DISTRIBUTION OF THE VERY FIRST POPULATION III STARS
AND THEIR RELATION TO BRIGHT $z \approx 6$ QUASARS

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ABSTRACT

We discuss the link between dark matter halos hosting the first Population III stars and the rare, massive halos that are generally considered to host bright quasars at high redshift ($z \approx 6$). The main question that we intend to answer is whether the supermassive black holes powering these QSOs grew out from the seeds planted by the first intermediate-mass black holes created in the universe. This question involves a dynamical range of $10^{13}$ in mass, and we address it by combining $N$-body simulations of structure formation to identify the most massive halos at $z \approx 6$ with a Monte Carlo method based on linear theory to obtain the location and formation times of the first-light halos within the whole simulation box. We show that the descendants of the first $\approx 10^6 M_\odot$ virialized halos do not, on average, end in the most massive halos at $z = 6$, but rather live in a large variety of environments. The oldest Population III progenitors of the most massive halos at $z \approx 6$ form instead from density peaks that are on average 1.5 $\sigma$ more common than the first Population III star formed in the volume occupied by one bright high-$z$ QSO. The intermediate-mass black hole seeds planted by the very first Population III stars at $z \approx 40$ can easily grow to masses $m_{BH} > 10^9 M_\odot$ by $z = 6$ assuming Eddington accretion with radiative efficiency $\epsilon \approx 0.1$. Quenching of the black hole accretion is therefore crucial to avoid an overabundance of supermassive black holes at lower redshift. This can be obtained if the mass accretion is limited to a fraction $\eta \approx 6 \times 10^{-3}$ of the total baryon mass of the halo hosting the black hole. The resulting high-end slope of the black hole mass function at $z = 6$ is $\alpha \approx -3.7$, a value within the 1 $\sigma$ error bar for the bright-end slope of the observed quasar luminosity function at $z = 6$.

Subject headings: cosmology: theory — early universe — galaxies: high-redshift — methods: $n$-body simulations

Online material: color figures

1. INTRODUCTION

Bright quasars at $z \approx 6$ are very luminous and rare objects that can be detected out to huge cosmological distances in very large area surveys such as the Sloan Digital Sky Survey (SDSS; Fan et al. 2004). Their estimated space density is $\approx 2.2 \times 10^{-9} \text{ (Mpc}^{-1} \text{h}^{-1})^{-3}$ (Fan et al. 2004), that is, about one object per about 200 deg$^2$ of sky, assuming a depth of $\Delta z = 1$ centered at $z = 6.1$ under the third-year Wilkinson Microwave Anisotropy Probe (WMAP) cosmology (Spergel et al. 2007). Their luminosity is thought to be due to accretion onto a supermassive black hole (e.g., see Hopkins et al. 2005).

A common expectation is that the luminous high-$z$ quasars are situated at the center of the biggest protoclusters at that time. Some observational evidence of overdensities of galaxies in two deep Hubble Space Telescope (HST) ACS fields containing a bright $z = 6$ quasar has been claimed (Stiavelli et al. 2005; Zhen et al. 2006), but it is unclear whether this is true in general. In fact, an ACS image only probes a long and narrow field of view of about $6 \times 6 \times 320$ (Mpc $h^{-1})^3$ in the redshift range $[5.6:6.6]$, so a significant number of detections may come from galaxies unrelated to the environment of the host halo of the bright quasar.

Numerical simulations that address the formation of bright quasars are extremely challenging, given their low number density. A huge simulation cube with edge of $\approx 700$ Mpc $h^{-1}$ is required just to expect, on average, one such object in the simulation box. A major computational investment, such as the Millennium Run (Springel et al. 2005), is required to resolve at high redshift (z $\approx 20$) virialized halos in this volume and to follow their merging history down to $z \approx 6$. Even assuming that the simulation volume is big enough that there is an expectation of finding halos hosting bright quasars, how can these halos be identified? In principle, two non–mutually exclusive alternatives appear plausible: either the supermassive black holes are hosted in the most massive halos with the corresponding number density of SDSS quasars or these black holes have grown from the first Population III intermediate-mass black hole seeds, therefore representing the descendants of the rarest density peaks that hosted first stars.

The first scenario implies that the $m_{BH}-\sigma$ relation (Ferrarese & Merritt 2000; Gebhardt et al. 2000) is already in place at high redshift (Volonteri et al. 2003; Hopkins et al. 2005; Di Matteo et al. 2005). In that case, multigrid simulations can be carried out to follow in detail the growth of the supermassive black hole (e.g., see Li et al. 2006). In the second scenario, the quasar progenitors would be traced back to the first Population III stars created in the universe within $\approx 10^6 M_\odot$ mass halos virialized at $z \approx 50$ (Bromm & Larson 2004; Abel et al. 2002). These Population III stars are very massive, $M > 100 M_\odot$, so after a short life of a few million years, they explode and may leave intermediate-mass black holes, plausible seeds for the supermassive black holes observed at lower redshift. Of course, the two scenarios can be consistent with each other if the first perturbations to collapse are also the most massive at $z = 6$. This
seems to be implied, e.g., in Springel et al. (2005), where the bright quasar candidate in the simulation is traced back to one of the 18 collapsed halos at \( z = 16.7 \).

In this paper we explore the link between the first Population III halos collapsed in a simulation box and the most massive halos at lower redshifts to gain insight to the scenarios of bright quasar formation. This is a numerically challenging problem, as the dynamical range of masses involved is very large: a simulation volume of \( 5 \times 10^8 \, (\text{Mpc} \, \text{h}^{-1})^3 \) has a mass of about \( 3.3 \times 10^{19} \, M_\odot \, \text{h}^{-1} \), that is, more than \( 10^{13} \) times the mass of a Population III dark matter halo. We have adopted an original approach to the problem, broadly inspired by the tree method of Cole et al. (1994). We first simulate at relatively low resolution the evolution of a simulation volume down to \( z = 0 \). Then, starting from the density fluctuations field at the initial conditions of the numerical simulation, we compute analytically the redshift distribution of the oldest Population III halo collapsed within each single grid cell. The information is then used as input for a Monte Carlo code to sample for each particle of the simulation the collapse redshift of the first Population III progenitor dark matter halo. The formation time of the oldest Population III remnant within the most massive halos identified at \( z \approx 6 \) is finally compared with that of the oldest Population III star sampled over the whole simulation volume, and the implications for the growth of supermassive black holes are discussed.

