Gravitational waves from Population III binary black holes formed by dynamical capture

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ABSTRACT

We use cosmological hydrodynamic simulations to study the gravitational wave (GW) signals from high-redshift binary black holes (BBHs) formed by dynamical capture (ex-situ formation channel). We in particular focus on BHs originating from the first generation of massive, metal-poor, so-called Population III (Pop III) stars. An alternative (in-situ) formation pathway arises in Pop III binary stars, whose GW signature has been intensively studied. In our optimistic model, we predict a local GW event rate density for ex-situ BBHs (formed at \(z > 4\)) of \(\sim 0.04 \text{ yr}^{-1} \text{ Gpc}^{-3}\). This is comparable to or even higher than the conservative predictions of the rate density for in-situ BBHs \(\sim 0.01 - 0.1 \text{ yr}^{-1} \text{ Gpc}^{-3}\), indicating that the ex-situ formation channel may be as important as the in-situ one for producing GW events. We also evaluate the detectability of our simulated GW events for selected planned GW instruments, such as the Einstein Telescope (ET). For instance, we find the all-sky detection rate with signal-to-noise ratios above 10 to be \(\lesssim 100 \text{ yr}^{-1}\) for the xylophone configuration of ET. However, our results are highly sensitive to the sub-grid models for BBH identification and evolution, such that the GW event efficiency (rate) is reduced by a factor of 4 (20) in the pessimistic case. The ex-situ channel of Pop III BBHs deserves further investigation with better modeling of the environments around Pop III-seeded BHs.

Key words: early universe – dark ages, reionization, first stars – gravitational waves

1 INTRODUCTION

The detection of gravitational waves (GWs) from merging compact objects, such as black holes (BHs) and neutron stars, has opened a new observational window in astrophysics, cosmology and fundamental physics (reviewed by, e.g. Barack et al. 2019). The statistics of GW events will place new constraints on a variety of astrophysical processes, such as cosmic star formation, the BH mass distribution, the formation and evolution of compact binaries, and cosmology (e.g. Fishbach et al. 2018; Vitale et al. 2019; Perna et al. 2019; Safarzadeh & Berger 2019; Farr et al. 2019; Adhikari et al. 2020; Tang et al. 2020; Safarzadeh 2020). The population of binary black holes (BBHs), as detected by the Laser Interferometer Gravitational-wave Observatory (LIGO) collaboration (Abbott et al. 2019a), is dominated by massive systems (\(\gtrsim 10 \text{ M}_\odot\)), including binaries with inferred total masses above \(\sim 40 \text{ M}_\odot\) (e.g. GW170729 and GW170817), which indicates that they originate from massive progenitor stars over a range of redshifts. However, it remains a mystery how such massive BBHs are formed and evolved to merge across cosmic time. Numerous scenarios have been proposed (e.g. Belczynski et al. 2016; Rodriguez et al. 2016b; Di Carlo et al. 2019; Conselice et al. 2019), involving a variety of astrophysical processes, such as the evolution of binary stars and mergers of ultra-dwarf galaxies.

Over the next decades, more advanced GW instruments will come into operation, including high-frequency ground-based detectors for stellar-mass BHs (SBHs), such as improved versions of LIGO and Virgo (Abbott et al. 2018, 2019b), as well as the Kamioka Gravitational Wave Detector (KAGRA). Intermediate-mass BHs (IMBHs) will be targeted with the third-generation instruments, such as the Einstein Telescope (ET; Punturo et al. 2010; Gair et al. 2011), the Cosmic Explorer (CE; Abbott et al. 2017), and the Decihertz-class Observatories (DOs; Arca Sedda et al. 2019; Kuns et al. 2019). Finally, low-frequency arrays in space will probe the high-mass end of the BBH range, such as the Laser Interferometer Space Antenna (LISA; Robson et al. 2019), and the TianQin observatory (Feng et al. 2019). These facilities will cover a large range in frequency and mass (\(\sim 1 - 10^7 \text{ M}_\odot\)), thus providing us a clear portrait of BH populations over cosmic time, in a wide spectrum of host systems. Combined with theoretical predictions, GW
observations will be a powerful probe of early structure formation (Sesana et al. 2009, 2011; Fragione et al. 2018a; Jani et al. 2019). Furthermore, the GW window ideally complements the electromagnetic (EM) one. The latter is biased towards massive/luminous systems at high redshifts, as EM signals decay rapidly with distance ($\propto d^{-2}_L$). While the amplitudes of GWs decay slower with distance ($\propto d^{-4}_L$), and BBHs formed in the early Universe can merge at lower redshifts, reflecting their long delay times.

On the theory side, the goal is to self-consistently predict the GW signals of high-z BBHs, originating from different channels of BH seeding and growth, as well as addressing the rich physics of BBH formation and evolution. A specific challenge is that physical processes on vastly different scales are involved, many of which are poorly understood. Currently, there are three main models for high-z BH seeds: (i) remnants of the first generation of massive, metal-free Population III (Pop III) stars with seed masses $M_{\text{BH}} \sim 40 – 140 M_\odot$ (e.g. Bond et al. 1984; Schneider et al. 2000; Madau & Rees 2001; Bromm & Yoshida 2011; Hirano et al. 2014), (ii) runaway collisions in dense star clusters with $M_{\text{BH}} \sim 10^3 – 10^4 M_\odot$ (e.g. Devecchi & Volonteri 2009; Katz et al. 2015); and (iii) rapid infall of primordial gas in peculiar environments leading to direct-collapse BHs (DCBHs) with $M_{\text{BH}} \sim 10^4 M_\odot$ (e.g. Bromm & Loeb 2003; Volonteri 2010; Johnson & Haardt 2016; Mais 2019; Smith & Bromm 2019; Inayoshi et al. 2019). The first two models produce relatively light seeds dominating in number, while seeds in the third class are believed to be rare, but important to explain the observed luminous quasars at high-z, powered by supermassive BHs (SMBHs) with masses up to $\sim 10^9 M_\odot$ (e.g. Schleicher et al. 2013; Dunn et al. 2018; Becerra et al. 2018; Wise et al. 2019; Regan et al. 2019; Basu & Das 2019).

For high-z BBHs in turn, there are two formation channels: (i) in-situ formation from binary Pop III stars, and (ii) ex-situ formation by dynamical capture of two BHs, either born into one dense star cluster, or from two originally separate formation sites (e.g. during galaxy mergers). The first channel has been intensely studied before and after the first LIGO detection (e.g. Kinugawa et al. 2014, 2015; Dvorkin et al. 2016; Hartwig et al. 2016; Inayoshi et al. 2016b; Belczynski et al. 2017; Mapelli et al. 2019). The local $(z \sim 0)$ intrinsic merger rate density of in-situ BBHs is predicted to be $\sim 0.1 – 100$ yr$^{-1}$ Gpc$^{-3}$, where the disagreement among different studies is dominated by uncertainties in the initial binary parameters and evolution models for Pop III binary stars (e.g. Stacy & Bromm 2013; Kinugawa et al. 2014; Belczynski et al. 2017). It remains unclear whether such in-situ Pop III-seeded BBHs contribute a significant fraction to the LIGO estimate of $9 – 240$ yr$^{-1}$ Gpc$^{-3}$ (Abbott et al. 2019a).

