The early growth of supermassive black holes in cosmological hydrodynamic simulations with constrained Gaussian realizations

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ABSTRACT
We examine the early growth of supermassive black holes (SMBHs) using constrained realization cosmological simulations. We reconstruct the initial conditions (ICs) in the large volume BlueTides (BT) hydrodynamic simulation and run them to \( z = 6 \). We compare the constrained simulations with BT to test the accuracy of this method for reproducing the first quasars and their environments. At the high redshifts of interest, non-linear mode coupling on the scale of even small simulation box sizes is not present. This allows our re-simulations in a volume of \((15 h^{-1} \text{Mpc})^3\) to correctly recover the evolution of large-scale structure, and the stellar and BH mass functions in the vicinity of a \( \sim 10^{12} M_\odot \) halo which we identified in BT at \( z \sim 7 \) to be hosting a \( \sim 10^9 M_\odot \) SMBH. Our re-simulations confirm that only with the lowest tidal field, high-density peaks in the ICs can induce the fastest BH growth required to explain the \( z > 6 \) quasars. We carry out three simulations with the same ICs but different BH seed masses of \( 5 \times 10^3 \), \( 5 \times 10^4 \), and \( 5 \times 10^5 h^{-1} M_\odot \) (the one used in BT) while keeping the halo to BH mass ratio fixed. We find that the BH mass converges to \( \sim 10^9 M_\odot \) by \( z = 6 \) regardless of the seeding procedure while their early growth histories at \( z > 10 \) differ. The simulations with small BH seeds lead to the emergence of a large population of BHs which merge frequently at early times (four BH mergers, with masses \( 10^4 \sim 10^6 M_\odot \) at \( z \gtrsim 12 \)). This is also accompanied by a few major BH mergers at \( z \lesssim 8 \) for intermediate and small BH seeds while there are no mergers in the large BH seed simulation. The increased BH merger rate for low mass BH seeds provides an exciting prospect for discriminating BH formation mechanisms with the advent of multi-messenger astrophysics and next-generation GW facilities.

Key words: black hole physics – methods: numerical – galaxies: high-redshift

1 INTRODUCTION
The formation of the first supermassive black holes (SMBHs) remains elusive in our standard paradigm of structure formation. SMBHs, as massive as those in galaxies today, are known to exist in the early universe, even up to \( z \sim 7.5 \). Luminous, extremely rare, quasars at \( z \sim 6 \) were initially discovered in the Sloan Digital Sky Survey (Fan et al. 2006; Jiang et al. 2009) and, until recently, the highest redshift quasar known (Wu et al. 2015) at \( z = 7.09 \) (Mortlock et al. 2011) has been surpassed by the discovery of a bright quasar at \( z = 7.54 \) (Bañados et al. 2018), which is currently the record holder for known high redshift quasars. A further sample of two \( z > 7 \) has also been recently discovered (Yang et al. 2018). The presence of luminous quasars observed within the first billion years of the Universe highlights that the BH seeds for the massive BH population must have assembled at the cosmic dawn, concurrently with the time of the formation of the first stars or galaxies.

However, the precise SMBH seed formation mechanism remains unknown, nor is it clear that there is only one seed formation channel at play over the entire SMBH seed mass spectrum of models. The current scenarios suggest that seed BHs are (a) remnants of the first generation of stars (PopIII) (e.g. Abel et al. 2002; Madau & Rees 2001; Johnson & Bromm 2007) or (b) direct gas collapse within the first massive halos (e.g. Lodato & Natarajan 2006; Begelman et al. 2006; Regan & Haehnelt 2009; Ferrara et al. 2014; Latif et al. 2008).
or (c) runaway collapse of dense nuclear star clusters (e.g. Begelman & Rees 1978; Devecchi & Volonteri 2009; Yajima & Khochfar 2016; Katz et al. 2015). The seed BHs then range in mass from a few hundred to a few $10^5 M_\odot$ for (b) and (c).

In large volume cosmological simulations, a common and widely used sub-grid model for SMBHs and active galactic nuclei (AGN) feedback has been proposed in Di Matteo et al. (2005). Since the SMBH seed formation processes (direct collapse, or stellar collapse; (see Regan & Haehnelt 2009, for a review)) are not resolved by cosmological simulations, it is assumed that every halo above a certain threshold mass hosts a central BH seed so that BHs are always well resolved. Halos are selected for seeding by regularly running the ‘Friends-of-Friends’ (FoF) halo finder on the dark matter distribution. The mass for the BH seed ($M_{\text{seed}}^*$) and that of the halo ($M_{\text{halo}}^\text{fof}$) that is seeded are parameters in the simulations. Although this is an ad-hoc seeding procedure, the initial seed BH mass subsequently grows in these simulations via mergers and accretion. Many simulations have adopted this or a similar scenario and gotten good agreements with observations such as ILLUSTRIS simulation (Vogelsberger et al. 2014), the Evolution and Assembly of Galaxies and their Environment (EAGLE) suite of SPH simulation (Schaye et al. 2015), the MASSIVEBLACK II simulation (Khandai et al. 2015), and the BLUETIDES simulation (Feng et al. 2016a).

