The impact of reionization on the formation of supermassive black hole seeds

Jarrett L. Johnson,† Daniel J. Whalen, Bhaskar Agarwal, Jan-Pieter Paardekooper and Sadegh Khochfar

1 X Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
2 Zentrum für Astronomie, Institut für Theoretische Astrophysik, Universität Heidelberg, Albert-Ueberle-Str. 2, D-69120 Heidelberg, Germany
3 Max-Planck-Institut für extraterrestrische Physik, Giessenbachstraße, D-85748 Garching, Germany
4 Institute for Astronomy, University of Edinburgh, Royal Observatory, Edinburgh EH9 3HJ, UK

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ABSTRACT

Direct collapse black holes (DCBHs) formed from the collapse of atomically cooled primordial gas in the early Universe are strong candidates for the seeds of supermassive BHs. DCBHs are thought to form in atomic cooling haloes in the presence of a strong molecule-dissociating, Lyman–Werner (LW) radiation field. Given that star-forming galaxies are likely to be the source of the LW radiation in this scenario, ionizing radiation from these galaxies may accompany the LW radiation. We present cosmological simulations resolving the collapse of primordial gas into an atomic cooling halo, including the effects of both LW and ionizing radiation. We find that in cases where the gas is not self-shielded from the ionizing radiation, the collapse can be delayed by \( \sim 25 \) Myr. When the ionized gas does collapse, the free electrons that are present catalyse \( \text{H}_2 \) formation. In turn, \( \text{H}_2 \) cooling becomes efficient in the centre of the halo, and DCBH formation is prevented. We emphasize, however, that in many cases the gas collapsing into atomic cooling haloes at high redshift is self-shielding to ionizing radiation. Therefore, it is only in a fraction of such haloes in which DCBH formation is prevented due to reionization.

Key words: ISM: molecules – quasars: supermassive black holes – cosmology: theory – early universe.

1 INTRODUCTION

The origin of the black holes (BHs) inhabiting the centres of massive galaxies (e.g. Gebhardt et al. 2000; Merritt & Ferrarese 2001) and powering luminous quasars at high redshift (e.g. Willott, McLure & Jarvis 2003; Fan et al. 2006; Mortlock et al. 2011) has long been an open question at the forefront of cosmology and galaxy formation. There is a strong possibility that many of these grew from seed BHs which were born with masses of \( 10^4 - 10^6 \) \( M_\odot \) in the centres of atomic cooling dark matter (DM) haloes in the early Universe (e.g. Natarajan & Volonteri 2012; Volonteri 2012). In this scenario, the primordial gas within the halo is unable to cool below \( \sim 10^4 \) K (e.g. Spaans & Silk 2006) because of low abundance of \( \text{H}_2 \) molecules, which implies that runaway gravitational collapse only occurs once up to \( \sim 10^6 \) \( M_\odot \) of gas has accumulated in the centre of the halo. The central objects that form from this collapse, likely short-lived supermassive stars (e.g. Fuller, Woosley & Weaver 1986; Hosokawa et al. 2013) or quasi-stars (e.g. Begelman, Rossi & Armitage 2008), grow at rates of up to \( 1 \) \( M_\odot \) yr\(^{-1} \) (Wise, Turk & Abel 2008; Regan & Haehnelt 2009; Shang, Bryan & Haiman 2010; Johnson et al. 2011; Latif et al. 2013a; Prieto, Jimenez & Haiman 2013) and are believed to typically leave behind BHs with masses of up to \( 10^6 \) \( M_\odot \) (e.g. Choi, Shlosman & Begelman 2013). BHs formed via this process are referred to as direct collapse black holes (DCBHs).