The second channel has been studied with semi-analytical models (e.g. Sesana et al. 2009, 2011; Dayal et al. 2019) in the context of cosmic structure formation. For instance, the detection rate for ET is predicted to be $\lesssim 2$ yr$^{-1}$ (Sesana et al. 2009) with signal-to-noise ratios (SNRs) above 6, while that for LISA (with SNR $> 7$ at $z > 4$) is $\sim 3 – 5$ yr$^{-1}$ (Dayal et al. 2019). However, in principle the dynamical capture process can only be modelled properly with cosmological simulations, as complex dynamics of BHs embedded in gas and stars is involved, which has been shown non-trivial in previous studies (e.g. Tremmel et al. 2015; Roškar et al. 2015; Tamfal et al. 2018; Pfister et al. 2019; Oguya et al. 2019).

In light of this, we use high-resolution cosmological hydrodynamic simulations to study the GW signals from ex-situ BBHs formed in the early Universe. We only consider the ex-situ BBHs involving two BHs from separate formation sites (i.e. star-forming clouds for Pop III seeded BHs), and defer the in-cluster scenario to future studies.2 We particularly focus on Pop III-seeded BHs in the mass range $M_{\text{BH}} \sim 40 – 600 M_\odot$, as they dominate the number counts. Besides, previous studies have shown that such light seeds can hardly grow via accretion at high redshifts (e.g. Johnson & Bromm 2007; Alvarez et al. 2009; Hirano et al. 2014; Smith et al. 2018), so that it is challenging to observe them as quasars with EM signals, and GW detection may be the only available probe. A technical reason is that light seeds originate from small-scale structures (i.e. minihaloes), for which a small simulation volume ($V \sim 100$ Mpc$^3$) is sufficient to provide a valid cosmological representation of the high-z Universe $(z \gtrsim 4)$, so that achieving high resolution is not computationally prohibitive. This work nicely complements the existing studies on the in-situ BBH formation channel, which also predominantly involves BH seeds of similar masses.

Our simulations are equipped with customized sub-grid models for Pop III and Population II (Pop II) star formation and feedback, as well as Pop III BH seeding, accretion, dynamical friction, capture and feedback. For completeness, we also adopt a sub-grid model to identify direct-collapse black hole (DCBH) candidates, similar to that used in the ROMULUS simulations (Tremmel et al. 2017). Any DCBH candidates in our simulations, however, may not be representative, considering our limits on volume, resolution and feedback modelling. Here, we carry out our simulations within the standard ΛCDM cosmology. It is also interesting to investigate the GW signals in alternative dark matter (DM) models, which we defer to future studies.

The paper is structured as follows. Section 2 describes our simulation setup and sub-grid models for stars and BHs. In Section 3, we compare our simulation results with observational constraints in the EM window, specifically the star formation and BH accretion histories, as well as halo-stellar-BH mass scaling relations, thus justifying our sub-grid models and choice of simulation parameters. In Section 4, we describe our model for ex-situ binary evolution, and the resulting GW detection rates from such ex-situ BBH mergers for selected future instruments. In Section 5, we summarize

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1 Binary supermassive stars can also be formed during direct collapse of primordial gas, which leads to in-situ formation of binary DCBHs (e.g. Latif et al. 2020). However, since DCBH formation only happens in rare peculiar environments, we expect the Pop III-seeded BBHs to dominate the in-situ channel.

2 In the local Universe, the in-cluster scenario is particularly relevant for globular clusters (e.g. Haster et al. 2016; Fragione et al. 2018a,b; Rodríguez & Loeb 2018; Kremer et al. 2019) and nuclear star clusters (e.g. O’Leary et al. 2009; Petrovich & Antonini 2017; Hoang et al. 2018), which lead to local merger rate densities of $n_{\text{GW,GC}} \sim 1 – 20$ yr$^{-1}$ Gpc$^{-3}$ and $n_{\text{GW,NSC}} \sim 5 – 15$ yr$^{-1}$ Gpc$^{-3}$, respectively.
our findings and discuss potential caveats, as well as promising directions for future work.

2 METHODOLOGY

We use the GIZMO code (Hopkins 2015), which couples new hydrodynamic algorithms with the parallelization and gravity solver of GADGET-3 (Springel 2005). We here adopt the Lagrangian meshless finite-mass (MFM) version of GIZMO (with a number of neighbours $N_{\text{nb}} = 32$), which is a hybrid of smoothed particle hydrodynamics (SPH) and grid-based hydro solvers. For physics beyond gravity and hydrodynamics, our simulations include the primordial chemistry, cooling and metal enrichment model from Jaacks et al. (2018), as well as a modified version of the star formation (SF) and stellar feedback model in Jaacks et al. (2018); Jaacks et al. (2019), further discussed in Sec. 2.2. Besides, we have implemented customized sub-grid models for the seeding, dynamical capture, accretion and feedback of BHs formed from Pop III stellar populations (Sec. 2.3)\(^3\), based on the BH model in GADGET-3 (Springel et al. 2005). With these numerical tools, we study the properties of Pop III-seeded BHs, especially their GW signals, in a series of cosmological simulations, whose characteristics are summarised below (Sec. 2.1).

2.1 Simulation setup

To explore both cosmic-average and overdense regions in the early Universe, our simulations are conducted in two simulation setups. The first setup (zoom-in region) is the zoom-in region adopted in Liu et al. (2019), which is defined around a halo of $\sim 10^{10} M_\odot$ at $z \sim 10$, with a co-moving volume $V_C \sim 4 h^{-3} \text{Mpc}^3$. While the second setup (box) is a cubic box with co-moving side-length $L = 4 h^{-1}\text{Mpc}$. The initial conditions for both setups in ACDM cosmology are generated with the MUSIC code (Hahn & Abel 2011) at the initial redshift $z_i = 99$ under the Planck cosmological parameters (Planck Collaboration et al. 2016): $\Omega_m = 0.315$, $\Omega_b = 0.048$, $\sigma_8 = 0.829$, $n_s = 0.966$, and $h = 0.6774$. The chemical abundances are initialized with the results in Galli & Palla (2013), following Liu et al. (2019) (see their Table 1). To better appreciate the effects of stellar feedback on Pop III-seeded BHs, in addition to the fiducial (FD) implementation of stellar feedback, we further explore an ‘extreme’ case in the zoom setup (under the same resolution), NSFDER, where photo-ionization heating and stellar winds from Pop II stars are turned off\(^3\). Besides, to evaluate the convergence of our methods, we conduct a higher-resolution (HR) simulation in the zoom setup, with the mass resolution for gas and DM particles increased by a factor of 8 compared with the fiducial runs. The basic information of the aforementioned simulations is summarised in Table 1. For illustration, Fig. 1 shows the thermal and DM structure in the center of the zoom-in region at $z = 4$, from one of our fiducial runs, in terms of temperature distribution and projected DM density field. We use the VT (Turk et al. 2010) and CAESAR (Thompson 2014) software packages to analyse simulation results.