Taking BLUETIDES, a large-scale and high-resolution cosmological hydrodynamic simulation with $2 \times 7040^3$ particles in a box of $400 h^{-1}$ Mpc on a side, as an example, SMBHs are modeled as the follows. For each FoF halo with a mass above $M_{\text{halo}}^\text{fof} = 5 \times 10^{10} h^{-1} M_\odot$, a SMBH is seeded with an initial seed mass $M_{\text{seed}}^* = 5 \times 10^5 h^{-1} M_\odot$ at the position of the local minimum potential if there is no SMBH in that halo. After being seeded, gas accretion proceeds according to Hoyle & Lyttleton (1939); Bondi & Hoyle (1944); Bondi (1952) while the BH accretion rate is limited to three times of the Eddington rate. When SMBHs are accreting, we assume that some fraction of the radiated luminosity can couple thermally and isotropically to surrounding gas in the form of feedback energy (Springel 2005).

Adopting this SMBH model with other sub-grid physics for the galaxy formation modeling, BLUETIDES simulation has predicted various quantities in good agreements with current observational constraints in the high-$z$ universe such as UV luminosity functions (Feng et al. 2016a; Waters et al. 2016a,b; Wilkins et al. 2017), the first galaxies and the most massive quasars (Feng et al. 2015; Di Matteo et al. 2017; Tenneti et al. 2018), the Lyman continuum photon production efficiency (Wilkins et al. 2016, 2017), galaxy stellar mass functions (Wilkins et al. 2018), angular clustering amplitude (Bhownick et al. 2018), BH-galaxy scaling relations (Huang et al. 2018), and gas outflows from the $z = 7.54$ quasar (Ni et al. 2018). Important for our work here, BLUETIDES, with its large volume and appropriate resolution, is currently the only cosmological hydrodynamical simulation that makes direct contact with the rare, first quasar population at $z > 7$.

However, an essential question for the SMBH sub-grid model is how different parameters (e.g. $M_{\text{seed}}^*$ or $M_{\text{halo}}^\text{fof}$) may affect the SMBH growth and local environment in cosmological simulations. Changing seed BH mass and re-running such a large simulation is completely prohibitive because that is too computationally expensive.

A common approach to reducing the demand on the computational resource is to run a “zoom-in re-simulation” with a higher resolution or different physical parameters from a certain region selected from a large volume lower resolution simulation. This allows people to focus on a specific environment numerically and has been applied to study SMBHs in simulations for various purposes (e.g. Li et al. 2007; Sijacki et al. 2009; Hopkins & Quataert 2010; Bournaud et al. 2011; Romano-Díaz et al. 2011; Bellovary et al. 2013; Dubois et al. 2013; Anglés-Alcázar et al. 2014; Costa et al. 2014; Feng et al. 2014). Other than the zoom-in re-simulation approach, here, we combine the technique of constrained Gaussian realizations (Hoffman & Ribak 1991; van de Weygaert & Bertschinger 1996, see also Section 2) and cosmological hydrodynamic simulations to study the growth of SMBHs. With the constrained Gaussian realization, we are able to constrain the initial density field by adding a desirable height of a density peak when generating the initial condition such that a more massive halo can form at later times in a smaller box compared with those large-volume (~ Gpc) cosmological simulations. For instance, we are able to grow a halo with a mass $\sim 10^{12} M_\odot$ in a box with $15 h^{-1}$ Mpc on a side at $z = 8$, whose mass is similar to the one hosting the most massive BH in BLUETIDES simulation ($400 h^{-1}$ Mpc on a side) under the same resolution, reducing the computational demand by a factor of $(400/15)^3 \sim 20000$.

This approach is a more general way to study the growth of SMBH compared to the zoom-in re-simulation method because the goal of the latter is to study a particular object/region exactly (for example, a particular halo). However, our approach is aiming to study an environment by creating one or more different realizations but with similar properties such as halo mass or tidal field to the object/region of our interest.

As we shall further demonstrate, besides the density constraint, we still need another condition to help us study SMBHs in cosmological simulations because SMBHs are much rarer than massive halos. For example, there is only one SMBH with a mass above $10^8 M_\odot$ in a halo with a mass $\sim 10^{12} M_\odot$ while there are $> 50$ halos more massive than that halo at $z = 8$. A possible quantity is the tidal field: it has been proposed that a lower tidal field is helpful for an SMBH to seed and to grow (Di Matteo et al. 2017). As a consequence, we also choose the realization with a lower tidal field around the local environment where the halo forms, which indeed helps more massive SMBHs grow in simulations (see Section 3.2).

After significantly decreasing the demand on the computational resource with the constrained Gaussian realizations and a lower tidal field realization, we are finally able to examine how sensitive the SMBH growth is to the BH seed mass in the sub-grid model by running multiple cosmological simulations. According to different hypotheses of BH formation scenario, the BH seed mass has been suggested from $10^2$ to $10^6 h^{-1} M_\odot$ (Haehnelt & Rees 1993; Loeb & Rasio 1994; Eisenstein & Loeb 1995; Bromm & Loeb 2003; Koushiappas et al. 2004; Begelman et al. 2006; Lodato & Natarajan 2006; Zhang et al. 2008; Volonteri 2010; Latif et al. 2013; Schleicher et al. 2013; Ferrara et al. 2014) so we study three
different seed masses: $5 \times 10^3$, $5 \times 10^4$, and $5 \times 10^5 h^{-1} M_\odot$ in this paper.

The paper is organized as follows. In Section 2, we describe how we use FastPM to generate initial conditions with constrained Gaussian realizations. In Section 3, we describe MP-Gadget (the source code of simulation) and how we determine simulation setups such as the height of the density peak and the effect of the tidal field. In Section 4, we show the main result of SMBHs in simulations with different BH seed masses. In Section 5, we conclude the paper.

