, but for 114 Mpc \( h^{-1} \) box with (left) grids of \( 64^3 \) and (right) \( 128^3 \).
is considerably worse in general when the temporal bias is not included, with typical differences of $\sim$20-50%. The only exception is the MH numbers in the low-resolution grid, where the agreement becomes better, indicating that the halo clustering is insensitive to the temporal bias in this limited case.

3.2 Sub-grid Modelling of Temporal Stochasticity in Multi-Scale reionization

We implement our fiducial method, namely assigning stochasticity sampled from a log-normal distribution with temporal correlations ($\S$2.5) in generating mock halo catalogues on a $300^3$-grid density field in a large volume of 500 Mpc $h^{-1}$ per side simulated with the CubeP$^3$M code (Harnois-Dérap et al. 2013). We have previously shown that a 500 Mpc $h^{-1}$ volume is sufficiently large to obtain very reliable statistics in various physical properties of EoR (Iliev et al. 2014), and a $300^3$-grid is optimal for simulating patchy reionization with reasonable computational resources. The size of the grid cell is also chosen to match the cell size of the $64^3$-grid in 114 Mpc $h^{-1}$-box we used above for the LMACHs collapsed fraction. This approach enables populating such a large volume, which is usually limited in realizing small-mass haloes due to numerical resolution limit, with LMACHs very reliably as shown in the previous sections.

In Figure 13 we show the modelled stochasticity with temporal correlations of the $f_{\text{coll,9.9}}$ over a range of redshifts, repre-
The figure shows the LMACH collapsed fraction $f_{\text{coll}, 8.9}$ per cell with respect to $\delta$ at $z = 17.848, 10.110$ and $7.570$ (left to right). The top panels correspond to the actual N-body simulation data from our $114 \ h^{-1} \text{Mpc}$ box on a $64^3$ grid, while the bottom panels show the generated mock haloes with temporal bias for $500 \ h^{-1} \text{Mpc}$ box on a $300^3$ grid. The color map shows the normalized density of data points in discretised bins of $\log_{10}(1+\delta)$ and $\log_{10} f_{\text{coll}, 8.9}$.

representative of the early, middle and late phases of reionization, respectively. The overall characteristics of the mock data are in good agreement with those of the N-body data, as intended. While not clearly shown in Figure[13] the large volume contains cells with $\delta$'s in the more extended tail ends of the PDF than the small box. We note that it is again difficult to simulate the apparent dip (dubbed as “indentation” in §3.1) shown in the N-body data with this prescription.

We compare the power spectra generated from the mock vs. N-body data (Figure[14]) to check the reliability of our approach for future reionization simulations. For the range of redshifts shown and wavenumbers $k \lesssim 1 \ h^{-1} \text{Mpc}$, the error is no larger than $\sim 10 - 30\%$. At the same wavenumber range, $P(k)$ of the mock data has a trend to be larger at high $z$ but gradually shifting to be smaller at low $z$ than that of the N-body data. Disagreement always exists for $k$’s around the Nyquist value, whose impact on reionization requires further investigation. However, we expect that the influence of this will be minor if one is only interested in relatively large-scale ($k \lesssim 1 \ h^{-1} \text{Mpc}$) phenomena.

4 SUMMARY AND DISCUSSION

In this work we present a novel scheme developed for creating realistic sub-resolution low-mass halo populations in large-scale N-body simulation volumes. The mock haloes produced by our method reproduce the correct average local numbers or collapsed fraction of the unresolved haloes very well, down to the smallest halo masses, as well as their spatial clustering and local population evolution. This new halo bias prescription can be used as a sub-grid model for studies of structure formation for a range of applications that would otherwise be limited in dynamic range, thereby enabling studies of the small-scale structures and their impact within large, cosmological volumes.

We achieve this by including not only the deterministic bias as a function of the local density environment (Ahn et al. 2015), but also an additional stochastic bias, which accounts for its other dependencies, which yields a more natural representation of the universe. Using very high-resolution N-body data, we have compared two distinct methods for realising this stochastic bias: (1) stochasticity reconstruction based on the current cell overdensity $\delta$ only and (2) one based on both $\delta$ and the past history of the halo population in that locality. We found the latter method, which we dubbed “temporal bias”, is superior to the former. Including the temporal bias yields mock halo catalogues with significantly better statistical properties than without it in terms of the local halo population evolution as well as the power spectrum $P(k)$ of the 3D halo-number field, both compared to the high-resolution N-body data where the relevant halo range is resolved.

There are a number of possible applications for our method. A direct application of this temporal bias is in simulations of cosmic reionization. They require very large dynamic range, since the H II region expansion is driven by low-mass galaxies, while proper statistics of the patchiness demands very large volumes to be followed (Iliev et al. 2014). Importantly, in this case, the evolution is cumulative and depends on the temporal evolution of structure for-
Stochastic bias

The lower panels show the $P(k)$ and the upper panels show the percentage of absolute difference of the $P(k)$ of $f_{\text{col,11.8:9}}$ at the indicated redshift between the N-body (114 Mpc $h^{-1}$, 64$^3$ grid, black dotted in lower panel) and mock data (500 Mpc $h^{-1}$, 300$^3$ grid; magenta dashed).

Figure 14. The lower panels show the $P(k)$ and the upper panels show the percentage of absolute difference of the $P(k)$ of $f_{\text{col,11.8:9}}$ at the indicated redshift between the N-body (114 Mpc $h^{-1}$, 64$^3$ grid, black dotted in lower panel) and mock data (500 Mpc $h^{-1}$, 300$^3$ grid; magenta dashed).

This study shows that the temporal correlation in stochasticity plays an important role in shaping the statistical properties of cosmological haloes. This is proven by the fact that the temporal bias (method 2 above) generates halo catalogues in much better agreement with the N-body halo data than method (1) in terms of $P(k)$ and cross-correlations. This also implies that even when one is to generate halo catalogues for the study of galaxy surveys, which seemingly requires an instantaneous halo bias, this temporal bias scheme can work as a very reliable solution. Further study along this line is warranted.

There are some caveats and room for improvement in our methodology. In our current approach, the temporal bias is based on the complete history of a given Eulerian cell, while in reality the stochasticity should only depend on the past history. Furthermore, advection of matter to and from neighbouring cells means that the Eulerian cell density does not contain the full information on the matter field evolution. For a better temporal bias prescription, one may instead adopt a scheme that takes a limited lookback-time history of an Eulerian cell to mitigate these two problems. This requires further investigation, which we will address in the near future. While our approach and results are general, the specific parameterisation of the temporal bias is based on empirical fits based on a specific structure-formation simulation. Therefore, if one were to apply this to a universe described by a different set of cosmological parameters, our approach would require a new small-box, high-resolution simulation resolving haloes of our interest. It would be preferable to find a more analytical scheme that allows deterministic temporal stochasticity in halo bias that could be easily re-calculated.

Regardless of this, our scheme provides significant improvement over existing methods, yielding a more accurate mock halo catalogues at high redshift, which will be very helpful in improved descriptions of the cosmic reionization process and interpretation of high-redshift observations. Using this approach will yield better answers on how much impact low-mass haloes, which have usually been neglected or treated with crude approximations, have on structure formation at high redshift and the history of cosmic reionization.

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