Our approach is tuned to investigate the formation and the subsequent remnant distribution of the first rare density peaks that hosted Population III stars at \( z \approx 30 \). In this respect, our study has a goal similar to Reed et al. (2005), with the important difference that we search for the first Population III star in the complete simulation box, not by means of progressive refinements around substructures that probe only a small fraction of the total box volume. As our method is tuned to finding very rare fluctuations, it is not easily applied to the significantly more common 3 σ peaks with mass \( \approx 10^{6} \, M_\odot \), that collapse at \( z \approx 20 \) and that might constitute the majority of Population III stars, if these are terminated by chemical feedback at \( z \approx 20 \) (e.g., see Greif & Bromm 2006) and not by photodissociation of molecular hydrogen at \( z \approx 25 \) (Haiman et al. 2000).

This paper is organized as follows. In § 2 we present the details of the numerical simulations carried out. In § 3 we analyze the numerical results, focusing on the merging history of the first Population III halos formed in the simulation box. In § 4 we review when the first stars epoch ends, while in § 5 we discuss the implications of the Population III distribution that we find for the buildup of the supermassive black hole population at \( z \lesssim 6 \). We conclude in § 6.

2. NUMERICAL METHODS

2.1. N-Body Simulations

The numerical simulations presented in this paper have been carried out using the public version of the PM-tree code Gadget-2 (Springel 2005). Our standard choice is to adopt a cosmology based on the third-year WMAP data (Spergel et al. 2007): \( \Omega_{\Lambda} = 0.74 \), \( \Omega_m = 0.26 \), and \( H_0 = 70 \, \text{km} \, \text{s}^{-1} \, \text{Mpc}^{-1} \), where \( \Omega_m \) is the total matter density in units of the critical density \( \rho_c = 3H_0^2/(8\pi G) \), where \( H_0 \) is the Hubble constant (parameterized as \( H_0 = 100 \, h \, \text{km} \, \text{s}^{-1} \, \text{Mpc}^{-1} \)), \( G \) is Newton’s gravitational constant (Peebles 1993), and \( \Omega_{\Lambda} \) is the dark energy density. As for \( \sigma_8 \), the root mean squared mass fluctuation in a sphere of radius \( 8 \, \text{Mpc} \, \text{h}^{-1} \) extrapolated at \( z = 0 \) using linear theory, we consider both \( \sigma_8 = 0.9 \) and 0.75, focusing in particular on the higher value, which provides a better match to the observed clustering properties of galaxies (Evrard et al. 2007).

The initial conditions have been generated using a code based on the Grafic algorithm (Bertschinger 2001). An initial uniform lattice is perturbed using a discrete realization of a Gaussian random field sampled in real space and then convolved in Fourier space with a \( \Lambda \)CDM transfer function computed using the fit by Eisenstein & Hu (1999) and assuming a scale invariant longwave spectral index \( n = 1 \). The initial density field is saved for later reprocessing through the first-light Monte Carlo code (see § 2.2). The particle velocities and displacements are then evolved to the desired starting redshift \( z_{\text{start}} = 70 / 3.7 \) (i.e., \( z_{\text{start}} = 0.015 \)) using the Zel’dovich approximation, and the evolution is followed using Gadget-2 (Springel 2005). Dark matter halos are identified in the simulations snapshots using the HOP halo finder (Eisenstein & Hut 1998).

To find the optimal tradeoff between mass resolution and box size, both critical parameters to establish a connection between Population III halos and the most massive halos identified at \( z = 6 \), we resort to simulations (see Table 1) with three different box sizes, all using \( N = 512^3 \) particles.

| ID | \( L_{\text{box}} \) (Mpc) | \( \sigma_8 \) | \( k_{\text{ref}} \) (h Mpc\(^{-1}\)) | \( M_0 \) (h M\(^{-1}\)) | \( N_{\text{MC}} \) |
|---|---|---|---|---|---|
| S1 | 60 | 0.9 | 5 | 8.6 \times 10^5 | 100 |
| S2 | 60 | 0.75 | 5 | 8.6 \times 10^5 | 100 |
| M1 | 512 | 0.9 | 40 | 1.0 \times 10^6 | 200 |
| L1 | 720 | 0.9 | 57 | 1.0 \times 10^6 | 600 |

Notes.—Summary table with the details of the numerical simulations carried out in this paper. Col. (1): the simulation ID; col. (2): the box size; col. (3): the value of \( \sigma_8 \) used to generate the initial conditions; col. (4): \( k_{\text{ref}} \), the refinement factor, that is, the ratio of the mass of a single particle in the N-body run to the mass assumed for a Population III star halo \( (M_0; \text{col. (5)}) \); col. (6): \( N_{\text{MC}} \), the number of different Monte Carlo realizations of the Population III halo density field for each N-body realization.

2.2. Monte Carlo Code for First-Light Sources

Given the initial density fluctuations field on the simulation grid, where a cell has a mass of order \( 10^{10} - 10^{11} \, M_\odot \, h^{-1} \), our goal is to estimate the redshift of the first virialized perturbation within each cell at the mass scale of early Population III dark matter halos (i.e., \( \leq 10^9 \, M_\odot \); see, e.g., Bromm & Larson 2004).
For this we resort to an analytical treatment based on a linear approximation for structure formation. The initial conditions for an N-body simulation in a box of size $L$ with $N$ particles and a single-particle mass $m_p$, define a Gaussian random field $\delta \rho$ for the $N$ cells (associated with the location of the $N$ particles) of the simulation grid. This density field is usually generated by convolving white noise with the transfer function associated with the power spectrum of the density perturbations (e.g., see Bertschinger 2001) and is used to obtain the initial velocity and position displacements for the particles (e.g., see eq. [5.115] in Peebles 1993). The density fluctuation in each cell has a contribution from different uncorrelated frequencies in the power spectrum. When the initial conditions for an N-body simulation are generated, the power spectrum has an upper cutoff around the Nyquist frequency for the grid used (i.e., around the frequency associated with the average interparticle distance) and a lower cutoff at the frequency associated with the box size (if periodic boundary conditions are enforced). A higher resolution version of the initial density field can be obtained by simply increasing the grid size and adding the density perturbations associated with the power spectrum between the old and the new cutoff frequencies.