2 INITIAL CONDITIONS

We use FastPM—a highly scalable approximated particle mesh (PM) N-body solver, which implements the PM scheme enforcing correct linear displacement evolution via modified kick and drift factors—to generate initial conditions for our simulations. More detail can be found in Feng et al. (2016b) and https://github.com/rainwoodman/fastpm.

We choose FastPM because it is able to generate initial density fields with constrained Gaussian realizations (Hoffman & Ribak 1991; van de Weygaert & Bertschinger 1996). With constrained density peaks in the initial conditions, heavier halos are able to form at later times in smaller simulation boxes, allowing us to study the early growth of SMBHs in these regions.

In FastPM, the constrained Gaussian density field is encoded in the form of

$$\delta(x) = \bar{\delta}(x) + \bar{\xi}(x) \bar{\xi}'(c_j - \bar{c_j})$$

(1)

where $\delta(x)$ is the constrained density field, $\bar{\delta}(x)$ is the unconstrained density field, $c_j$ and $\bar{c_j}$ are the density constraint and the unconstrained value at $\bar{c_j}$ respectively, $\bar{\xi}(x) = \langle \delta(x)c_j \rangle$, and $\bar{\xi}'(c_j) = \langle \bar{\xi}(x)c_j \rangle$.

In Figure 1, we illustrate the density fields in a given realization of initial conditions with and without (the right and left panels respectively) a constrained density peak in the dense region (near the bottom-left corner of the image) of a box with a side of $15 h^{-1}$ Mpc. As expected, we find that the density indeed increases in the region where we put the constraint (near the bottom-left corner) while the overall pattern of the density field remains the same.

Since this work is the first one to use FastPM to generate a constrained initial condition for cosmological simulations, we examine the difference of the power spectrum $(\Delta P(k) = (P(k) - P_{no}(k))/P_{no}(k))$ where $P_{no}(k)$ is $P(k)$ without any constraints) with different density constraints in Figure 2. In the left panel, we find that $\Delta P(k)$ is higher as the height of the constrained peak is higher at smaller $k$ while the difference at other scales is less than 3%.

To illustrate the differences in $P(k)$ at low $k$, we look into the relation between $\Delta P(k) = 0.5 h^3$ Mpc) $(\Delta P(k)$ is almost constant as $k < 0.6 h$/Mpc) and the height of the constrained peak $(\delta_{peak})$ in the right panel of Figure 2. We find that $\Delta P(k)$ is perfectly fit by $\Delta P(k) = 0.5 h^3$ Mpc) = $a_0^2 + b_{peak} + c$ where $a_0 = (2.7 \times 10^{-3}, 2.7 \times 10^{-3}, 5.3 \times 10^{-3})$. A quadratic relation is expected because the change of $P(k)$ can be derived from Equation 1 in $k$-space.

The reason we need to employ a constrained Gaussian realization of the initial conditions is of course due to the fact that the first quasars are extremely rare and hence the massive halos hosting these first SMBHs also has to be commensurately rare. To study such rare early objects, one needs extremely large volume simulations (such as BlueTides). For instance, there is only one SMBH with a mass above $10^8 M_\odot$ in a halo with a mass of $\sim 10^{13} M_\odot$ at $z = 8$ in BlueTides simulation ($400 h^{-1}$ Mpc on a side of cube). With the knowledge from the uniform cosmological hydrodynamic BlueTides volume we can assess directly the height of the constrained density peak (and other properties) and further proceed the study of the early growth of SMBHs by 'reproducing' it in our constrained realizations.

In summary, we first reconstruct the initial conditions based on our reference BlueTides simulation and then run the reconstructed initial conditions forward in time until $z = 6$. In the next section, we then compare the resulting constrained simulations with the original simulation at $z = 8$ to test the accuracy of this method for the problem at hand.

3 SIMULATION SETUP

We use MP-Gadget—a massively parallel cosmological smoothed particle hydrodynamic (SPH) simulation software—to run all the simulations throughout this paper. Its hydrodynamics solver adopts the new pressure-entropy formulation of SPH (Hopkins 2013). Main sub-grid models are (1) star formation based on a multiphase star formation model (Springel & Hernquist 2003) with modifications following Vogelsberger et al. (2013), (2) gas cooling through radiative processes (Katz et al. 1996) and metal cooling (Vogelsberger et al. 2014), (3) formation of molecular hydrogen and its effects on star formation (Krumholz & Gnedin 2011), (4) type II supernovae wind feedback (Nelson et al. 2015), (5) a model of ‘patchy’ reionization (Battaglia et al. 2013) yielding a mean reionization redshift $z \sim 10$ (Hinshaw et al. 2013), and incorporating the UV background estimated by Faucher-Giguère et al. (2009), and (6) BH growth and AGN feedback (Di Matteo et al. 2005). More detail about MP-Gadget can be found in Feng et al. (2016a) and https://github.com/bluetides-project/MP-Gadget.