In DCBH formation, the \( \text{H}_2 \) fraction is typically considered to be suppressed by a strong molecule-dissociating, Lyman–Werner (LW) radiation field (e.g. Haiman, Abel & Rees 2000; Glover & Brand 2001; Machacek, Bryan & Abel 2001; Ahn et al. 2012). While an elevated LW radiation field is likely required to sufficiently suppress \( \text{H}_2 \) cooling during the collapse of the gas (e.g. Bromm & Loeb 2003; Shang et al. 2010; Van Borm & Spaans 2013; Visbal, Haiman & Bryan 2014a), the results of both semi-analytic models (e.g. Dijkstra et al. 2008; Agarwal et al. 2012; Petri, Ferrara & Salvaterra 2012; Fernandez et al. 2014; Ferrara et al. 2014; Visbal, Haiman & Bryan 2014b) and cosmological simulations (Agarwal et al. 2014) suggest that such fields may have been produced regularly in the early universe and therefore that DCBH formation may

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1 We note that a small fraction of supermassive stars may instead explode as powerful supernovae and leave behind no remnant (e.g. Montero, Janka & Müller 2012; Chen et al. 2014).

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have been relatively common. This conclusion has been strengthened by complementary modelling of the growth (e.g. Johnson et al. 2012; Latif et al. 2013b; Regan, Johansson & Haehnelt 2014) and evolution (e.g. Begelman 2010; Hosokawa, Omukai & Yorke 2012; Hosokawa et al. 2013; Inayoshi, Hosokawa & Omukai 2013; Schleicher et al. 2013) of the supermassive stellar progenitors of DCBHs, which suggests that their growth to mass scales of up to $10^8 \, M_\odot$ is not likely impeded by radiative feedback or pulsational instability. Indeed, there is a strong possibility that DCBH remnants still reside in present-day galaxies (Koushiappas, Bullock & Dekel 2004; Bellovary et al. 2011; Devecchi et al. 2012; Greene 2012; Reines et al. 2014), including our Milky Way (Rashkov & Madau 2014) and its satellites (van Wassenhove et al. 2010).

While the elevated LW radiation fields required for widespread DCBH formation may have been produced in the early Universe, it is likely that in many cases other forms of radiation accompanied them. In particular, given that the sources of this radiation were likely early star-forming galaxies, ionizing radiation from stars, X-rays from young accreting BHs and cosmic rays from early supernovae may have commonly been present, in addition to LW radiation. Using one-zone models of primordial gas collapse in atomically cooled haloes, Inayoshi & Omukai (2011) addressed the role that X-rays and cosmic ray ionization may have played in the process of DCBH formation, finding that the free electron population generated deep in the cores of the haloes could have catalysed the rapid formation of H$_2$ molecules, leading to cooling of the primordial gas to temperatures well below $10^4$ K and preventing DCBH formation. In addition, Yue et al. (2014) have recently developed a semi-analytic model in which DCBH formation is halted once the Universe becomes reionized, due to the photoevaporation of the gas from atomic cooling haloes.

Here, we address the effects of ionizing radiation on the formation of DCBHs using cosmological simulations that track both the elevated LW radiation field required for DCBH formation as well as an accompanying ionizing radiation field. In Section 2, we describe the methodology used to model the effects of background ionizing and LW radiation fields. In Section 3, we present the results of our simulations. Finally, in Section 4, we give a brief discussion of our results.

2 METHODOLOGY

Here, we describe the approach that we have taken to model the impact of a photoionizing background on the process of DCBH formation. We have carried out two cosmological simulations employing the same version of the smoothed particle hydrodynamics (SPH) code GADGET (Springel, Yoshida & White 2001; Springel & Hernquist 2002) that we have employed in previous work (see e.g. Johnson et al. 2011, 2013). We make use of the same initial conditions as in those previous works, namely a 1 Mpc$^3$ (comoving) cosmological volume which is initialized at $z = 100$ and within which an atomic cooling halo is identified at $z \cong 15$, at which time its DM mass is $\cong 4 \times 10^7 \, M_\odot$ (corresponding roughly to a 3$\sigma$ fluctuation). It is the evolution of the primordial gas during its collapse into this halo that is the focus of our study.

In both of these simulations, we use the same prescription for the LW background radiation field that we have employed in the previous works cited above. This consists of a constant uniform background LW field with an intensity characterized by $J_{21} = 10^3$, with a spectrum characterized by a temperature of $\sim 10^4$ K (Shang et al. 2010). We account for the self-shielding of H$_2$ molecules to this radiation by calculating the H$_2$ self-shielding factor, which expresses the fraction of the unattenuated background LW flux to which a gas parcel is exposed, using an estimate based on the local column density of H$_2$ molecules (Bromm & Loeb 2003; see also Shang et al. 2010; Wolcott-Green, Haiman & Bryan 2011).