2.2 Star formation and feedback

Since individual stars cannot be resolved in our cosmological simulations, each stellar particle represents a stellar population whose member stars are sampled from the input initial mass function (IMF). We use the same Pop III and Pop II stellar population models as those used in Jaacks et al. (2018); Jaacks et al. (2019); Liu et al. (2019). Pop III stars are sampled on-the-fly from a top-heavy IMF $\Phi(M) \propto M^{-\alpha} \exp(-M_{\text{cut}}/M^2)$ with $\alpha = 0.17$ and $M_{\text{cut}} = 20 M_\odot$ in the mass range $1 - 150 M_\odot$. While for Pop II stellar populations, we pre-calculate all needed physical quantities (e.g. luminosity of ionizing photons) per unit stellar mass, by integrations of a Chabrier IMF over a mass range $0.08 - 100 M_\odot$ (see table 2 and eq. (7) in Jaacks et al. 2019 for details), and assume that all Pop II stellar particles are identical. Again, following Jaacks et al. (2019), a gas particle will be identified as a SF candidate when the number density of hydrogen exceeds $n_{th} = 100 \text{cm}^{-3}$, while the temperature $T$ remains below $T_{th} = 10^4$ K. However, in this work, in order to better simulate the interactions between BHs and stars, we do not turn SF candidates directly into stellar particles\(^5\). Instead, we let SF candidates spawn stellar particles in a stochastic manner (see Sec. 2.2.1). A Pop III stellar population is assigned to the newly-born stellar particle when its metallicity is below a critical value, $Z < Z_{\text{crit}} = 10^{-4} Z_\odot$ (Safranek-Shrader et al. 2010; Schneider et al. 2011); otherwise, a Pop II stellar population is assigned. Furthermore, we include stellar winds from Pop II stars, using the methodology in Springel & Hernquist (2003) (see Sec. 2.2.5). In the following subsections, we briefly describe our implementations of SF and stellar feedback, focusing on the modifications with respect to the original model in Jaacks et al. (2018); Jaacks et al. (2019). Equipped with these sub-grid models and primordial chemistry and cooling, our simulations can capture the multi-phase features of interstellar and intergalactic media (ISM and IGM) (see Fig. 2 for an example of the temperature-density phase diagram in the box setup, in the post-reionization era). The resulting star formation and BH accretion histories are also consistent with observational constraints at high-$z$ (Sec. 3).

\(^3\) We did not model Pop II-seeded BHs as they are typically less massive ($M_{\text{BH}} \lesssim 10 M_\odot$) and suffer from strong SN natal kicks, such that their accretion, mergers and feedback are inefficient. We also did not consider X-ray binaries whose effect on Pop III star formation has been found negligible, although their feedback may affect early BH accretion and reionization (e.g. Jeon et al. 2014; Ryu et al. 2015).

\(^4\) We never turn off the feedback from Pop III stars and the LW radiation from Pop II stars, as this leads to significant (a factor of $3 - 5$) overproduction of Pop III stellar populations, and thus, BH seeds, relative to the FD case, so that the results will be of no comparison power. Note that the Pop III stellar mass densities in our FD runs are consistent with observational constraints (see Sec. 3).

\(^5\) In Jaacks et al. (2019), a stellar particle represents not only the stellar population associated with it, but also the underlying interstellar medium (ISM) assumed to be coupled with the stellar population. In this work, we treat stars and their natal ISM separately to better model the dynamical friction of BHs by stars.
2.2.1 Stochastic star formation

For each SF candidate, we calculate the corresponding probability of SF as

\[ p_{\text{SF}} = \frac{m_{\text{SF}}}{m_*} \left[ 1 - \exp(-\eta_* dt / t_{\text{ff},i}) \right], \]

where \( m_{\text{SF}} \) and \( m_* \) are the masses of the SF candidate and stellar particle to be spawned, \( \eta_* \) is the star formation efficiency (SFE), \( dt \) is the current simulation timestep, and \( t_{\text{ff},i} = \sqrt{3\pi/4\mu G \rho_*} \) is the free-fall timescale of the SF candidate with a gas density \( \rho_* \). Here we set \( \eta_{*, \text{PopIII}} = 0.05 \) for Pop III stars and \( \eta_{*, \text{PopII}} = 0.1 \) for Pop II stars, consistent with Jaacks et al. (2019). A random number \( p \) following a uniform distribution in \([0, 1]\) is generated, and a stellar particle will be spawned if \( p < p_{\text{SF}} \). We set \( m_* \approx 600 \, M_\odot \), based on the results from high-resolution simulations of Pop III star formation in individual minihaloes (Bromm 2013; Stacy et al. 2016) and observational constraints from the global 21-cm absorption signal (Schauer et al. 2019), showing that the characteristic mass of Pop III stellar populations is \( 500 \sim 1000 \, M_\odot \). For simplicity, we adopt the same \( m_* \) for both Pop III and Pop II stellar populations, having verified that the choice of \( m_* \) has little impact on processes involving Pop II stars.

This stochastic implementation of SF is based on the assumption that the local SF rate density (SFRD) within gas of density \( \rho_g \) can be written as (e.g. Katz 1992; Stinson et al. 2006)

\[ \frac{d\rho_*}{dt} = \eta_* \frac{\rho_g}{\tau_g}, \]

where \( \tau_g \) is the characteristic timescale for gas inflow during the collapse of the star-forming cloud. This formalism is incorporated into our simulations with \( \rho_g = \rho_i \) and \( \tau_g = t_{\text{ff},i} \).

2.2.2 Lyman-Werner radiation

Similar to Jaacks et al. (2018), we calculate the contributions to the global uniform Lyman-Werner (LW) background from Pop III and Pop II stars with (Johnson 2013)

\[ J_{\text{LW}, \text{PopIII}}(t) \approx \frac{hc}{4\pi} \eta_{\text{LW}} \langle \dot{\rho}_s(t) \rangle t_* X / m_{\text{BH}} \]

where \( t_* \) is the typical lifetime of (massive stars in) the stellar population, \( \langle \dot{\rho}_s(t) \rangle \) is the global (physical) SFRD at time \( t \), \( \eta_{\text{LW}} \) is the number of LW photons produced per stellar baryon, and \( X = 0.76 \) is the mass fraction of hydrogen in primordial gas. We adopt \( \eta_{\text{LW}, \text{PopIII}} = 2 \times 10^4 \), \( t_* \text{PopIII} = 3 \, \text{Myr} \).

| Run       | \( V_C \) [Mpc\(^3\)] | \( m_{\text{gas}} \) [M\(_\odot\)] | \( m_{\text{DM}} \) [M\(_\odot\)] | \( m_* \) [M\(_\odot\)] | \( \epsilon_{\text{gas/DM}} \) [h\(^{-1}\)kpc] | \( \epsilon_{\text{BH}} \) [h\(^{-1}\)kpc] | FDBKPopII |
|-----------|-------------------------|-----------------------------|-----------------------------|-------------------------|-----------------------------|-----------------------------|------------|
| FDzoom    | 10.9                    | 9.4 \times 10^3             | 5.2 \times 10^4             | 586                     | 0.2                         | 0.02                        | ✓          |
| NSFDBzoom | 10.9                    | 9.4 \times 10^3             | 5.2 \times 10^4             | 586                     | 0.2                         | 0.2                         | ✓          |
| FDbox     | 205.9                   | 9.4 \times 10^3             | 5.2 \times 10^4             | 586                     | 0.2                         | 0.2                         | ✓          |
| FDzoomHR  | 10.9                    | 1.2 \times 10^3             | 6.5 \times 10^3             | 586                     | 0.1                         | 0.02                        | ✓          |