Throughout the paper, we adopt the cosmological parameters based on the Nine-Year Wilkinson Microwave Anisotropy Probe Observations (Hinshaw et al. 2013) (see Table 1). Note that all our simulations have the same cosmology and resolution as BlueTides does (see Table 1) also which we need to use to assess the validity of our new constrained simulations. There are two box sizes that we use for our simulations: $10$ and $15 h^{-1}$ Mpc on a side of the cubes. Each of them contains $2 \times 176^3$ and $2 \times 264^3$ particles with a gravitational smoothing length $\epsilon = 1.5 h^{-1}$ kpc (same as in BlueTides). All simulations are run from $z = 99$ to $z = 6$ as we are primarily interested in SMBH seeds and early growth at high-$z$.

| $h$ | $\Omega_{\text{matter}}$ | $\Omega_{DM}$ | $M_{\odot}$ |
|-----|-------------------------|--------------|-----------|
| 0.697 | 0.2814 | 1.2 $\times 10^7 h^{-1} M_{\odot}$ |

| $\sigma_8$ | $\Omega_{\text{baryon}}$ | $M_{\text{gas}}$ | $M_{\odot}$ |
|------------|--------------------------|------------------|-----------|
| 0.820 | 0.0464 | 2.36 $\times 10^6 h^{-1} M_{\odot}$ |

| $n_s$ | $\Omega_{\Lambda}$ | $\epsilon$ | $1.5 h^{-1}$ kpc |
|--------|---------------------|----------|-------------------|
| 0.971 | 0.7186 | 1.5 $h^{-1}$ kpc |
Figure 1. Slices of density fields of the initial conditions with the same realization number. Left: without any constraints. Right: with a constrained density peak at the densest region of the original field (near the bottom-left corner). The dimensions are both 15Mpc/h \times 15Mpc/h with a thickness of 1Mpc/h.

Figure 2. Left: the difference of the power spectrums: \( \Delta P(k) = (P(k) - P_{no}(k))/P_{no}(k) \) where \( P_{no}(k) \) is \( P(k) \) without any constraints with different density constraints. Right: the relation between \( \Delta P(k = 0.5h/Mpc) \) and the constrained density peaks \( \delta_{peak} \). The black curve is the quadratic best fit.

3.1 Box size of simulations

Using the technique of constrained Gaussian realization, we are able to grow a more massive halo by adjusting the constrained density peak in the initial density field, allowing us to study rare objects (heavier halos and SMBHs) within smaller boxes (compared to large volume cosmological simulations). In order to assess if our box sizes are sufficient to follow the growth of the SMBHs, we need for the problem at hand we test against the growth histories of the halo we are trying to reproduce in BlueTides.

First, we check how far the farthest particle in the halo with the most massive BH in BlueTides has traveled from \( z = 99 \) to \( z = 8 \), finding that it was \( \sim 4.7h^{-1}\text{Mpc} \) away at \( z = 99 \) from where the SMBH is at \( z = 8 \). Given this, our two chosen box sizes: 10 and 15h^{-1}\text{Mpc} on a side should be sufficiently large enough to produce a converged assembly history.

To check this more quantitatively by directly using the halo and galaxy populations we have, Figure 3 shows the halo (\( \Phi_{\text{halo}} \)) and stellar mass functions (\( \Phi_{\star} \)) in the left and right panels respectively at \( z = 6, 8, \) and 10, compared with BlueTides (the black dash curves). As expected, there is one particular object in the very massive end of these functions since we have constrained a density peak to grow a heavier object. Aside this massive object, both mass functions are consistent with the ones from BlueTides at \( z = 8 \) and 10, indicating that the two box sizes are likely appropriately capturing the growth of the halo and stellar mass function as (statistically) expected.

We then look into the growth history of the most massive BHs and their hosts in the two simulations in Figure 4. In the left panel, we show the evolution of halo mass \( M_{\text{halo}} \) and stellar mass \( M_{\star} \) in comparison with the ones in BlueTides. By constraining an appropriate density peak, we can get a halo hosting a galaxy with a similar mass to the one
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Figure 3. Halo mass functions ($\Phi_{\text{halo}}$) and stellar mass functions ($\Phi_\star$) (the left and the right panels respectively) of the simulations with box sizes $10$ and $15\,h^{-1}\text{Mpc}$ in comparison with the measurements from BlueTides at $z = 6$, $8$, and $10$.

Figure 4. Left: the growth history of halo ($M_{\text{halo}}$) and galaxy ($M_\star$) hosting the most massive BH in the simulations with box sizes $10$ and $15\,h^{-1}\text{Mpc}$. Right: the growth history of the most massive BH ($M_\bullet$) in each simulation. The grey dashed curves are the quantities of the most massive BH in BlueTides.

However, based on the growth history of the most massive BHs in the two simulations in the right panel of Figure 4, we can see the slightly different evolution after $z \sim 9$. That is, a more/less massive BH forms in a bigger/smaller box. More than that, the evolution of the SMBH in $15h^{-1}\text{Mpc}$ box shows better convergence with the one in BlueTides, resulting us to use $15h^{-1}\text{Mpc}$ boxes to conduct main simulations for the study of BH seed in Section 4. On the other hand, we still utilize the smaller box ($10h^{-1}\text{Mpc}$) to study the influence of tidal field on the growth of SMBHs in Section 3.2 since (i) it is still a valid simulation and (ii) it is less computationally expensive.

3.2 Tidal fields of SMBHs

While a highly biased region (as in our constrained simulations) is a necessary condition for growing a massive BH, it is not sufficient. We can inspect this directly in BlueTides, where for example we find that among the $50$ most massive halos (of mass similar or greater than the one hosting the most massive BH) only one of them has a BH more massive than $10^8M_\odot$. Indeed, as we shall show, not all of the constrained Gaussian realizations able to grow massive halos guarantees to also grow SMBHs in them.

Di Matteo et al. (2017) has identified that the local tidal field as the environmental property is the most strongly correlated to the growth of the first quasars. The tidal field is of course also directly related to the initial conditions in the density field. In these findings, the extreme early growth depends on the early interplay of high gas densities and the tidal field that shapes the mode of accretion in those halos.