Along with this constant (in time) and uniform LW radiation field, we model the effect of an accompanying constant uniform ionizing radiation field. We adopt the following value for the local photoionization rate, assuming a ratio of ionizing photons to LW photons appropriate for a low-metallicity stellar population with an age of $\sim 10^7$ yr (Leitherer et al. 1999)

$$\Gamma_{\ion} = 1.5 \times 10^{-11} \mathrm{e}^{-\tau_{\ion}} \, \mathrm{s}^{-1},$$

(1)

where $\tau_{\ion}$ is the local optical depth to ionizing photons, estimated as described below. The value this obtains for the unattenuated photoionization rate (with $\tau_{\ion} = 0$) is chosen to be consistent with our choice of $J_{21} = 10^3$ for the unattenuated LW flux, assuming a value for the ratio of the escape fraction of ionizing photons to the escape fraction of LW photons for the galaxies producing the radiation of $f_{\text{esc}} / f_{\text{esc}, \text{LW}} \sim 0.3$, which is in broad agreement with estimates gleaned from simulations of early dwarf galaxies (e.g. Ricotti, Gnedin & Shull 2001; Kitayama et al. 2004; Wise & Cen 2009; Razoumov & Sommer-Larsen 2010; Paardekooper, Khochar & Dalla Vecchia 2013). For the corresponding photoheating rate, we conservatively assume that $\sim 2$ eV is deposited in the gas as heat for each photoionization.

We adopt a local approximation for the flux of ionizing photons to which a given parcel of gas is exposed, by estimating the optical depth to ionizing photons as

$$\tau_{\ion} = \sigma_{\ion} n_{\text{H}} r_{\text{char}} \simeq 10^2 \left( \frac{h \nu}{13.6 \, \text{eV}} \right)^{-3} \left( \frac{n_{\text{H}}}{1 \, \text{cm}^{-3}} \right) \left( \frac{r_{\text{char}}}{5 \, \text{pc}} \right),$$

(2)

where $\sigma_{\ion} \simeq 6 \times 10^{-18} \, \text{cm}^{-2} (h \nu/13.6 \, \text{eV})^{-3}$ is the cross-section for photoionization of neutral hydrogen, $n_{\text{H}}$ is the local density of neutral hydrogen atoms and $r_{\text{char}}$ is the physical size-scale appropriate for the parcel of gas, which we take to be defined in terms of the mass $m_{\text{SPH}} = 120 \, M_\odot$ of an SPH particle in our simulation

$$r_{\text{char}} = \left( \frac{3 m_{\text{SPH}}}{4 \pi \rho} \right)^{1/3} \simeq 10 \left( \frac{n_{\text{H}}}{1 \, \text{cm}^{-3}} \right)^{-1/3} \, \text{pc}.$$

3 We refer to the standard convention and assign to $J_{21}$ units of $10^{-21}$ erg s$^{-1}$ cm$^{-2}$ Hz$^{-1}$ sr$^{-1}$.

4 While the LW background radiation is turned on at $z = 100$ in our simulations, the ionizing background is turned on at $z = 30$ in our fiducial case. In Appendix A, we discuss the impact of turning the ionizing background on later, at $z = 20$.

5 We note that if a smaller fraction of ionizing photons relative to LW photons escape from source galaxies or if the stellar population is much older than $\sim 10^7$ yr, then the photoionization rate we have adopted will be an overestimate. In particular, the rate, normalized to the LW flux, may be roughly two orders of magnitude lower for a population age of $\sim 10^7$ yr (e.g. Leitherer et al. 1999), although we emphasize that in the early Universe (e.g. at $z \gtrsim 6$) the stars producing the bulk of the LW flux are likely much younger than this.

6 We evaluate this cross-section at $h \nu = 15.6$ eV, consistent with the 2 eV that we assume is deposited in the gas for each photoionization.
where \( \rho \) is the gas density at the location of the SPH particle. Note that we have normalized equations (2) and (3) for a neutral primordial gas; in particular, the optical depth can be \( \tau_{\text{ion}} \ll 1 \), where the gas is highly ionized.