In linear approximation, one can use the field $\delta \rho$ to obtain the redshift of virialization of a structure of mass $M_h > m_p$ at a given position $x$ in the grid. To do this, one averages the field $\delta \rho$ using a spherical window centered at $x$ with a radius such that the window encloses a mass $M_h$ and, assuming linear growth, computes the redshift at which the average density within the window reaches $\delta \rho = 1.69$ (in units such that the average density of the box is 1). In fact, for a spherical collapse model, when $\delta \rho = 1.69$ in linear theory, the halo has reached virial equilibrium under the full nonlinear dynamics. This concept is at the base of the various proposed methods for computing algorithmically the mass function of dark matter halos (e.g., see Press & Schechter 1974; Bond et al. 1991; Sheth & Tormen 1999).

We apply this idea to estimate the formation rate and the location in the simulation volume of dark matter halos at a mass scale below the single-particle mass used in the simulation. A straightforward implementation consists of first generating the density field associated with the N-body simulation and then refining at higher resolution the field by means of a constrained realization of the initial conditions used in the N-body run (e.g., see Bertschinger 2001). This provides exact and complete information on the whole density field, but the price to pay is the execution of very large fast Fourier transforms on the refined grid. If the goal is to compute density fluctuations down to a mass of $10^9 h^{-1}$ over a box of edge $720$ Mpc $h^{-1}$, a grid of $29,184^3$ is needed, which would require about 100 TB of RAM, which is well beyond the current memory capabilities of the largest supercomputers.

A shortcut is, however, available, if one trades information for numerical complexity. Given a realized numerical simulation, we are in fact not interested in getting a detailed picture of the dynamics at subgrid resolution, but only in identifying for each grid point the redshift of virialization of its first progenitor at a given subgrid mass scale. For example, given a simulation with single-particle mass of $10^{10} M_\odot h^{-1}$, our aim is to quantify the redshift of virialization of the first dark matter halo of mass $10^9 M_\odot h^{-1}$ within the volume associated with the $10^{10} M_\odot h^{-1}$ particle. In that case, if we were to have the full subgrid information, we would search for the maximum realized value of the density within the $10^4$ subgrid cells of mass $10^9 M_\odot h^{-1}$ that constitute our $10^{10} M_\odot h^{-1}$ single-particle cell. As the density fluctuation field is a Gaussian random field, the density in subgrid cells will be a Gaussian centered at the density of the parent cell with variance given by integrating the power spectrum of density fluctuations truncated between the Nquist frequency of the parent cell and that of the subcells.

Therefore, for a single cell of mass $m_p$, the redshift of collapse of a subgrid progenitor at a mass scale $m_p$ can be obtained simply by sampling from the probability distribution of the maximum of the subgrid fluctuations of the $k = m_p/m_{\text{grid}}$ subcells of mass $m_p$ that are within a cell of mass $m_p$. The probability distribution for the maximum of these fluctuations is available in analytic form when the field is Gaussian, as in the case considered here. In fact, given a probability distribution $p(x)$, with partition function $P(x)$,

$$P(x) = \int_{-\infty}^{x} p(a) da,$$  \hspace{1cm} (1)

the probability distribution $q(m, k)$ for the maximum $m$ of $k$ random numbers extracted from $p(x)$ $[m = \max (x_1, \ldots, x_k)]$ is the derivative of the partition function for $m$, which in turn is simply the $k$th power of the partition function $P(x)$. Therefore, we have

$$q(m, k) = kp(m)p(m)^{k-1}.$$  \hspace{1cm} (2)

Equation (2) has a simple interpretation: the probability that the maximum of $k$ random numbers lies in the interval $[m, m + \delta m]$ is given by the probability of sampling one of the $k$ numbers exactly in that interval and all the other numbers below $m$.

With the aid of equation (2), we can sample the distribution of the maximum of the additional subgrid density fluctuations that need to be considered in order to probe the mass scale of Population III halos. The variance $\sigma_{g}$ to be used in $p(x)$ may be computed from the power spectrum of the density fluctuations by considering an upper cutoff at the wavelength of one cell size in the initial conditions. Or, equivalently, if the complete power spectrum of density fluctuations has variance $\sigma(M_{\text{grid}})$ at the mass scale of one grid cell and variance $\sigma(M_{\text{PopIII halo}})$ at the mass scale of a halo hosting a first star, we set $\sigma_{g}$ such that

$$\sigma_{g}^2 = \sigma(M_{\text{PopIII halo}})^2 - \sigma(M_{\text{grid cell}})^2.$$  \hspace{1cm} (3)

Therefore our recipe for estimating the age of the earliest progenitor formed in each cell is the following:

1. Starting from the initial density fluctuation field on the grid used to initialize the N-body run, compute the mass refinement factor $k$ to go from the mass of a single particle (i.e., the mass within one grid cell) to that of a Population III star halo ($k = M_{\text{grid cell}}/M_{\text{PopIII halo}}$).
2. Given the power spectrum of the density fluctuations, $M_{\text{grid cell}}$ and $M_{\text{PopIII halo}}$, compute $\sigma_{g}$.
3. Extract one random number $r$ from $q(m, k)$ (see eq. [2]), where $p(m)$ is a Gaussian distribution with zero mean and variance $\sigma_{g}$.
4. Sum $r$ to the value of the density field in the cell to obtain $(\delta \rho_\text{g}/\rho)_\text{max}$ in the cell. From the value of $(\delta \rho_\text{g}/\rho)_\text{max}$, it is then straightforward to compute the nonlinear redshift for that perturbation, i.e., the redshift $z_{\text{nl}}$ when the linear density contrast reaches a value $(\delta \rho_\text{g}/\rho)_\text{max}(z_{\text{nl}}) = 1.69$.