Figure 1. Gas temperature distribution (left) and projected DM density field (right) for a slice of thickness \( 400 \, h^{-1}\)kpc from FDzoom_Lseed (see Sec. 2.3.1 for the meaning of Lseed) at \( z = 4 \). In the left panel, stellar BHs from Pop III progenitors are labelled with green dots. In the right panel, the DM haloes above the H\(_2\) cooling threshold (identified with the standard friends-of-friends method) are shown by circles whose size scales with halo mass. \( N \) denotes the number of DM particles in a pixel of size \( 1 \, h^{-1}\)kpc, such that column density is given in units of \( \Sigma_U = 2.4 \times 10^4 \, M_\odot \, \text{kpc}^{-2} \).
for Pop III and $n_{\text{H},\text{PopIII}} = 4 \times 10^3$ Myr for Pop II stellar populations, consistent with our IMFs. To better simulate the formation of Pop III stars, we also consider the local LW field under the optically thin assumption. That is to say, each newly-born stellar particle is labelled active for $t_\star$, during which it contributes to the local LW field with

$$J_{\text{LW}}(r) = \frac{(L_\nu)m_\star}{16\pi r^2}, \quad (L_\nu) \approx \frac{\hbar \nu \eta_{\text{LW}} X}{m_\text{H} t_\star}.$$  

(4)

where $(L_\nu)$ is the specific luminosity of LW radiation per stellar mass averaged across the stellar population, $m_\star$ is again the mass of the stellar particle, and $r$ is the distance to it. The total LW intensity at any position $x$ in the simulation region is then estimated via

$$J_{\text{LW}}(t, x) = J_{\text{LW}, \text{log}}(t) + J_{\text{LW, local}}(t, x),$$  

(5)

$$J_{\text{LW, local}}(t, x) = \sum_i \frac{(L_i) m_i}{16\pi |x_i - x|^2}.$$  

(6)

In the second line, the summation extends over all active stellar particles at time $t$ that are within 200 kpc around $x$ and have contributions to the local LW intensity above $10^{-3} J_{\text{LW, log}}(t)$. The choice of 200 kpc is based on the results from Regan et al. (2019), which show that the LW radiation of star-forming galaxies has little effect (on the evolution of primordial gas) beyond 200 kpc (see also Johnson et al. 2007).

The LW intensity distribution is then used to calculate the dissociation rates of the main molecular coolants $H_2$ and HD in our chemical network for each gas particle. The effect of self-shielding is approximated with dimensionless factors (Wolcott-Green et al. 2011; Wolcott-Green & Haiman 2011), based on the local $H_2$ column density $N_{H_2} \simeq n_{H_2} L_1$, where

$$L_1 = \sqrt{\frac{15k_B T}{4\pi \rho G m_\text{H}}}$$  

is the local Jeans length (see equ. (12) in Wolcott-Green et al. 2011, as well as equ. (12) and table 1 in Wolcott-Green & Haiman 2011 for details).

2.2.3 Photo-ionization heating

Similar to Jaacks et al. 2019, globally, heating by the UV background is calculated with the redshift-dependent photo-ionization rate $\langle \zeta(x) \rangle$ from Faucher-Giguere et al. (2009), taking into account self-shielding. Locally, photo-ionization (PI) heating is applied to the gas particles on-the-fly in the spherical region around each active stellar particle within the Strömgren radius

$$R_{\text{ion}} = \left(\frac{3\langle N_{\text{ion}}\rangle m_\star}{4\pi n_{\text{H}}^2} \right)^{1/3},$$  

(7)

where $\langle N_{\text{ion}}\rangle$ is the ionization luminosity per unit stellar mass, $n_{\text{H}}$ is the typical average number density of hydrogen in the surrounding interstellar medium (ISM), and $n_{\text{H}} = 2.50 \times 10^{-13} \text{ cm}^{-3} \text{ s}^{-1}$ is the case-B recombination coefficient.

Based on our IMFs, we have $\langle N_{\text{ion,PopIII}} \rangle \sim 10^{46} \text{ s}^{-1} \text{ M}_\odot^{-1}$ for Pop III and $\langle N_{\text{ion,PopII}} \rangle \sim 10^{47} \text{ s}^{-1} \text{ M}_\odot^{-1}$ for Pop II. We set $n_{\text{H,PopIII}} = 0.01 \text{ cm}^{-3}$ for Pop III while $n_{\text{H,PopII}} = 1 \text{ cm}^{-3}$ for Pop II, considering the scenario that ionization fronts around Pop III stars can break out of the host minihaloes and thus impact lower-density gas, compared with the case of Pop II stars whose $H_\text{II}$ regions are confined by the gravitational potentials of the host galaxies. The resulting radii are $R_{\text{ion,PopIII}} \simeq 2 \text{ kpc} \times [m_\star/(500 \text{ M}_\odot)^{1/3}]$ and $R_{\text{ion,PopII}} \simeq 0.2 \text{ kpc} \times [m_\star/(500 \text{ M}_\odot)^{1/3}]$.

As pointed out by Liu et al. (2019), since $n_{\text{H}}$ is fixed regardless of the actual environments around stellar particles in the simulation, our model tends to over-predict the volume of dense $H_\text{II}$ regions around Pop II stars by neglecting the effect of self-shielding against ionizing photons in dense clumps. To avoid this problem, we restrict PI heating from Pop II stars to gas particles with hydrogen number densities below $n_{\text{H,PopII}} = 10^3 \text{ cm}^{-3}$ except in an inner sphere around each Pop II stellar particle. This inner sphere captures the ‘realistic’ dense $H_\text{II}$ region, whose radius $R_{\text{inner}}$ is estimated from Equation (7) by replacing $n_{\text{H}}$ with the density of the stellar particle’s nearest gas neighbour.

2.2.4 Supernova legacy feedback

As in Jaacks et al. (2018); Jaacks et al. (2019), our simulations cannot resolve the process of shell expansion in supernova (SN) explosions. We instead ‘paint’ the chemical and thermal legacy of supernovae onto the affected simulation particles. When a stellar population dies (i.e. $t_\star$ after it was born), we calculate the final radius of shell expansion $r_{\text{final}}$ based on the total SN energy $E_{\text{tot}}$ with the fitting formula (see fig. 4 in Jaacks et al. 2018 for details)

$$r_{\text{final}} \simeq 0.8 \text{ kpc} \left(\frac{E_{\text{tot}}}{10^{52} \text{ erg}}\right)^{0.38}.$$  

(8)

Metals produced by SNe are evenly (mass-weighted) distributed to the gas particles within $r_{\text{final}}$ around the stellar particle. The total SN energy and ejected metal mass $M_Z$ are calculated on-the-fly by counting progenitors (i.e.
core-collapse and pair-instability SNe) for each Pop III stellar population (see Table 3 of Jaacks et al. 2018). Whereas for Pop II stellar populations, we assign $E_{\text{tot}} \approx 10^{52}$ erg $\times m_\star/(10^3 M_\odot)$ and $M_Z = 0.016 m_\star$.

In addition to metal enrichment, we also model the thermal legacy of Pop III SNe by applying thermal energy injection (corresponding to a temperature increase of $T_c \approx 2 \times 10^4$ K) and instantaneous ionization of hydrogen to the gas particles within $R_{\text{ion}}$ around each Pop III stellar particle at the end of its lifetime. This thermal legacy, combined with photo-ionization heating, is sufficient to capture the effect of Pop III feedback on surrounding gas, as exemplified in Fig. 3, consistent with the results in high-resolution simulations (e.g. Johnson et al. 2007; Ritter et al. 2012, 2015).