While this method provides a simple approximation for the local ionization and heating rates, as discussed further in Appendix A, we expect that our local estimate for the optical depth to ionizing photons (equation 2) is valid. This is supported by the fact that the results of our simulations for the gas density and collapse redshift required for self-shielding from ionizing radiation are in very good agreement with the detailed estimates recently presented by Noh & McQuinn (2014, see their equations 6 and 7). Our results are also consistent with those found by Dijkstra et al. (2004) for the conditions required for the gas in high-redshift haloes to self-shield against an intergalactic photoionizing background. These authors found that the gas self-shields more readily at high redshift due to the higher densities in virialized haloes. The atomic cooling halo we focus on in our simulations, and into which gas does collapse in the presence of an ionizing background, has a circular velocity of \( \simeq 20 \, \text{km s}^{-1} \) at \( z \simeq 15 \), which is higher than the minimum circular velocity that Dijkstra et al. (2004) find is required to retain gas in the presence of a photoionizing background at this redshift.

Furthermore, this is also consistent with the results of Okamoto, Gao & Theuns (2008), who found from cosmological simulations that haloes with circular velocities \( \gtrsim 10 \, \text{km s}^{-1} \) are able to retain a large fraction of their baryonic mass at \( z \gtrsim 10 \). This agreement with previous work gives us confidence that our approach produces reliable results.

### 3 Results

Here, we compare the results of our two simulations, highlighting the effects of the ionizing background on the evolution of the primordial gas. As we shall see, this radiation can profoundly alter the final outcome of the collapse of the gas.

Fig. 1 shows the properties of the gas within a 10 pc (physical) slice of the simulation volume, centred on the atomic cooling halo, the location of the virial radius of which is denoted by the white dashed circles (but is suppressed in the bottom-right panel, for clarity). From left to right, we show the temperature, number density of hydrogen atoms and the radial velocity if the gas relative to the centre of the halo, for our simulation with LW and ionizing radiation included (top) and for our simulation including only LW radiation (bottom). The impact of the ionizing background radiation is to heat the gas in the IGM and to evaporate it out of the filaments that feed the central halo. This results in slower infall of gas into the centre of the halo, as evidenced by the smaller infall (negative) velocities in the case with ionizing radiation included, as compared to the LW only case. This results in a delay of \( \Delta z \simeq 1 \) (\( \simeq 25 \, \text{Myr} \)) in the onset of runaway gravitational collapse at the centre of the halo.
The same as Fig. K to which the gas can cool in \( \sim 200 \) K, roughly showing the properties of the gas in the central halo, as in the case with just LW radiation, at large distances the gas is highly ionized and is almost entirely heated to temperatures up to \( \sim 10^4 \) K. At distances \( \lesssim 100 \) pc, the gas is self-shielded to the ionizing radiation and can collapse to high densities. Due to the higher free electron fraction of the collapsing gas in the case with ionizing radiation, at high densities the formation of H\(_2\) is catalysed (via the same reactions through which H\(_2\) is generally formed in the primordial gas; see e.g. Bromm & Larson 2004) and a much larger fraction of H\(_2\) is generated than in the case with just LW radiation.

Due to the higher H\(_2\) fraction in the case with ionizing radiation, the gas is able to cool via molecular transitions down to \( \sim 200 \) K, as is typical for Population (Pop) III star formation in minihaloes (see e.g. Clark et al. 2011; Greif et al. 2011). These temperatures are much lower than the \( \sim 10^4 \) K to which the gas can cool in the case with LW radiation only. The corresponding accretion rates on to the objects that form via the runaway gravitational collapse of the gas at the centre of the halo are expected to be very different, because of the large difference in the gas temperature (e.g. Omukai & Palla 2003)

\[
\frac{dM_{\text{acc}}}{dt} \sim 10^{-3} \left( \frac{T}{200 \text{ K}} \right)^{3/2} M_\odot \text{ yr}^{-1}.
\]