The particles of the simulation now carry the additional information of the redshift at which their first Population III star dark
In fact, if we are interested in identifying the most massive halos \( M \) of mass \( \Omega_c \) at low redshift \( z \approx 6 \) using numerical tests presented in Appendix A. This method has two main advantages:

1. It allows us to use relatively inexpensive “low resolution” simulations to identify the largest objects at low redshift \( z \lesssim 6 \). In fact, if we are interested in identifying the most massive halos at \( z \approx 6 \), we have assumed a box of 720 Mpc \( h^{-1} \) and a mass scale of \( M_{\text{qh}} = 4.3 \times 10^{12} M_\odot h^{-1} \), which implies \( k = 180^3 \). This represents the probability distribution for the mass scale of a Population III progenitor of a 5.7 \( M_\odot \) halo virialized. These are limitations that we need to accept, as the nonlinear evolution could be followed over the whole box only at the price of running a simulation prohibitively intensive in CPU and memory resources, with at least 10^5 times more particles than in the Millennium Run (Springel et al. 2005). This appears unfeasible for the time being, even considering next-generation dedicated supercomputers, such as the GRAPE-DR (Makino 2005).

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3. THE FATE OF THE FIRST POPULATION III HALOS

### 3.1. Analytical Considerations

The general picture for the connection between first halos and the most massive halos at \( z \approx 6 \) can be obtained using analytical considerations that will be later confirmed in 3.2 by the results of our numerical investigation. Following the choice for our large-box simulation, we consider a volume of \( (720 Mpch^{-1})^3 \) of mass \( M_{\text{box}} \), large enough to host a bright \( z \approx 6 \) quasar. We estimate from the Press-Schechter formalism (see also the masses of the \( z = 6 \) halos in our “large” box simulation in 3.2) that the most massive halo at \( z \approx 6 \) has a mass (which we call \( M_{\text{qh}} \)) of about \( 10^{12} - 10^{13} M_\odot h^{-1} \) (see also Springel et al. 2005). Since the most massive halo is the first at its mass scale to be formed, through the use of equation (2) we can obtain the distribution of its initial density fluctuation (see Fig. 1). If we assume \( M_{\text{qh}} = M_{\text{box}}/180^3 = 4.3 \times 10^{12} M_\odot h^{-1} \) (in agreement with Springel et al. 2005), this halo is expected to have originated from a density fluctuation in the range \( [5.5:7] \sigma(M_{\text{qh}}) \) at 90% of confidence level. We now consider the volume initially occupied by the mass \( M_{\text{qh}} \), and we compute from the primordial power spectrum the variance \( \sigma_8 \) of density perturbations at the mass scale of a Population III halo \( (M_{\text{fs}} = 10^6 M_\odot h^{-1}) \), considering only contributions from wavelengths at a scale below the volume enclosed by \( M_{\text{qh}} \) (eq. [3]). We obtain \( \sigma_8 = 4.85 \sigma(M_{\text{qh}}) \). From equation (2), it follows that the maximum of 160^3 Gaussian random numbers with variance \( \sigma_8 \) is distributed in the range \( [23.4:27.0] \sigma(M_{\text{qh}}) \) at 90% of confidence level. Combining the two 90% confidence level intervals, this means that the first Population III progenitor of a bright quasar originated from a perturbation in the range \( [28.4:32.7] \sigma(M_{\text{qh}}) \). If we consider instead a random subcell among the 160^3, the probability that the maximum subgrid perturbation is smaller than 32.7 \( \sigma(M_{\text{qh}}) \) is only 0.99995, so several hundreds of the 180^3 cells among the whole simulation volume are expected to have a Population III progenitor formed before that of the most massive \( z = 6 \) halo. In fact, from integration of equation (2), the sigma peak associated with the first star in the box is expected to be greater than 35.5 \( \sigma(M_{\text{qh}}) \) at 99.99% of confidence level [and in the interval \( [36.2:38.8] \sigma(M_{\text{qh}}) \) at 90% of confidence level]. Therefore, the rarity of the earliest Population III progenitor of the most massive halo at \( z = 6 \) is about 1.5 \( \sigma_8 \) less than that of the first Population III star formed in the simulation volume. In terms of formation redshift, the first Population III star dark matter halo in the simulation volume virializes in the redshift interval \( z \in [49:53] \), while the earliest Population III progenitor of the QSO halo is formed at \( z \in [38:44] \) (both intervals at 90% of confidence level and computed for \( \sigma_8 = 0.9 \).
averaged over the 10 most massive halos at perturbation, while the dotted line refers to the collapse redshift of the 100th Population III in the box. The local density around each particle is constructed using a 16 particle smoothing kernel. For the regrouping algorithm, we use $\delta_{\text{peak}} = 240, \delta_{\text{saddle}} = 180, \delta_{\text{outer}} = 100$, and a minimum group size of 20 particles. In the large simulation box (run L1 in Table 1), we identify 47 halos with 20 particles or more, and the most massive halo (37 particles) has a mass of $6.9 \times 10^{12} M_\odot h^{-1}$. In the medium simulation box (run M1 in Table 1), the higher mass resolution allows us to identify 694 halos with at least 20 particles, and the most massive halo has 92 particles, for a total mass of $6.1 \times 10^{12} M_\odot h^{-1}$, consistent with the results from the larger box. Finally, in the small-box simulations (runs S1 and S2 in Table 1), there are 14,972 halos with at least 100 particles in S1 ($\delta_{\text{avg}} = 0.9$), and 7531 halos with at least 100 particles in S2 ($\delta_{\text{avg}} = 0.75$). The most massive halo has a mass of $2.4 \times 10^{12} M_\odot h^{-1}$ in S1 and $7.1 \times 10^{11} M_\odot h^{-1}$ in S2. The $z = 6$ halo mass distribution for these two simulations is well described (with displacements within $\approx 15\%$) by a Sheth & Tormen (1999) mass function.