### 2.2.5 SN-driven winds

Above, we present our implementations of thermal and radiation feedback. However, mechanical (or kinematic) feedback is also crucial for simulating self-regulated SF and the state of the ISM, especially for Pop II stars. In light of this, we further include SN-driven winds for Pop II stars based on Springel & Hernquist (2003). For each Pop II SF candidate (gas particle) with a mass $m_{\text{SF}}$ about to spawn a stellar population, we calculate a probability

$$ p_w = 1 - \exp(-\eta_w m_\star/m_{\text{SF}}) $$

for the gas particle to be launched as a wind particle, where $\eta_w$ is the wind-launching factor. Similar to our stochastic SF model (Sec. 2.2.1), a random number is then generated to decide whether to launch a wind particle based on $p_w$. Once launched, the gas particle receives a kick of $v_{w,\text{SF}} \sim 170$ km s$^{-1}$ in a random direction. Here $v_{w,\text{SF}}$ is calculated as (Springel & Hernquist 2003):

$$ v_{w,\text{SF}} = \frac{\sqrt{2 \gamma \varepsilon_{\text{SN}}}}{(1 - \beta) \eta_w} \frac{K_{\text{SN}}}{m_{\text{BH}}}, $$$$ u_{\text{SN}} = \frac{1}{\mu} \frac{d_{\text{SN}}}{m_{\text{BH}}}, $$

where we adopt $\beta = 0.16$, $\chi = 0.05$ as the efficiencies for SN-hot-gas and hot-gas-wind energy couplings. Furthermore, $u_{\text{SN}}$ is the specific SN explosion energy, written in terms of the initial SN blast wave temperature $T_{\text{SN}} \approx 1.5 \times 10^8$ K, the adiabatic index $\gamma = 5/3$, and the mean molecular weight $\mu$ ($\approx 0.63$ for ionized primordial gas)$^6$. The wind particle is negligible to become a SF or DBCBH candidate, unless a time interval of $t_w$ has past or its (hydrogen number) density is below $n_w$. Here we set $t_w = 0.1 H^{-1}(t)$ and $n_w = 0.1 n_{\text{H}} = 10$ cm$^{-3}$ for wind-ISM recoupling, where $H^{-1}(t)$ is the local Hubble time. To be conservative, we only apply this sub-grid wind model to Pop II stars, as the effect of SN blast waves from Pop III stars has already been captured by the photo-ionization and thermal energy injection (see Sec. 2.2.3 and 2.2.4). We set $\eta_w = 2$ and $\chi = 0.05$ to reproduce the observed SFRD at $z \lesssim 10$ (see Sec. 3 for details).

### 2.3 Black hole model

In this section, we briefly describe our numerical methods of simulating Pop III-seeded BHs at high redshifts, which are mostly based on existing models designed for SMBHs (Tremmel et al. 2015, 2017; Negri & Volonteri 2017). Following the BH model in GADGET-3 (Springel et al. 2005), we calculate physical quantities reflecting the environment of each BH particle based on the simulation particles within a specific search radius $h_{\text{BH}}$. Here $h_{\text{BH}}$ is adjusted on-the-fly such that $N_{\text{gas}} \approx 2N_{\text{pop}}$ gas particles are enclosed, but cannot exceed the upper limit $h_{\text{max}} = 5r_{\text{gas}} = 1 h^{-1}$kpc (in co-moving coordinates). This upper limit is adopted to avoid over-predicting the BH accretion rate in low-density regions$^7$. For conciseness, below we denote the physical (i.e. non-comoving) gravitational softening length of BH particles as $\epsilon_{g} \equiv 2.5h_{\text{BH}}$, beyond which scale the force is completely Newtonian, where $a$ is the cosmic scale factor.

#### 2.3.1 Black hole seeding

As mentioned in Section 2.2, each Pop III population is sampled from a top-heavy IMF, where we identify stars in the mass range $40 \leq M/M_\odot \leq 140$ as BH progenitors, consistent with our feedback model. Stars with $M > 140$ $M_\odot$ will evolve into pair-instability SNe, leaving no remnant behind, while the majority of stars with masses below 40 $M_\odot$ will not end up in black holes. Besides, even for the stars that become core-collapse SNe at last and give birth to BHs with some fractions of their stellar masses (i.e. for $8 M_\odot < M < 40 M_\odot$), the resulting BHs are low-mass in nature, and the SN natal kicks (with typical velocities above 100 km s$^{-1}$, e.g. Repetto et al. 2012) can eject them out of the host minihaloes, which will significantly suppress their participation in mass growth and mergers (Whalen & Fryer 2012). We assume that Pop III stars in the range $40 \leq M/M_\odot \leq 140$ will convert all their stellar mass into BH mass, and that natal kicks are negligible. Note that our stellar population models do not explicitly include binary stars, as we here focus on the GW signals from ex-situ BH binaries (formed by dynamical capture) with members from different stellar populations.

Given the small number of Pop III BH progenitors with $40 \leq M/M_\odot \leq 140$ from IMF sampling, there are still uncertainties in the resulting mass spectrum of BH seeds, because of small-scale dynamical interactions between stars, beyond our resolution. It remains unknown whether/how these progenitors will merge to form more massive BHs or eject some of them out of the host halo, since simulations resolving individual stars are computationally expensive and only able to track their evolution for up to $\sim 10^3$ yr (e.g. Stacy & Bromm 2013; Susa et al. 2014; Machida & Nakamura 2015; Stacy et al. 2016; Hirano & Bromm 2017; Sugimura et al. 2020b). For simplicity and generality, we consider two extreme cases.

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$^6$ The values of $\beta$ and $T_{\text{SN}}$ are consistent with our IMF for which the total energy and mass of SN are $E_{\text{tot}} \sim 10^{52}$ erg $\times m_\star/(10^3 M_\odot)$ and $M_{\text{SN}} = 0.16 m_\star$, such that $u_{\text{SN}} = E_{\text{tot}}/M_{\text{SN}} \approx 3 \times 10^{16}$ cm$^2$ s$^{-2}$.

$^7$ Without this upper limit, the median value of $h_{\text{BH}} \approx 0.5 h^{-1}$kpc in presence of stellar feedback, so that the simulation results are insensitive to $h_{\text{max}}$ for $h_{\text{max}} \gtrsim 0.5 h^{-1}$kpc.
with relatively heavy (Hseed) and light (Lseed) BHs as the final products. In Hseed, we assume that all BH progenitors will coalesce to form one BH in the end, resulting in seed masses (~300 – 590 $M_⊙$, see Fig. 4) that are on average ~ 80% of the total initial stellar mass $m_\star$. Such a coalescence process can be driven by runaway stellar collisions or gas inflows (e.g. Lupi et al. 2014; Giersz et al. 2015; Sakurai et al. 2017). In Lseed, we only keep track of the most massive BH progenitor (for accretion and feedback), while the rest is assumed to be inactive in terms of accretion, feedback and dynamical capture. The typical seed mass (~80 – 140 $M_⊙$, see Fig. 4) is then only ~ 20% of $m_\star$. When a Pop III stellar population reaches the end of its life, we turn it into a BH particle with a mass assigned with the methods above. For Hseed, the dynamical mass is unchanged when the stellar particle is turned into a BH particle, under the assumption that the remaining ~ 20% of mass is locked-up in low-mass stars (and/or their remnants) bound to the BH. While for Lseed, the dynamical mass is set to $f_m \simeq 0.6$ of the original stellar mass $m_\star$, according to the finding that on average ~ 0.4 of Pop III protostars are ejected out of the SF disc (Stacy & Bromm 2013).