Using the temperatures at the centre of the halo shown in Figs 2 and 3, for the cases with and without ionizing radiation, this corresponds roughly to \( \sim 10^{-3} \) and \( \sim 10^{-4} M_\odot \text{ yr}^{-1} \), respectively. Again, the former is consistent with Pop III star formation in which H\(_2\) cooling is effective, while the latter is consistent instead with the formation of a supermassive star (or binary supermassive stars; see e.g. Regan & Haehnelt 2009; Whalen et al. 2013) with a mass of \( \sim 10^5 M_\odot \) (e.g. Wise et al. 2008; Shang et al. 2010; Johnson et al. 2012; Latif et al. 2013b). From this, we can conclude that when there is only LW radiation it is likely that a supermassive star (and subsequently a DCBH) will form, while in the case with both LW and ionizing radiation a small galaxy composed of Pop III stars with masses \( \lesssim 10^5 M_\odot \) will likely form instead (e.g. Hirano et al. 2014).

Fig. 4 shows the enclosed mass of H\(_2\) as a function of distance from the centre of the halo, in both simulations. The much higher H\(_2\) mass in the case with ionizing radiation, leads to strong self-shielding of the gas to LW radiation, as shown in Fig. 5. This effective self-shielding in turn implies that the H\(_2\) photodissociation rate in the centre of the halo is much lower than in the case with just LW radiation. This leads to a higher H\(_2\) fraction, which in turn leads to stronger self-shielding of the gas. Thus, there is a runaway process of H\(_2\) formation and self-shielding, set up by the fact that the gas collapses into the halo with an elevated free electron fraction because it was photoionized in the IGM. The slower formation of H\(_2\) in the case with just LW radiation leads to weaker self-shielding and, ultimately, to the weak molecular cooling and higher temperatures that set the stage for the formation of a DCBH.

Fig. 6 shows both the mass enclosed and the radially averaged Jeans mass of the gas, as a function of the distance from the centre of the halo, for both simulations. Runaway gravitational collapse is...
Figure 4. The mass in $\text{H}_2$ molecules enclosed, as a function of distance from the centre of the atomic cooling halo, in our two simulations at the same redshifts as shown in the previous figures. Due to the elevated free electron fraction in the case with photoionization, a larger mass of $\text{H}_2$ builds up than in the case with just LW radiation. This leads to the gas becoming self-shielding to LW radiation, as shown in Fig. 5.

Figure 5. The factor by which the $\text{H}_2$-dissociating LW flux is decreased due to local self-shielding of the $\text{H}_2$ molecules, as a function of distance from the centre of the host halo. Shown are the radially averaged values of this factor, for LW and photoionizing background radiation fields (blue) and for just an LW background radiation field (orange), at the same times as shown in the previous figures. The elevated $\text{H}_2$ fraction in the simulation including ionizing radiation leads to much stronger self-shielding of the molecules, which allows for efficient formation of $\text{H}_2$.

possible when the enclosed mass exceeds the Jeans mass. As shown in Figs 6 and 7, there is a factor of a few less gas in the centre of the halo in the case with ionizing radiation. However, due to the lower temperatures of the gas in this case, we expect that the central $\lesssim 10^4 \, M_\odot$ of gas becomes Jeans unstable and undergoes runaway gravitational collapse, while in the case with just LW radiation the gas is Jeans unstable at a much larger mass scale of $\sim 10^5 \, M_\odot$. This is again consistent with our expectation that a supermassive star, and subsequently a DCBH, will form in the case with just LW radiation, while a small Pop III galaxy will instead form in the case including ionizing radiation.

Figure 6. The mass enclosed (solid lines) and the radially averaged Jeans mass (dotted lines), as functions of the distance from the centre of the host atomic cooling halo, with LW and photoionizing background radiation fields (blue) and with just an LW background radiation field (orange), at the same times as shown in previous figures. Also shown is the mass contained in the SPH smoothing kernel in our simulations, $m_{\text{res}}$, which roughly corresponds to the minimum mass that can be resolved. The gas is only able to collapse under its own gravity when the enclosed mass is larger than the Jeans mass. In the case with LW and ionization this occurs at a mass scale of a few $\times 10^3 \, M_\odot$, whereas in the case with only LW radiation this occurs at a mass scale of $\sim 10^5 \, M_\odot$. In the former case, the mass scale is too small for the formation of a DCBH, whereas it is sufficiently large for a DCBH to form in the latter.