The tidal field is characterized by the three eigenvalues ($t_1$, $t_2$, $t_3$) of the local tidal tensor $T_{ij} = S_{ij} - \frac{1}{3} S_{ii} S_{jj}$, where the strain tensor is the second derivative of the potential,
$S_{ij} = \nabla_i \nabla_j \phi$. According to Dalal et al. (2008), $S_{ij}$ is calculated in Fourier space as $\hat{S}_{ij} = \frac{k_i k_j}{k^2} \hat{\delta}$. The three eigenvalues are by definition $t_1 > t_2 > t_3$ and satisfy $t_1 + t_2 + t_3 = 0$ so that $t_1$ is always positive and $t_3$ is negative. Thus, the tidal field stretches material along $t_1$ and compresses material along $t_3$, where $(t_1, t_2, t_3)$ are the corresponding eigenvectors. Following the standard usage, we use $t_1$ as the indicator of the local tidal field strength.

In order to further evaluate (and confirm the results from BLUETIDES) the role of the tidal field in the growth of the first massive SMBHs, we perform three ($10h^{-1}\text{Mpc}$ on side) simulations with the same height of the density peak but with different realizations that give different tidal fields around the peak. We then measure $t_1$ and the mass of the most massive BHs in the three simulations in Figure 5 (the orange, blue, and green curves for low, medium, and high $t_1$ respectively). In the left panel, we show $t_1$ measured at different scales at $z = 6$ in the inner panel and the evolution of $t_1$ measured at $1h^{-1}\text{Mpc}$ in the outer panel. It indicates that the three BHs have different $t_1$ and that the one with a lower/medium/higher $t_1$ has been always lower/medium/higher across redshifts. In the right panel, we show the growth history of the most massive BHs, finding that the tidal field indeed affects the growth of the SMBH. That is, a SMBH can grow more/less massive when it is in a lower/higher $t_1$ surrounding environment (in particular, by $z = 6$, $M_\odot$ of the BHs can differ by a factor of 10).

By showing that a lower tidal field environment indeed helps a more massive growth of a SMBH, (i) we strengthen the findings from BLUETIDES (Di Matteo et al. 2017): the local tidal field of the environment is strongly correlated to the growth of the first quasars. (ii) We further have the random number of the realization that provides low $t_1$ after constraining the density field, which will be using for our main simulations in the following sections.

**4 SIMULATION SUITES**

**4.1 Different BH seed masses**

After combining the constrained Gaussian realization technique (Section 2) and a lower tidal field realization (Section 3), we have shown that our simulations are able to recreate an initial condition that grows a similar massive halo as well as the most massive BH in BLUETIDES. The density field for the initial condition for such a peak is shown in the right panel Figure 1.

As mentioned in Section 1, the goal of this paper is to study the effect of the choice of BH seed mass in simulations (a parameter in the SMBH sub-grid model) on the early growth of SMBHs. Using the same initial conditions, we carry out three simulations with different BH seed masses: $M_{\text{seed}}^* = 5 \times 10^5, 5 \times 10^6, 5 \times 10^7h^{-1}\text{M}_\odot$. For each BH seed mass, we also adjust the minimum halo mass accordingly. We name the simulations as B3H8, B4H9, and B5H10 to indicate each of these cases, so, for example, B4H9 is the run for a BH of $5 \times 10^6h^{-1}\text{M}_\odot$ seeded in a newly forming halo of $5 \times 10^7h^{-1}\text{M}_\odot$ and so on (see Table 2 for the specific names with corresponding seed and halo masses information for each of the three simulations).

In Figure 7, we show the halo mass functions $\Phi_{\text{halo}}$ and the stellar mass functions $\Phi_*$ (the left and the right panels respectively) of the simulations with BH seed masses $M_{\text{seed}}^* = 5 \times 10^5, 5 \times 10^6, 5 \times 10^7h^{-1}\text{M}_\odot$ (blue: B3H8, green: B4H9, and orange: B5H10 respectively) in comparison with the measurements from BLUETIDES (the grey dash curves) at $z = 6, 8,$ and 10. We find that all the mass func-

**Table 2. Simulation naming rule according to the BH seed mass ($M_{\text{seed}}^*$) and minimum halo mass ($M_{\text{halo}}^*$).**

| Name  | $M_{\text{seed}}^* [h^{-1}\text{M}_\odot]$ | $M_{\text{halo}}^* [h^{-1}\text{M}_\odot]$ |
|-------|------------------------------------------|------------------------------------------|
| B3H8  | $5 \times 10^5$                         | $5 \times 10^8$                         |
| B4H9  | $5 \times 10^6$                         | $5 \times 10^9$                         |
| B5H10 | $5 \times 10^7$                         | $5 \times 10^{10}$                      |
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Figure 6. Slices of the gas density fields weighted by the gas temperature of simulations B3H8, B4H9, and B5H10 (from the left to the right) at $z = 10$, $8$, and $6$ (from the top to the bottom) with dimensions of $7.5\,\text{Mpc}/h \times 7.5\,\text{Mpc}/h$ with a thickness of $1\,\text{Mpc}/h$. The yellow marks show the BHs and are sized according to their masses. The orange marks show the most massive BH in each run.