For DCBH candidates, we design a set of criteria to capture the hot, dense and metal-poor phase in which the collapse is almost isothermal, leading to formation of BH seeds with $M_{BH} \gtrsim 10^4 M_⊙$. We turn a gas particle into a DCBH candidate, when its (hydrogen number) density reaches $n_{DCBH} = 2 \times 10^3 \text{ cm}^{-3}$ with a temperature $7000 < T/K < 10^4$, a metallicity $Z < Z_{DCBH} = 2 \times 10^{-4} Z_⊙$ and a H$_2$ abundance $x_{H_2} < 1 \times 10^{-6}$. The criteria here are based on the predictions from our one-zone model with the same cooling functions and chemical network as adopted in the simula-

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**Figure 3.** Evolution of gas density, temperature, H$_2$ abundance and radial velocity profiles (clockwise) around a Pop III stellar particle. The median values at $t \simeq 0.1, 3, 12$ and 24 Myr are plotted with solid, dashed, dashed-dotted and dotted lines, on top of individual gas particles denoted by orange, blue, green and yellow dots, respectively, where $t$ is the time after the formation of the Pop III stellar population. For $t \leq t_f = 3$ Myr, photo-ionization heating reduces the central density by a factor of 10, and generates inner ($r \lesssim 100$ pc) outflows with velocities up to ~ 30 km s$^{-1}$. Then the H$_2$ region keeps expanding for ~ 20 Myr before re-collapse, during which process gas cools to ~ $10^3$ K in the inner region with $n_H \gtrsim 0.1$ cm$^{-3}$, and the H$_2$ abundance reaches up to ~ $10^{-3}$ by enhanced H$_2$ formation catalysed by free electrons. The decrease in H$_2$ abundance from $t \simeq 12$ Myr to $t = 24$ Myr is caused by external LW radiation. Note that, in our case, $J_{LW,bg} \sim 10^{-21}$ erg s$^{-1}$ cm$^{-2}$ Hz$^{-1}$ sr$^{-1}$ at $z \sim 1.5$. 

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$^8$ The untracked BH progenitors can either remain within or be ejected from the original SF disc/host halo.
tions (Jaacks et al. 2019; Liu & Bromm 2018), in which the critical density \( n_{\text{DCBH}} \) is a bifurcation point, such that gas in the metal-poor, \( H_2 \)-poor and hot phase described by the above criteria remains hot (\( T \sim 7500 \) K), even when as dense as \( n_4 \sim 10^{10} \) \( \text{cm}^{-3} \); otherwise, gas can cool to \( T < 10^5 \) K and fragment during collapse, resulting in normal star formation. In reality, this metal-poor, \( H_2 \)-poor and hot phase occurs under strong gas inflows and/or LW fields. Similar to Tremmel et al. (2017), our criteria are used to select the regions where BH seeds can form and grow quickly to large masses, regardless of the specific formation pathways at unresolved scales, such as supermassive stars (e.g. Schleicher et al. 2013; Sakurai et al. 2016). As the initial mass growth (and feedback) cannot be resolved in our simulations, we set the initial (candidate) DCBH mass to the mass of the parent gas particle for simplicity (\( M_{\text{BH}} \simeq m_{\text{g,initial}} \simeq 10^4 \, M_\odot \) under fiducial resolution), and use sub-grid models to keep track of the subsequent evolution (see below).

2.3.2 Black hole capture

Once two black hole particles (with dynamical masses \( m_1 \) and \( m_2 \)) get closer than two softening lengths \( \Delta r < 2\epsilon_b \), and meanwhile remain gravitationally bound to each other (when the relative velocity \( \Delta v \) is smaller than the escape speed \( v_{\text{esc}} = \sqrt{2G(m_1 + m_2)}/\Delta r \)), they are combined into one simulation BH particle. The resulting BH particle then represents a BH binary or multiple system. Here the combination of two simulations particles represents the formation of a gravitationally bound system by dynamical capture, whose subsequent internal evolution is beyond our resolution, and it is by no means equivalent to the final coalescence of two or multiple BHs that would result in GW emission. In reality, it can take several billion years for the BH binary to harden and eventually produce GW signals (e.g. Sesana & Khan 2015; Conselice et al. 2019).

Note that the binaries identified in this way may not be hard binaries, while only hard binaries will be hardened to become BH-BH mergers. Therefore, the resulting GW rates should be regarded as optimistic estimations. We discuss the difference between this optimistic model with a more ‘pessimistic/realistic’ model that only considers hard binaries in Section 4.3. Since we cannot resolve the hardening processes of BH binaries in our cosmological simulations, we estimate the lifetime of each BH binary analytically from observed/simulated scaling relations (see Sec. 4.1 for details). To do so, we record the masses of the primary (\( M_1 \)) and secondary (\( M_2 \)) members, as well as the initial (orbital) eccentricity \( e \) for each newly-formed binary/multiple BH system.

2.3.3 Dynamical friction

In our simulations, the masses of Pop III BH particles are usually comparable to that of stellar particles (\( m_{\text{BH}} \sim m_0 \)), and much smaller than the masses of gas and DM particles (\( m_{\text{BH}} \sim 0.1m_{\text{gas}} \sim 0.02m_{\text{DM}} \)). Under this condition, the corresponding gravitational softening lengths of background particles must be large enough to avoid spurious collisionality, which meanwhile will suppress dynamical friction (DF) by preventing close encounters with BH particles. Thus, DF of BHs by background objects is not naturally simulated with the gravity solver on scales smaller than the background gravitational softening length, which is a common problem in cosmological simulations with limited mass/spatial resolution. Since dynamical interactions are crucial for BH mergers, we adopt the sub-grid model from Tremmel et al. (2015) to better simulate DF of BHs by background stars.

For each BH particle, the additional acceleration from the sub-grid DF model is (Tremmel et al. 2015)

\[
\mathbf{a}_{\text{DF}} = -4\pi G^2 M_{\text{BH}} \rho_s(<v_{\text{BH}}) \ln \Lambda \frac{v_{\text{BH}}}{v_{\text{BH}}} ,
\]

where \( v_{\text{BH}} \) is the velocity of the BH relative to the local background center of mass (COM) \( \rho_s(<v_{\text{BH}}) \) is the mass density of stars with velocities relative to the COM smaller than \( v_{\text{BH}} \), and \( \ln \Lambda \) is the Coulomb logarithm. In our case, \( \rho_s(<v_{\text{BH}}) \) is estimated with

\[
\rho_s(<v_{\text{BH}}) = \frac{M_s(<v_{\text{BH}})}{[4\pi r_{\text{DF}}^2/3]} ,
\]

where \( M_s(<v_{\text{BH}}) \) is the total mass of stellar particles within \( r_{\text{DF}} \) (physical) around the BH, whose velocities relative to the COM are smaller than \( v_{\text{BH}} \). We set \( r_{\text{DF}} = ah_{\text{BH}} \). The Coulomb logarithm is

\[
\ln \Lambda = \ln (1 + b_{\text{max}}/b_{\text{min}}) ,
\]

\[
b_{\text{max}} = \epsilon_g , \quad b_{\text{min}} = \frac{G M_{\text{BH}}}{v_{\text{BH}}} .
\]

\[\text{Figure 4. Distributions of Pop III BH seed masses for Hseed (purple) and Lseed (blue), measured with the Pop III particles in Fizoom_Hseed at } z = 4.\]

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\(9\) The metallicity threshold \( Z_{\text{DCBH}} = 2 \times 10^{-4} Z_\odot \) is consistent with the results in the early semi-analytical study by Omukai et al. (2008) and the empirical choice in the Romulus simulations (Tremmel et al. 2017).