The link between the halos identified in the snapshots and the first-light sources is established using the Monte Carlo method described in § 2.2. For the large box, we consider a refinement factor $k = 57$ to move from the single-particle mass of the simulation to a typical Population III halo mass, so that $M_{\text{fs}} = 1.0 \times 10^6 M_\odot h^{-1}$. For the first 10 most massive halos at $z = 6$, we show in Figure 2 the distribution of the redshift at which the oldest progenitor crosses the virialization density contrast threshold in linear theory ($\delta/\rho = 1.69$) and the distribution of the ranking of the collapse time computed over all the Population III progenitors of the simulation particles. The collapse rank of the first Population III progenitor of the most massive $z = 6$ halo is in the interval $[474:45075]$ at 90% of confidence level, with median 8535. The corresponding virialization redshifts are in the interval $[39.3:44.1]$ with median 41.1. For comparison, the first Population III halo in the box virializes in the

![Figure 2](image)

**Figure 2.** Left: Distribution for the ranking of the collapse epoch for the oldest Population III halo progenitor (with $M_{\text{fs}} = 10^8 M_\odot h^{-1}$) of the most massive halo and averaged over the 10 most massive halos at $z = 6$ in the (720 Mpc $h^{-1}$)$^3$ box simulation. The cardinality is measured over 600 Monte Carlo realizations. Right: As in the left, but distribution of the collapse time $z_{\text{nl}}$ for the oldest Population III progenitor. The line represents the collapse redshift of the first Population III star perturbation, while the dotted line refers to the collapse redshift of the 100th Population III in the box. [See the electronic edition of the Journal for a color version of this figure.]

From these simple analytical estimates, it is clear that the most massive and rarest structures that collapsed around $z \approx 6$ do not descend from the rarest sigma peaks at the first-light mass scale in the simulation volume, when the simulation box represents a significant fraction of the Hubble volume. Conversely, the black hole remnants of the first Population III stars in the universe do not provide the seeds for supermassive black holes within the most massive halos at $z \leq 6$. The descendants of first Population III stars are instead expected to be found at the center of a variety of halos, as we quantify in § 3.2 by means of N-body simulations.

**3.2. Simulations Results**

In constructing the $z = 6$ halo catalogs, we adopt the following parameters for the HOP halo finder (Eisenstein & Hut 1998). The local density around each particle is constructed using a 16 particle smoothing kernel. For the regrouping algorithm, we use $\delta_{\text{peak}} = 240, \delta_{\text{saddle}} = 180, \delta_{\text{outer}} = 100$, and a minimum group size of 20 particles. In the large simulation box (run L1 in Table 1), we identify 47 halos with 20 particles or more, and the most massive halo (37 particles) has a mass of $6.9 \times 10^{12} M_\odot h^{-1}$. In the medium simulation box (run M1 in Table 1), the higher mass resolution allows us to identify 694 halos with at least 20 particles, and the most massive halo has 92 particles, for a total mass of $6.1 \times 10^{12} M_\odot h^{-1}$, consistent with the results from the larger box. Finally, in the small-box simulations (runs S1 and S2 in Table 1), there are 14,972 halos with at least 100 particles in S1 ($\delta_{\text{avg}} = 0.9$), and 7531 halos with at least 100 particles in S2 ($\delta_{\text{avg}} = 0.75$). The most massive halo has a mass of $2.4 \times 10^{12} M_\odot h^{-1}$ in S1 and $7.1 \times 10^{11} M_\odot h^{-1}$ in S2. The $z = 6$ halo mass distribution for these two simulations is well described (with displacements within $\approx 15\%$) by a Sheth & Tormen (1999) mass function.
redshift interval [49.0:52.7] with median 50.3; the 100th first light in the box collapses in the redshift range [45.5:45.8] with median 45.7. These results from the combined $N$-body simulation and Monte Carlo code are in excellent quantitative agreement with the analytical estimates of $x$ of 3.1 and confirm that in a large simulation box the most massive halos at $z = 6$ do not derive from the rarest sigma peaks at the first-light mass scale. This result is robust with respect to the adopted typical mass for Population III halos. In Figure 3 we show the results obtained by changing the mass of the halos hosting the first stars and considering larger halos ($M_{\text{fs}} = 3.4 \times 10^6 \, M_\odot \, h^{-1}$ with $k = 38^3$) and smaller halos ($M_{\text{fs}} = 3.0 \times 10^5 \, M_\odot \, h^{-1}$ with $k = 85^3$). The formation redshift varies as the first halos are formed earlier, when they are less massive, but the relative ranking between the first Population III halo in the box and the first Population III progenitor of the most massive structures at $z = 6$ remains similar. In passing, we note that our distribution of the formation redshift for the first $3 \times 10^5 \, M_\odot$ progenitor of the most massive $z = 6$ halo (formed at $z \approx 46$) is in agreement with the results by Reed et al. (2005) obtained by means of $N$-body simulations with adaptive refinements. However, this halo is not the first one formed in the simulation box, as we find that the first structure on this mass scale is formed at $z \approx 55$ (see Fig. 3).

The results are similar for the medium box, which has a volume only 3 times smaller than the large one (see Fig. 4). The refinement factor used here is $k = 40$, which gives $M_{\text{fs}} = 1.0 \times 10^6 \, M_\odot \, h^{-1}$. The first Population III halo in the box virializes in the redshift range [48.3:52.4] with median 49.7, while the oldest Population III progenitor of the most massive halo virializes in the redshift range [38.5:43.2] (median 40.4) and has a collapse ranking in the range [574:37499] at 90% of confidence level with median 7261.

The picture changes significantly (see Fig. 5) for the small box, which has a volume more than $10^3$ times smaller than the large box. Here we use a refinement factor $k = 5$, which leads to $M_{\text{fs}} = 8.6 \times 10^5 \, M_\odot \, h^{-1}$. The collapse rank of the first-light progenitor of the most massive $z = 6$ halo is in the range [1:103] at the 90% confidence level with median 13. The correlation between the first Population III star and the most massive structure at $z = 6$ is therefore strong due to the small volume of the box. This means that locally the oldest remnants of first stars are expected to be within the largest collapsed structures.

![Fig. 3](image1.png)

![Fig. 4](image2.png)
From the medium-sized box numerical simulation, we have also characterized the fraction of first Population III remnants that end in identified halos at \( z = 0 \). If we consider one of the first 100 first-light halos collapsed in the box, there is an average probability of 0.72 of finding its remnant in a halo identified at \( z = 0 \) with more than 100 particles (that is, of mass above \( 6.7 \times 10^{12} M_\odot h^{-1} \)). The median distribution for the mass of a halo hosting one of the remnants of these first-light sources is \( \approx 3 \times 10^{13} M_\odot h^{-1} \). At 95% of confidence level, the remnants are hosted by a halo of mass less than \( 3.6 \times 10^{14} M_\odot h^{-1} \). For comparison, the most massive halo in the simulation has a mass of \( 4.4 \times 10^{16} M_\odot h^{-1} \), and there are about 15,000 halos more massive than \( 3 \times 10^{12} M_\odot h^{-1} \). This is a consequence of the poor correlation between first Population III halos and most massive halos at low redshift.