Table 3. Number of BHs ($N_*$) in the three simulations (B3H8, B4H9, and B5H10) at different redshifts.

|       | $N_{B3H8}^*$ | $N_{B4H9}^*$ | $N_{B5H10}^*$ |
|-------|--------------|--------------|---------------|
| $z = 10$ | 1678         | 36           | 1             |
| $z = 8$  | 4994         | 135          | 2             |
| $z = 6$  | 12210        | 488          | 11            |

We will now look more specifically into the growth history of these high mass halos of interest in our constrained simulations. In the left panel of Figure 8, we show the growth history of halo mass $M_{\text{halo}}$ and stellar mass $M_*$ for the most massive BH in each of the simulations B3H8, B4H9, and B5H10. We find that, under the density-constrained initial condition, we indeed grow a halo hosting a galaxy with the expected masses: $M_{\text{halo}}$ and $M_*$ are consistent with the history of the host halo and galaxy in the BlueTides (the grey dashed curve). Moreover, the halos and the galaxies have a very similar growth history among the three new simulations, showing that the choice of BH seed mass does not affect the growth of the hosts in any significant way.
Figure 7. Halo mass functions (\(\Phi_{\text{halo}}\)) and stellar mass functions (\(\Phi_{\star}\)) (the left and the right respectively) of simulations B3H8, B4H9, and B5H10 (\(M_{\text{tot}} = 5 \times 10^3, 5 \times 10^4, \text{ and } 5 \times 10^5 h^{-1} M_{\odot}\)) respectively in comparison with the measurements from BlueTides at \(z = 6, 8, \text{ and } 10\).

Figure 8. Left: the growth history of halo \(M_{\text{halo}}\) and galaxy \(M_{\star}\) hosting the most massive BH in simulations B3H8, B4H9, and B5H10 (\(M_{\text{tot}} = 5 \times 10^3, 5 \times 10^4, \text{ and } 5 \times 10^5 h^{-1} M_{\odot}\) respectively). Right: the growth history of the most massive BH in each simulation. The grey dashed curves are the quantities of the most massive BH in BlueTides.

Figure 9. The evolution of BH accretion rate (the left panel) and star formation rate (the right panel) of the most massive BHs in simulations B3H8, B4H9, and B5H10 (\(M_{\text{tot}} = 5 \times 10^3, 5 \times 10^4, \text{ and } 5 \times 10^5 h^{-1} M_{\odot}\) respectively) in comparison with BlueTides (the grey dashed curves).
4.2 The growth of the most massive BHs

By directly comparing our new simulations with the BlueTides simulations, we have established that our re-
simulations are able to correctly recover the evolution of the environment and growth history of the host halos of the mas-
svie BHs and the basic properties of the galaxy population.

We now look into the growth history of the most massive BHs within the three simulations (blue: B3H8, green: B4H9,
and orange: B5H10) and compare those with that of the most massive BH in BlueTides (the grey curve in the right
panel of Figure 8). The horizontal lines denote the different
BH seed masses $M_{\text{seed}}^*$ so that a smaller BH seed emerges in a lower mass halo at earlier times than a corresponding higher mass one.

For example, when a BH seed of $10^5 M_\odot$ is placed in halos of mass $10^8 M_\odot$ it is seeded at $z = 20$. In addition, as this mass halo is not so rare, not only one seed emerges, as in the case of $10^5 M_\odot$.

To illustrate the general features of the three simulations with different seeding scenarios, in Figure 6, we show the projected gas density field in our simulations weighted by the gas temperature of simulations B3H8, B4H9, and B5H10 (from the left to the right) at $z = 10, 8$, and 6 (from the top to the bottom) with dimensions of $7.5 Mpc/h \times 7.5 Mpc/h$ with a thickness of $1 Mpc/h$. The yellow circles show the BHs (where the size of the symbol is scaled with the BH masses) and the orange circle show the most massive BH in each simulation. One of the most noticeable features in Figure 6 is the marked difference in the amounts of BHs in the three different simulations. Since we have adjusted the minimum halo as well to decrease commensurately with the BH seed mass (see Table 2) the simulation with the smaller seed mass places the BHs in less massive and increasingly more common halos than the large seed BH simulation. As a result, we end up with much more BHs in the left panels (B3H8) than in the right panels (B5H10). The number of BHs in each simulation is summarized in Table 3. It is evident, however, that even though the seed population and the total number of BHs are different in the three runs, the largest BH in the center of the high-density region grows significantly and reaches similar mass in all three simulations.

More quantitatively, in Figure 8 we find that the growth of the most massive BH in each simulation starts to converge to the same value at $z \sim 8$ and reaches a mass of about $10^9 M_\odot$ by $z = 6$ in all cases. This shows that the choice of the BH seed mass is not a particularly important parameter for the growth of the most massive BHs (at least as far as we can test and in the expected range of $10^7 \sim 10^8 h^{-1} M_\odot$). However, we note that the early ($z > 10$) growth of the SMBH in the three different simulations can be faster or slower. The low and high seed BHs start to have larger masses at early times while the intermediate seed is the one that remains at the seed mass the longest but once it starts growing it catches up fast to the other two. Another remarkable feature is that the growth history of B3H8 contains discrete jumps, indicating lots of mergers even at the early times compared to the other two.

In Figure 9, we show the evolution of the BH accretion rate (the left panel) and the star formation rate (the right panel) of each of the most massive BHs that grow in our constrained runs with different seed BH masses (B3H8, B4H9 and B5H10 respectively) and compare them to the respective quantities for the most massive BH in BlueTides. We find that the BH accretion rates of the three SMBHs in the three separate runs (i) have the same overall evolution in the accretion rate: with an initial, typically low accretion phase, followed by a close to exponential (Eddington) growth phase and a final quenched, feedback regulated phase. It is noticeable that (ii) while the early and intermediate phases differ somewhat, the accretion gradually converges after $z \sim 10$, which is about the time the three SMBHs enter the feedback regulated phase. At this point, their BH mass growth saturates somewhat and the BH masses in the three different runs start converging too.