\(10\) Such situations are rare even in over-dense regions. For instance, there are typically a few DCBH candidates while \( \sim 2000 \) stellar BH particles formed at \( z > 4 \) in Fizoom runs.

\(11\) We only apply the sub-grid DF model to stars because they are the dominant source for DF, and our resolution for gas and DM particles is too low for the sub-grid model to work.

\(12\) The local COM velocity is defined with all stellar particles around the BH within \( h_{\text{BH}} \).
Here we use \( b_{\text{max}} = \varepsilon_g \varepsilon \equiv 2.8 a_c \), and multiply the acceleration \( n_{\text{DP}} \) by a factor \( 1/[1 + M_{\text{BH}}/(5 m_g)] \) to avoid double counting the frictional forces on resolved (larger) scales.\(^{13}\)

### 2.3.4 Black hole accretion

We adopt a modified Bondi-Hoyle formalism developed by Tremmel et al. (2017) to calculate the BH accretion rate \( \dot{M}_{\text{acc}} \), which takes into account the angular momentum of gas. For each BH particle, the characteristic rotational velocity of surrounding gas \( \varepsilon_g \) away from the BH is estimated as \( \nu_g = j / \varepsilon_g \), where \( j \) is the specific angular momentum of gas particles in the radius range \( 3h_{\text{acc}} - 4h_{\text{acc}} \), and \( h_{\text{acc}} = \min(\varepsilon_g h_{\text{BH}}/4) \). Then \( \nu_g \) is compared with the characteristic bulk motion velocity \( v_{\text{bulk}} \), approximated by the smallest relative velocity of gas particles within \( h_{\text{BH}} \). When \( \nu_g \leq v_{\text{bulk}} \), the effect of angular momentum is negligible, so that the original Bondi-Hoyle accretion formula is used:

\[
\dot{M}_{\text{acc}} = \frac{4\pi (GM_{\text{BH}})^2 \rho_h}{(c^2 + \nu_g^2)^{3/2}}, \quad (14)
\]

where \( \rho_h \) is the gas density computed from the hydro kernel and \( c \) is the sound speed and \( v_g \) the mass-weighted average relative velocity of gas with respect to the BH. Here \( c \) is calculated with the mass-weighted average temperature of surrounding gas. While for \( \nu_g > v_{\text{bulk}} \), a rotation-based formula is used (Tremmel et al. 2017):

\[
\dot{M}_{\text{acc}} = \frac{4\pi (GM_{\text{BH}})^2 \rho_h c}{(c^2 + v_g^2)^{3/2}}, \quad (15)
\]

We also place an upper limit on \( \dot{M}_{\text{acc}} \) as 10 times the Eddington accretion rate (for primordial gas with \( \mu \simeq 1.22 \))\(^{14}\)

\[
\dot{M}_{\text{Emd}} = 2.7 \times 10^{-6} M_\odot \text{ yr}^{-1} \left( \frac{M_{\text{BH}}}{1000 M_\odot} \right) \left( \frac{\varepsilon_0}{0.1} \right)^{-1}, \quad (16)
\]

where \( \varepsilon_0 \) is the default radiation efficiency. Here we set \( \varepsilon_0 = 0.125 \).

Given \( \dot{M}_{\text{acc}} \), we update the BH mass at each timestep via \( \delta M_{\text{BH}} = \dot{M}_{\text{acc}} \delta t \). The dynamical masses of BH particles are also updated smoothly\(^{15}\) with \( \delta m_{\text{BH}} = \delta M_{\text{BH}} / M_{\text{BH,res}} \) for \( M_{\text{BH}} < M_{\text{BH,res}} = 10^4 M_\odot \sim m_{\text{gas}} \). While for \( M_{\text{BH}} \geq M_{\text{BH,res}} \), we adopt the algorithm from Springel et al. 2005 (see their equ. (35)), in which BH particles swallow nearby gas particles stochastically, and the dynamical masses are only updated when gas particles are swallowed instead of smoothly at each timestep. As in Springel et al. (2005), here we also apply drag forces from accretion to BH particles according to momentum conservation.

\(^{13}\) The factor \( 1/[1 + M_{\text{BH}}/(5 m_g)] \) is only significant for DCBH candidate particles with \( M_{\text{BH}} \sim m_{\text{gas}} \gtrsim 10 m_g \). The Coulomb logarithm \( \ln A \) is around 8 in our simulations, as \( M_{\text{BH}} \sim 10^2 \sim 10^3 M_\odot, \varepsilon_g h_{\text{BH}} \sim 30 \text{ km s}^{-1} \) and \( \varepsilon_g \sim 8 \text{ pc} \), typically.

\(^{14}\) Throughout our simulations, accretion is always highly sub-Eddington, especially for Pop III-seeded BHs. We include this upper limit for completeness, although it is never invoked here.

\(^{15}\) This implies that mass conservation is not explicitly enforced in our simulations. Nevertheless, the effect is negligible since \( M_{\text{BH,res}} \sim m_{\text{gas}} \), and the total number of BH particles is much smaller than the total number of gas particles. Besides, the fraction of accreted mass in BH mass is typically less than one percent in our simulations.

#### 2.3.5 Black hole feedback

We include both thermal and mechanical feedback from BH accretion in our simulations. Following Springel et al. (2005), the thermal feedback is implemented as internal energy injection into gas particles within \( h_{\text{BH}} \) for each BH particle. The total amount of energy to be distributed among gas particles within the hydro kernel of size \( h_{\text{BH}} \), over a timestep \( \delta t \), is \( \delta E = \varepsilon \eta L_{\text{BH}} \delta t \), where \( \varepsilon \) is the efficiency of radiation-thermal coupling, and \( L_{\text{BH}} \) is the luminosity from BH accretion

\[
L_{\text{BH}} = \varepsilon_{EM} \dot{M}_{\text{acc}} c^2 . \quad (17)
\]

Instead of using a fixed radiation efficiency \( \varepsilon_{EM} \), we here use the method in Negri & Volonteri (2017) to calculate \( \varepsilon_{EM} \) as

\[
\varepsilon_{EM} = \frac{\varepsilon_0 A_\eta}{1 + A_\eta}, \quad \eta \equiv \frac{\dot{M}_{\text{acc}}}{\dot{M}_{\text{Edd}}}, \quad (18)
\]

where \( A = 100 \) and \( \varepsilon_0 = 0.125 \). This approach takes into account the transition from optically thick and geometrically thin, radiatively efficient accretion discs, to optically thin, geometrically thick, radiatively inefficient advection dominated accretion flows (Negri & Volonteri 2017). We set \( \varepsilon_0 = 0.02 \) as a conservative choice, based on the calibration with SMBHs in Tremmel et al. (2017).