Finally, combining the results from three all of our simulation boxes, we construct in Figure 6 the Population III star formation rate at high \( z \). The total number of Population III halos that virialize is decreasing with redshift, from a number density of \( \approx 0.1 \) (Mpc \( h^{-1} \))\(^{-3} \) at \( z \approx 30 \). In our small-box simulation, this means that the average density of Population III halos is \( \approx 10^{-3} \) per grid cell. Therefore there is a very small probability of having two collapsed halos within the same cell, an event that would not be captured in our model.

4. WHEN DOES THE FIRST STARS EPOCH END?

In § 3 we show that the most massive halos at \( z = 6 \) have first-light progenitors that were formed when several thousand other Population III stars already existed. Are these progenitors still entitled to be called first stars? That is, when does the “first stars” epoch end? Here we review the question, adopting two different definitions to characterize the transition from the first to the second generation of stars, namely, (1) a threshold for the transition given by the destruction of molecular hydrogen and (2) a metallicity-based threshold.

4.1. Molecular Hydrogen Destruction

One criterion for the end of the first-light epoch can be based on the destruction of molecular hydrogen in the interstellar medium (ISM) due to photons in the Lyman-Werner energy range (\( [11.15:13.6] \) eV) emitted by Population III stars. \( H_2 \) is in fact needed for cooling of the gas in dark matter halos of mass \( \approx 10^6 \) (e.g., see Bromm & Larson 2004). The flux in the Lyman-Werner band is about 7.5% of the ionizing flux (i.e., with an energy range
above 13.6 eV). A Population III star is expected to emit a total of about $7.6 	imes 10^{61}$ photons per solar mass (Stiavelli et al. 2004), so if we assume $300 M_{\odot}$ as a typical mass, we have about $1.7 \times 10^{63}$ H$_2$-destroying photons emitted over the stellar lifetime. Only a fraction $\approx 0.15$ of these photons can effectively destroy an H$_2$ molecule, as the most probable outcome of absorption of a Lyman Werner photon is a first decay to a highly excited vibrational level that later returns to the ground state, with resulting reemitted photons below the 11.15 eV threshold (Shull & Beckwith 1982; Glover & Brand 2001). Therefore we estimate that $\approx 2.5 \times 10^{62}$ H$_2$ molecules will be destroyed by a Population III star. Given the neutral hydrogen number density $6.2 \times 10^{66}$ Mpc$^{-3}$, this means that a Population III star destroys H$_2$ over a volume $4 \times 10^{-5}$ Mpc$^3$/H$_2$, where $\xi$ is the ratio of molecular to atomic hydrogen. Assuming a primordial molecular hydrogen fraction $\xi \approx 10^{-5}$ (e.g., see Peebles 1993), we obtain that a Population III star has the energy to destroy primordial H$_2$ in a volume of $\approx 14$ (Mpc $h^{-1}$)$^3$ (see also the detailed radiative transfer simulations by Johnson et al. 2007). From Figure 6, it is immediately seen that by $z \approx 30$ the Population III number density has reached the critical level of $0.1$ (Mpc $h^{-1}$)$^{-3}$, and therefore around that epoch the radiation background destroys all the primordial H$_2$. Once all the primordial H$_2$ has been cleared, the universe becomes transparent in the Lyman Werner bands, and the new H$_2$ formed during the collapse of gas clouds is dissociated by the background radiation. In fact, assuming that the abundance of H$_2$ formed during collapse is $\xi_{\text{coll}} \approx 5 \times 10^{-4}$ (e.g., see Haiman et al. 2000), this means that a collapsing $10^6 M_{\odot}$ halo produces about $1.3 \times 10^{59}$ H$_2$ molecules, a negligible number with respect to the $2.5 \times 10^{62}$ H$_2$ molecules that are destroyed. Our simple estimate therefore suggests that around $z \approx 30$ the star formation rate of Population III stars in $10^6 M_{\odot}$ halos is greatly suppressed and proceeds in a self-regulated fashion, in which only a fraction $\approx 10^{-3}$ of the collapsing halos are actually able to cool and lead to the formation of massive Population III stars. Eventually, the Lyman Werner background is maintained by Population III stars formed in more massive halos ($M \approx 10^8 M_{\odot}$), cooled by atomic hydrogen and, at later times, by Population II stars.

Inspired by these ideas, we set the end of the primordial epoch for Population III formation at the point where the primordial H$_2$ has been destroyed, that is, around $z \approx 30$. Of course, this is only an order-of-magnitude estimate, and to fully address the feedback due to photodissociating Lyman Werner photons, realistic radiative transfer cosmological simulations are needed, which may even lead to positive feedback (e.g., see Ricotti et al. 2001). In particular, our estimate does not take into account the effects of self-shielding and the fact that the formation timescale for H$_2$ during the halo collapse may be shorter than the timescale for photodissociation by the background radiation. Thus, it is possible that the Population III star formation rate at $z \approx 30$ is not suppressed as much as predicted by our argument. However, our estimate seems to be in broad agreement with the more realistic model by Haiman et al. (2000), which predicts the onset of a significant negative feedback at $z \approx 25$, depending on the assumed efficiency of Lyman Werner photon production.

### 4.2. Metal Enrichment

Another possibility to end the first-star epoch is based on a ISM metallicity threshold. However, in this case a clear transition epoch is missing (e.g., see Scannapieco et al. 2003; Furlanetto & Loeb 2005). This is because metal enrichment, driven by stellar winds whose typical velocities are many orders of magnitude lower than the speed of light, is mainly a local process. Therefore pockets of primordial gas may exist in regions of space that have experienced relatively little star formation, such as voids, even when the average metallicity in the universe is above the critical threshold assumed to define the end of the Population III era.