In contrast, the evolution of $M_\star$ is rather similar at the early time but differs more significantly in the later phase during the feedback regulated phase. In particular, the smallest BH mass seed models exhibit a rather bursty star formation history at $z < 10$ with variations of up to a factor of 10 in SFR compared to the other two larger BH seed simulations, whose SFR remain close to constants at a level of a few hundred $M_\odot/\text{yr}$.

4.3 BH Mergers

As shown in Figure 6 and in Table 3, there is a major difference in the BH population of our three runs with different seed mass. Particularly in the B3H8, when small mass seeds are implemented in our simulation, there is a huge difference in the BH population in the environment of the most massive BH. In this case, the BH is surrounded by a large population of other BHs (since we adjusted the minimum halo as well for the seeding). As expected, these BHs merge with each other as evidenced by the BH mass assembly history and its step-like features that appear when any BHs merge into the main central one. To show more clearly the differences in the BH merger history of the three runs with different seeding pro-
cedures in Figure 10, we show the BH merger history for the run with $M_{\text{seed}}^* = 5 \times 10^5 M_\odot$ (B3H8; left panel) and $5 \times 10^4 h^{-1} M_\odot$ (B4H9; right panel) compared to the one with $5 \times 10^5 h^{-1} M_\odot$ (B5H10; black solid curves). Whenever a BH merger hap-
pens, the color of the growth history changes. Plus, we show the merger tree illustration of the BH projected positions in Figure 11. The size of the data points illustrates the mass of BHs. We find that there are 8 and 6 BH mergers in B3H8 and B4H9 respectively while there is no merger in B5H10 by $z = 6$ (although a merger is likely to occur below this redshift as the closest BH below 100 kpc distance from the most massive one).

At $z > 12$, interestingly, we find that there are 4 mergers happen for the SMBH in B3H8 while there are no mergers occur in the other two simulations. This possibly explains why the SMBH in B3H8 grows faster than the other two SMBHs at the early times. However, the early growth is dominated by mergers rather than accretion. This is interesting, as it implies that while a small mass seed may be expected to grow slower at the early times, our simulation shows that if smaller mass seeds are more common, a lot of the early growth can still occur via mergers. The small mass seed may then grow and catch up to a more massive, rarer
seed rather quickly, as we show for the B3H8 model case. The different BH merger history obtained in the seed models we have investigated here is the primary reason for the differences in the early growth of the SMBHs at the early times. So while the final BH mass reaches very similar value, different seeding procedures are expected to produce significantly different BH populations and associated merger rates that can discriminate the different scenarios at early times \( z > 10 \). At \( 6 < z < 10 \) models with BH seeds within the range of \( 10^3 - 10^4 M_\odot \) tend to undergo few major (\( M_1/M_2 \sim \) to a few) BH mergers. For the largest, rarest seed models (\( \sim 10^5 M_\odot \)), in such a region the massive black hole is not expected to experience any merger until \( z < 6 \).

These marked differences in the predictions of the merger history for the first massive black holes constitute an interesting prospect for constraining BH seed masses/models for the first quasars that will become within reach with the planned LISA mission.

5 CONCLUSIONS

In this paper, we have investigated cosmological simulations designed to reproduce the environments and large-scale structure relevant for the growth of the first quasars at \( z \geq 6 \). In particular, we have focused on the effects of different choices of BH seed mass (a parameter in the SMBH subgrid model) on the growth history of the SMBH at the early time. To do so, we have applied the technique of constrained Gaussian realizations (Hoffman & Ribak 1991; van de Weygaert & Bertschinger 1996) in order to be able to reconstruct initial conditions to reproduce the large-scale structure of the most massive BHs in BlueTides, the only cosmological hydrodynamic simulation with a sufficient resolution and
a very large volume which makes direct predictions for the first, rare observed quasars (Di Matteo et al. 2017; Ni et al. 2018). The first quasars are extremely rare objects and in BlueTides simulation, 400h−3Mpc on a side, there are only 4 SMBHs with mass \( \sim 10^9 M_\odot \) by \( z = 7 \).

We have first reconstructed the initial conditions of this reference simulation and then run the reconstructed initial conditions forward in time until \( z = 6 \). We have compared the resulting constrained simulations with the original BlueTides simulation to test the accuracy of this method. With the significant decreases on the computational resources by \((400/15)^3 \sim 20000\) times less (keeping the same resolution as in BlueTides), we have conducted a series of re-simulations.

At the high redshifts of interest, non-linear mode coupling on the scale of even small simulation box sizes is not present. We have shown that our re-simulations (in boxes of 10 and 15h−1Mpc on a side) are able to correctly recover the evolution of the large scale structure, and halo, stellar mass functions as well as the growth history of the most massive BH and host galaxy (the initial condition conditions of which were reconstructed). The halo, stellar, and BH mass from the BlueTides simulation are recovered in our re-simulations within a factor of 1.5 in mass. The halo hosting the massive BH has a mass \( \sim 10^{12} M_\odot \), a stellar mass \( \sim 4 \times 10^9 M_\odot \) and an SMBH \( \sim 4 \times 10^8 M_\odot \) forms at \( z = 8 \), fully consistent with BlueTides.