Figure 7. The ratio of the mass enclosed in the simulation including both LW and ionizing radiation to that including only LW radiation, as a function of distance from the centre of the host atomic cooling halo. Due to the higher pressure of the gas in the simulation including ionizing radiation, the accretion rate into the centre of the halo is lower than in the case without it and the mass enclosed within the virial radius at $r \approx 500$ pc is lower by a factor of $\approx 3$. Note that, as shown in Fig. 6, the mass within $r \approx 2$ pc is not well resolved in our simulation.

4 DISCUSSION

We have presented a pair of cosmological simulations which demonstrate that it is possible for ionizing radiation to prevent DCBH formation in atomic cooling haloes. We find that this is due to the
large free electron fraction in the photoionized gas, which leads to the rapid formation of H$_2$ and ultimately to effective molecular cooling that stabilizes the halo for DCBH formation. We expect that a small Pop III galaxy with up to $\sim10^5$ M$_\odot$ in primordial stars may form, instead, similar to previously studied cases of Pop III star formation in atomic cooling haloes including just a background LW radiation field (e.g. Oh & Haiman 2002; Trenti & Stiavelli 2009; Safranek-Shrader et al. 2012).

We emphasize that this effect relies on the gas being photoionized before its collapse into the centre of the halo. In cases where the ionizing radiation turns on at relatively late times, when the gas in the halo has already collapsed to densities at which it is self-shielded from the ionizing radiation, we do not expect that a large H$_2$ fraction develops, and indeed it is likely that DCBH formation is still able to take place in this case. In Appendix B, we present one such case, in which the ionizing background turns on at $z = 20$, by which time the dense gas in the halo is already self-shielded from the ionizing radiation. Indeed, we find that in this case the collapse of the self-shielded gas proceeds almost identically to the case with just LW radiation (compare Figs 3 and B1). Because many atomic cooling haloes may be self-shielding to ionizing radiation, especially in the early stages of reionization (see e.g. Noh & McQuinn 2014), DCBH formation may still take place readily at $z \gtrsim 15$ even in photoionized regions.

We note that this picture is in basic agreement with that presented by Yue et al. (2014), who argue that in photoionized regions the gas cannot be retained by atomic cooling haloes at $z \lesssim 14$, and so DCBHs will not likely form in photoionized regions below this redshift. Our result is related, but distinct – we find that if the gas in atomically cooling haloes is subject to an elevated ionizing radiation background and cannot self-shield against it, then DCBH formation can be prevented even if the gas is retained in the halo. We also emphasize that, because reionization is an inhomogeneous process, it should in principle be possible for DCBHs to form at redshifts $z \lesssim 14$ in regions which are not yet reionized; consistent with this, Agarwal et al. (2014) find that DCBHs may form down to at least $z \sim 9$.

Our results suggest that, when ionizing radiation accompanies a background LW radiation field the critical LW flux required for DCBH formation is likely to be significantly higher than in the absence of ionizing radiation. As we adopted $J_{21} = 10^3$ for our simulations, it appears that the critical flux for photoionized gas may be well above this value, although this is likely to vary with redshift and may be a function of the growth history of the halo (see e.g. Latif et al. 2014). This correction could lead to reduced estimates of the prevalence of DCBHs in the early Universe, as compared to previous results (see e.g. Dijkstra et al. 2008; Shang et al. 2010; Agarwal et al. 2012, 2014; Latif et al. 2014), at least in reionized regions.

Related to the question of the critical LW flux, we note that here we have followed the approach of similar works (e.g. Bromm & Loeb 2003; Shang et al. 2010) and adopted the approximation given by Draine & Bertoldi (1996) for the H$_2$ self-shielding factor. As shown by Shang et al. (2010) and Wolcott-Green et al. (2011), this likely overestimates the shielding factor, and so may lead to overestimates of the critical LW flux required to suppress molecular cooling (but see also Richings, Schaye & Oppenheimer 2014). Therefore, the critical flux for the halo in our simulations may in fact be significantly lower than the $J_{21} = 10^3$ that we adopted. As we have used the same self-shielding prescription in our simulations both with and without ionizing radiation, we do not expect that using an improved prescription would qualitatively change our central results pertaining to the effects of ionizing radiation. That said, it may be crucial to model in great detail both the photodissociation of H$_2$ molecules and the transfer of the H$_2$ line emission that can cool the gas (e.g. Greif 2014), in order to determine the final fates of atomic cooling haloes exposed to elevated levels of LW radiation.