In any case, this definition provides a longer duration for the first-star era. In fact, to enrich the local metallicity above the $Z = 10^{-4} Z_{\odot}$ threshold, relevant for stopping Population III formation by chemical feedback (see Bromm & Larson 2004), one $300 M_{\odot}$ supernova (SN) must explode for every $\approx 2 \times 10^{8} M_{\odot}$ total mass volume (DM+baryons), assuming on average a Population III mass of $300 M_{\odot}$ with yield 0.2. For a Milky Way–like halo, this means that about 3000 first-star SNe are needed to enrich the intergalactic medium (IGM) to the critical metallicity. According to this definition, the Population III epoch would end within a significant fraction of the total simulated volume around $z \approx 20$, when there is the collapse of dark matter halos originating from 3 $\sigma$ peaks at the $10^9 M_{\odot}$ mass scale (e.g., see Madau & Rees 2001), if the suppression in the Population III star formation rate due to lack of H$_2$ cooling is neglected. A further caveat is that very massive stars may end directly in intermediate-mass black holes without releasing the produced metals in the IGM (Heger & Woosley 2002; Santos et al. 2002).

### 5. Growth of the Population III Black Hole Seeds

From our investigation, it is clear that, before the first Population III progenitor of the most massive halo at $z = 6$ is born, several thousands of intermediate-mass ($m_{\text{BH}} \approx 10^2 M_{\odot}$) black hole seeds are planted by Population III stars formed in a cosmic volume that will on average host a bright $z = 6$ quasar. This result does not allow establishing an immediate correlation between the very first Population III stars created in the universe and the bright $z = 6$ quasars, but neither does it exclude such a link, as the formation epoch for the quasar seed is still at very high redshift ($z \approx 40$), when radiative feedback from other Population III stars already formed is unlikely to affect the formation and evolution of the seed (see § 4.1). Here we investigate with a simple merger tree code what the fate of the black holes seeds formed up to the formation time of the quasar seed is and what the implications are for the observed quasar luminosity function.

We assume Eddington accretion for the black hole (BH) seeds, so that the evolution of the BH mass is given by

$$m_{\text{BH}} = m_0 \exp\left[(t - t_0)/t_{\text{Sal}}\right],$$

where $m_0$ is the mass at formation time $t_0$ and $t_{\text{Sal}}$ is the Salpeter time (Salpeter 1964),

$$t_{\text{Sal}} = \frac{\epsilon m_{\text{BH}} c^2}{(1 - \epsilon)H_{\text{rad}}} = 4.507 \times 10^8 \text{ yr} \frac{\epsilon}{1 - \epsilon},$$

where $\epsilon$ is the radiative efficiency.

Using equation (5), we can immediately see that a difference of $\Delta t \lesssim 2 \times 10^7$ yr, that is, of $\Delta z \approx 10$ at $z = 40$, in the formation epoch of the BH seed of a bright quasar is not too important in terms of the final mass that can be accreted by $z = 6$, as this
corresponds to about half a folding time. Assuming $\epsilon = 0.1$ until $z = 6.4$, the highest redshift in the SDSS quasar sample (Fan et al. 2004), we obtain a ratio of final to initial mass $m_{\text{BH}}/m_0 = 2.62 \times 10^7$ for $z = 50$ and $m_{\text{BH}}/m_0 = 1.78 \times 10^7$ for $z = 40$. Therefore in both cases there has been enough time to build up a $z \approx 6$ supermassive black hole with mass $m_{\text{BH}} \gtrsim 10^9$ starting from a Population III remnant.

This estimate, however, highlights that only a minor fraction of the Population III BH seeds formed before $z = 40$ can accrete mass with high efficiency; otherwise, the number density of supermassive black holes at low redshift would greatly exceed the observational constraints. The first BH seeds in the box are distant from each other, so they evolve in relative isolation, possibly without merging among themselves. Therefore other mechanisms must be responsible for quenching accretion of the first BH seeds. Interestingly, if we were to assume that accretion periods are Poisson-distributed in time for each seed, we would not be able to explain the observed power-law distribution of BH masses at $z \lesssim 6$ around the high-mass end. A Poisson distribution would in fact give too little scatter around the median value and a sharp (faster than exponential) decay of the displacements from the mean accreted mass. An exponential distribution of the accretion efficiency is instead required to match the observed BH mass function. In addition, it is necessary to assume that the duty cycle of the BH accretion is roughly proportional to the mass of the halo it resides in. This is sensible, since an accretion model unrelated to the hosting halo mass may lead to the unphysical result of possibly accreting more mass than the total baryon mass available in that halo. In fact, a BH seed formed at $z \approx 40$ is within a halo of median mass $\approx 10^{11} M_{\odot} h^{-1}$ at $z = 6$, and a few percent of the seeds may be in halos with mass below $\approx 10^9 M_{\odot} h^{-1}$ at that redshift.

To explore this possibility, we follow the merging history of Population III halos formed at $z = 40$ by means of a merger tree code based on Lacey & Cole (1993). We implement a BH growth based on equation (5), but at each step of the tree we limit the BH mass to $m_{\text{BH}} \leq \eta m_{\text{bar}}$, where $m_{\text{bar}}$ is the total baryon mass of the halo that hosts the BH. The results are reported in Figure 7. If the BH growth is not constrained (or only mildly constrained), then a significant fraction of the seeds grow above $10^{10} M_{\odot}$, which would result in an unrealistic number density of supermassive black holes at $z = 6$. However, if $\eta \approx 6 \times 10^{-3}$ (as in Yoo & Miralda-Escudé 2004; see also Wyithe & Loeb 2003), then we obtain an expected mass for the BH powering bright $z = 6$ quasars of $\approx 5 \times 10^9 M_{\odot}$, which is in agreement with the observational constraints from SDSS quasars (Fan et al. 2004).

By fitting a power-law function to the BH mass function in the range $[0.055: 0.2] \times 10^{10} M_{\odot}$, we obtain a slope $\alpha \approx -2.6$, while the slope is $\alpha \approx -3.7$ in the mass range $[0.2: 1.0] \times 10^{10} M_{\odot}$, a value that is consistent within the 1σ error bar with the slope of the bright end of the quasar luminosity function measured by Fan et al. (2004).