By running a set of three different realizations (each of them has different local tidal field), we have further shown that a low tidal field environment is crucial for the growth of the earliest and most massive SMBHs, which is consistent with the BlueTides result in Di Matteo et al. (2017). For our highest tidal field realization, the mass of the most massive BH is a factor of a few hundred times lower (reaching only \( \sim 3 \times 10^6 M_\odot \) at \( z = 8 \)) than in our lowest tidal field realization. Among the simulations, the SMBH in the lowest tidal field environment (tidal field strength \( t_\epsilon \sim 0.6 \) measured at 15h−1Mpc) has a mass 10 times more than the one in the highest tidal field environment (\( t_\epsilon \sim 1.2 \)) by \( z = 6 \).

Finally, by selecting the initial condition that best recovers the original quasar environment (i.e. with low tidal fields) in BlueTides, we have run another set of simulations to investigate the effects of the choice of BH seed mass on the growth of these first massive objects. In BlueTides simulation, the seed mass was chosen to be \( 5\times10^5 h^{-1}M_\odot \), which is at the high end of the predicted mass for seed BHs. With the same initial condition, we run three simulations with different SMBH seed masses: \( 5\times10^5, 5\times10^6 \) and \( 5\times10^5 h^{-1}M_\odot \) (the latter is the same as the one in BlueTides).

We have found that under our assumptions (i) the final mass of the SMBH (at \( z = 6 \)) is insensitive to the initial seed mass. The mass of SMBH (or first quasar) in our re-simulation is \( \sim 10^9 M_\odot \) at \( z = 6 \) irrespective of the choice of seed mass. (ii) The value of the seed mass has important signatures in the early (\( z > 10 \)) growth and merger history of a SMBH. The less massive seeds may tend to grow slower initially, but if seeded in more common, less massive, earlier forming halos they merge efficiently. A significant fraction of the early growth then, in a low mass seed scenario, occurs in this mode. This effectively allows the SMBH growth history to catch up with that of a later, more massive seed. There are 4 SMBH mergers occur at \( z \gtrsim 12 \) for the most massive SMBH with the lowest seed mass while no mergers happen for the other two runs, which possibly explains the result that the smallest seed grows faster at early times. The significant differences in the early merger rates provide an interesting discriminating feature for low versus high BH seed models at the early time. The space-based gravitational wave telescope LISA will open up new investigations into the dynamical processes involving SMBHs and new exciting prospects for tracing the origin, merger history of SMBHs across cosmic ages.

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REFERENCES

Abel T., Bryan G. L., Norman M. L., 2002, Science, 295, 93
Anglés-Alcázar D., Davé R., Özel F., Oppenheimer B. D., 2014, ApJ, 782, 84
Bañados E., et al., 2018, Nature, 553, 473
Battaglia N., Trac H., Cen R., Loeb A., 2013, ApJ, 776, 81
Begelman M. C., Rees M. J., 1978, MNRAS, 185, 847
Begelman M. C., Volonteri M., Rees M. J., 2006, MNRAS, 370, 289
Bellovary J., Brooks A., Volonteri M., Governato F., Quinn T., Wadsley J., 2013, ApJ, 779, 136
Blomnick A. K., Di Matteo T., Feng Y., Lanusse F., 2018, MNRAS, 474, 5393
Bondi H., 1952, MNRAS, 112, 195
Bondi H., Hoyle F., 1944, MNRAS, 104, 273
Bournaud F., Dekel A., Teyssier R., Cacciato M., Daddi E., Juneau S., Shankar F., 2011, ApJ, 741, L33
Bromm V., Loeb A., 2003, ApJ, 596, 34
Costa T., Sijacki D., Trenti M., Haehnelt M. G., 2014, MNRAS, 439, 2146
Dalal N., White M., Bond J. R., Shirokov A., 2008, ApJ, 687, 12
Devecchi B., Volonteri M., 2009, ApJ, 694, 302
Di Matteo T., Springel V., Hernquist L., 2005, Nature, 433, 604
Di Matteo T., Croft R. A. C., Feng Y., Waters D., Wilkins S., 2017, MNRAS, 467, 4243
Dubois Y., Pichon C., Devriendt J., Silk J., Haehnelt M., Kimm T., Slyz A., 2013, MNRAS, 428, 2885
Eisenstein D. J., Loeb A., 1995, ApJ, 443, 11
Fan X., et al., 2006, AJ, 132, 117
Faucher-Giguère C.-A., Lidz A., Zaldarriaga M., Hernquist L., 2009, ApJ, 703, 1416
Feng Y., Di Matteo T., Croft R., Khandai N., 2014, MNRAS, 440, 1865
Feng Y., Di Matteo T., Croft R., Tenneti A., Bird S., Battaglia N., Wilkins S., 2015, ApJ, 808, L17
Feng Y., Di-Matteo T., Croft R. A., Bird S., Battaglia N., Wilkins S., 2016a, MNRAS, 455, 2778
Feng Y., Chu M.-Y., Seljak U., McDonald P., 2016b, MNRAS, 463, 2273
Ferrara A., Salvadori S., Yue B., Schleicher D., 2014, MNRAS, 443, 2310
Haehnelt M. G., Rees M. J., 1993, MNRAS, 263, 168
Hinsch G., et al., 2013, ApJS, 208, 19
Hoffman Y., Ribak E., 1991, ApJ, 380, L5
Hopkins P. F., 2013, MNRAS, 428, 2840

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