We expect that the Pop III galaxies that form in cases in which ionizing radiation prevents DCBH formation may contain significantly more mass in primordial stars than the stellar clusters formed in smaller minihaloes. This follows from the fact that the relatively deep DM gravitational potential wells of atomic cooling haloes allow the gas to be more readily retained in the face of stellar feedback than in the case of Pop III star formation in minihaloes (see e.g. Bromm & Yoshida 2011). Due to their higher masses, we expect that Pop III galaxies formed in atomic cooling haloes may be among the most luminous Pop III star-forming objects, with distinct observational signatures that could be detected by future missions such as the James Webb Space Telescope (see e.g. Schaerer 2003; Johnson 2010; Inoue 2011; Zackrisson et al. 2011; Pawlik, Milosavljević & Bromm 2013).

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APPENDIX A: LOCAL APPROXIMATION FOR THE PHOTOIONIZATION RATE

Our approach to modeling the impact of an ionizing background radiation field, as described in Section 2, relies on a simple, local estimate of its attenuation. In particular, it is assumed that the attenuation of the field largely takes place over a length-scale comparable to, or smaller than, that of an individual SPH particle. Here, we show that this assumption is valid.

The optical depth to ionizing radiation over the length-scale of a parcel of gas represented by a single SPH particle, under the assumption of a neutral medium, is given by equation (2). Evaluated at a photon energy of 15.6 eV (as we assume in our calculations; see Section 2) and expressing this length-scale following equation (3), the optical depth becomes

$$\tau_{\text{ion}} \simeq 1.3 \times 10^2 \left( \frac{n_{\text{H}}}{1 \text{ cm}^{-3}} \right)^{2/3}.$$  \hspace{1cm} (A1)

As shown in Figs 2 and 3, the density profile of the atomic cooling halo in our simulations can be approximated as isothermal, with the number density of hydrogen nuclei approximated as $n_{\text{H}} \simeq 10^5 (r/\text{pc})^{-2}$. Using this expression in the above formula for optical depth, we obtain

$$\tau_{\text{ion}} \simeq 3 \times 10^3 \left( \frac{r}{\text{pc}} \right)^{-4/3}.$$  \hspace{1cm} (A2)

where $r$ is the distance from the centre of the halo. This implies that in neutral regions the optical depth is large, i.e. that $\tau_{\text{ion}} \gtrsim 1$, over the length-scale of an SPH particle at $r \lesssim 10^4 \text{ pc}$. Therefore, we expect our approximation to be valid in the dense central regions of the halo, at $r \sim 100 \text{ pc}$, within which we find the gas to be optically thick to the external ionizing radiation field.

APPENDIX B: EVOLUTION OF SELF-SHIELDED GAS

Here, we briefly highlight the results of a simulation in which the ionizing background turns on at $z = 20$, in order to highlight the dependence of our results on the state of the halo when first subjected to the ionizing background. By this redshift, the dense gas in the halo is already self-shielding to the ionizing radiation and it is never photoionized. We note that the gas becoming self-shielded already by $z = 20$ in this halo is consistent with the recent analytical estimates presented by Noh & McQuinn (2014), as well as with the results of previous numerical simulations cited in Section 2 (Dijkstra et al. 2004; Okamoto et al. 2008).
Fig. B1. The same as Figs 2 and 3, but for our simulation in which the photoionizing background is turned on at $z = 20$. In this case, the gas in the halo has already collapsed to relatively high density by this redshift and the dense core of the halo is self-shielding to the ionizing radiation. As a result, the free electron fraction in the dense gas is not elevated relative to the case with just LW radiation and the $\text{H}_2$ fraction also remains low (compare to Fig. 3). Therefore, in this case and in others where the dense gas in the core of the halo is not self-shielding to the radiation and never becomes photoionized, we expect that DCBH formation is not prevented and likely proceeds just as in the case with only LW radiation.