Another contribution to ease overproduction of bright quasars may be given by the suppression of the early growth of the Population III BH seeds for the first $\approx 10^8$ yr after formation, that is, for about 2$t_{\text{Sal}}$ (Johnson & Bromm 2007). In fact, the radiation from a Population III star may evacuate most of the gas from its host halo, so that the subsequent BH growth is quenched until a merger provides a new gas reservoir to enable growth at near the Eddington rate (Johnson & Bromm 2007). Also the BH seeds situated in more massive halos would probably be more likely to replenish their gas supply earlier.

6. CONCLUSION

In this paper we investigate the link between the first Population III halos collapsed in a simulation box and the most massive structures at $z \approx 6$, with the aim of establishing the relationship between the first intermediate-mass black holes created in the universe and the supermassive black holes that power the emission of bright $z = 6$ quasars. We show that almost no correlation is present between the sites of formation of the first few hundred $10^5 M_{\odot} h^{-1}$ halos and the most massive halos at $z \lesssim 6$, when the simulation box has an edge of several hundred Mpc. Here the Population III progenitors (halos of mass $M_\odot \approx 10^6 M_{\odot}$) of massive halos at $z \lesssim 6$ formed from density peaks that are $\approx 1.5 \sigma(M_\odot)$ more common than that of the first Population III star in the $(512 \text{ Mpc})^3$ simulation box. These halos virialize around $z_{\text{Sal}} \approx 40$, to be compared with $z_{\text{Sal}} \approx 48$ of the first Population III halo.

This result has important consequences. We show that if bright quasars and supermassive black holes live in the most massive halos at $z \approx 6$, then their progenitors at the $10^6 M_{\odot}$ mass scale are well within the Population III era, regardless of the Population III termination mechanism. On the other hand, if the $m_{\text{BH}}$--$z$ relationship is already in place at $z = 6$, then bright quasars are not linked to the remnants of the very first intermediate-mass black holes (IMBHs) born in the universe, as their IMBH progenitors form when already several thousands of Population III stars have been created within the typical volume that hosts a bright $z = 6$ quasar. The IMBH seeds planted by these very first Population III stars have sufficient time to grow up to $m_{\text{BH}} < [0.2: 1] \times 10^{10} M_{\odot}$ by $z = 6$ if we assume Eddington accretion with radiative efficiency $\epsilon \lesssim 0.1$. Instead, quenching of the BH accretion is required for the seeds of those Population III stars that will not end in massive halos at $z = 6$; otherwise, the number density of supermassive black holes would greatly exceed the observational constraints. One way to obtain growth
consistent with the observations is to limit the accreted mass at a fraction $\eta \approx 6 \times 10^{-3}$ of the total baryon halo mass. This gives a slope of the BH mass function $\alpha = -3.7$ in the BH mass range $m_{\text{BH}} \in [0.2:1] \times 10^{10} \, M_\odot$, which is within the 1 $\sigma$ uncertainty of the slope of the bright end of the $z = 6$ quasar luminosity function ($\alpha \approx -3.5$) measured by Fan et al. (2004).

Another important point highlighted by this study is that rich clusters do not preferentially host the remnants of the first Population III stars. In fact, the remnants of the first 100 Population III stars in our medium-sized simulation box (volume of $(512 \, \text{Mpc} \, h^{-1})^3$) end at $z = 0$ on halos that have a median mass of $3 \times 10^{13} \, M_\odot \, h^{-1}$. This suggests caution in interpreting the results from studies that select a specific volume of the simulation box, such as a rich cluster, and then progressively refine smaller and smaller regions, with the aim of hunting for the first lights formed in the whole simulation (see, e.g., Reed et al. 2005). Only by considering refinements over the complete volume of the box can the rarity and the formation ranking of these progenitors be correctly evaluated.

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**APPENDIX A**

TESTS FOR THE FIRST-LIGHT MONTE CARLO METHOD

To verify the validity of our Monte Carlo method, we perform two main tests. First, we compare the maximum overdensity at the first-light halo mass scale identified over the whole simulation box, using different grid resolutions, including the analytical expectation (that is equivalent to assuming that the whole box is just one cell). The results are reported in Figure 8 and confirm indeed that the method is independent of the grid size, with an excellent match between all the probability distributions computed. The figure was obtained by first generating a Gaussian random field with $\sigma = 0.1$ on a $N = 64^3$ grid and adopting $\sigma_{\text{fs}} = 0.008$ and $k = 4$. Then we progressively bin grid cell values to obtain lower resolution versions of the original field. The variance in the low-resolution grids scales as $(N/64^3)^{1/2}$, and the values for $\sigma_{\text{fs}}$ and $k$ are correspondingly increased. As a second test, shown in Figure 9, we realized a constrained low-resolution ($N = 128^3$) version of the initial conditions for our S1 simulation, and we have then carried out the run down to $z = 6$. From the snapshot at $z = 6$, we identify the most massive halos in this simulations, verifying that there is a good spatial and mass match with the original 512$^3$ run. The redshift distribution of the first Population III progenitor for the most massive halos was computed using our method and compared with that of the original run. The agreement is very good, especially considering that the dynamics of the dark matter halos was followed at a resolution 64 times lower.

![Fig. 8.—Probability distribution for the maximum density fluctuation at first-light scale ($\sigma_n$) in a synthetic test of the refinement method obtained generating first a Gaussian random field with $\sigma = 0.1$ on a $N_0 = 64^3$ grid, and then applying our MC method with a refinement factor of 4, subgrid fluctuations $\sigma_{\text{fs}} = 0.08$, and 400 Monte Carlo realizations. We progressively downgrade the resolution of the simulation grid to $N_0 = 32$ and 16, increasing $\sigma_{\text{fs}}$ following our prescription. The MC sampling results are compared with the theoretical probability distribution for $\sigma_n$ (dashed line). [See the electronic edition of the Journal for a color version of this figure.]](image_url)
Fig. 9.—Probability distribution for the earliest Population III star in the two most massive halos of the S1 run obtained from the full resolution (dashed line) and from a lower resolution constrained realization of the same initial conditions (solid line). [See the electronic edition of the Journal for a color version of this figure.]

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