The mechanical feedback in terms of broad absorption line (BAL) winds is only applied to BHs with \( M_{\text{BH}} \geq M_{\text{BH,res}} = 10^4 M_\odot \). Once turned on, the probability of swallowing gas particles is boosted by a factor of \( 1/f_{\text{acc}} \). For each swallowed gas particle with mass \( \delta m \) above (below) the accretion plane\(^{16}\), a wind gas particle with mass \( m_w = (1 - f_{\text{acc}}) \delta m \) is launched with a kick velocity of \( v_w \) relative to the swallowed particle, along (opposite to) the direction of the angular momentum of surrounding gas. Here we assume that \( v_w = 200 \text{ km s}^{-1} \left( M_{\text{BH}}/M_{\text{BH,res}} \right)^{1/2} \), and calculate \( f_{\text{acc}} \) with (Negri & Volonteri 2017)

\[
f_{\text{acc}} = \frac{1}{1 + \eta_w}, \quad \eta_w = 2 c_w \frac{c_w^2}{v_g^2}, \quad \varepsilon_w = \frac{\varepsilon_{\text{wd}} A_w \eta}{1 + A_w \eta}, \quad (19)
\]

where \( \varepsilon_{\text{wd}} = 10^{-4} \) and \( A_w = 1000 \). Note that since accretion is insignificant for the dominant Pop III-seeded BHs under stellar and BH feedback, we always have \( M_{\text{BH}} \lesssim M_{\text{BH,res}} \), except for rare DCBH candidates, and BAL winds have little effect in our simulations.

### 3 SIMULATION RESULTS

In this section we summarize the main features of our simulations in the EM window, in terms of star formation histories, BH growth and halo-stellar-BH mass scaling relations, in comparison with observational constraints and previous theoretical predictions. For conciseness, we here only show the results for the fiducial stellar feedback model and resolution under the \textit{seed} BH seeding scenario. The results for \textit{seed} are similar. The effects of stellar feedback and resolution are discussed in appendices A and B. We will discuss the GW signals in the next section.

16 The accretion plane is orthogonal to the (specific) momentum of surrounding gas.
3.1 Star formation history

Fig. 5 shows the (co-moving) SFRDs for all stars (left panel, including both Pop III and Pop II) and Pop III stars (right panel) measured in FDBox\_Lseed. We compare our simulated SFRDs with the results from Jaacks et al. (2019), semi-analytical models in Hartwig et al. (2016), de Souza et al. (2011) and Mirocha & Furlanetto 2019 (based on the observed 21-cm absorption signal), and (extrapolated) observational results from Wei et al. (2014), Madau & Dickinson (2014) and Finkelstein (2016). In the box setup, the total SFRD is dominated by Pop II stars at $z \lesssim 18$. Despite the different implementations of SF and stellar feedback, our total SFRD agrees well with that of Jaacks et al. (2019), whose simulation setup is identical to our box run. It is also within the range of observational constraints at $z \lesssim 10$, with an upper limit from Wei et al. (2014) based on Swift long gamma-ray bursts and a lower limit from Madau & Dickinson (2014); Finkelstein (2016) based on UV and IR galaxy surveys. However, it is lower than the semi-analytical models from Mirocha & Furlanetto (2019) and Hartwig et al. (2016) (by up to 2 orders of magnitude) in the Pop III-dominated regime at $z \gtrsim 18$. One explanation is that our simulations have more realistic/stricter conditions for Pop III star formation, while semi-analytical models use idealized criteria (based on efficient H$_2$ cooling) to identify star-forming mini-haloes, which may overproduce the abundance of Pop III hosts and thus, the resulting Pop III SFRD. We do not expect these uncertainties at the highest redshifts to play an important role in inferring the GW signals from Pop III-seeded BBHs, for which the SFRD at lower redshifts is more relevant.

For Pop III stars, the simulated SFRD reaches a peak at $z \sim 11$ and declines rapidly thereafter. We fit our Pop III SFRD to the form $\dot{\rho}_*\,\text{PopIII}(z) [M_{\odot}\,\text{yr}^{-1}\,\text{Mpc}^{-3}] = a (1 + z)^b / (1 + [(1 + z)/c]^d)$ and find the best-fitting parameters $a = 765.7$, $b = -5.92$, $c = 12.83$ and $d = -8.55$ for FDBox\_Lseed. By integrating this best-fitting SFRD to $z = 4$, which is assumed as the end of metal-free SF\(^{17}\), we obtain a total density of Pop III stars formed across FDbox\_Lseed $a = 4$, which is assumed as the end of metal-free SF\(^{17}\), the total SFRD only $\rho^z \,\text{PopIII}(z) \gtrsim 7 \times 10^4 M_{\odot} \text{Mpc}^{-3}$, which is consistent with the constraints in Visbal et al. (2015) set by Planck data. However, the discrepancies among different models for Pop III SFRD are significant. For instance, our result is lower than that of Jaacks et al. (2019) by up to one order of magnitude at $z \lesssim 17$. The reason is that we have implemented stronger stellar feedback such as local LW fields, suppressing H$_2$ formation, and SN-driven winds (which enhance metal enrichment in the IGM). When compared with the semi-analytical Pop III SFRDs in de Souza et al. (2011) and Hartwig et al. (2016), which are widely used to derive the GW signals of in-situ Pop III BBHs, disagreements of up to a factor of 10 occur (at $z \lesssim 7$ and $z \gtrsim 15$ for Hartwig et al. 2016 and $z > 4$ for de Souza et al. 2011). Since direct measurement of the Pop III SFRD remains challenging even in the JWST era, we regard the agreement with the indirect constraint on $\rho^z \,\text{PopIII}(z) \gtrsim 7 \times 10^4 M_{\odot} \text{Mpc}^{-3}$ from Planck data (Visbal et al. 2015) as a consistency check for our SFRD. Note that the indirect constraints from the Planck optical depth are sensitive to assumptions on the escape fraction of ionizing photons $f_{\text{esc}}$, and the Pop III ionization efficiency $\eta_{\text{ion}}$. The constraint in Visbal et al. (2015) of $\lesssim 10^{-4.5} M_{\odot} \text{Mpc}^{-3}$ is on the strong side. Weaker constraints are also possible, e.g. $\lesssim 10^6 M_{\odot} \text{Mpc}^{-3}$ for $f_{\text{esc}} = 0.1$ and $\eta_{\text{ion}} = 5 \times 10^4$ (Inayoshi et al. 2016b). To be self-consistent, when comparing the GW signals of our simulated ex-situ BBHs with those of in-situ BBHs in the literature, we rescale the latter results to meet the same integral condition. The BH seeding models have little effect on star formation in our simulations, as BH accretion is always unimportant and the relevant feedback is also too weak to make any difference.

3.2 Black hole growth

Throughout our simulations, accretion is mostly sub-Eddington for Pop III-seeded BHs in the presence of stellar and BH feedback. For instance, Fig. 6 shows the distribution of Eddington ratio $M_{\text{acc}}/M_{\text{Edd}}$ in FDBox\_Lseed at $z = 4$, which has a log-normal-like shape and peaks at $M_{\text{acc}}/M_{\text{Edd}} \sim 10^{-6}$. This is consistent with the results in high-resolution 3D simulations with detailed BH feedback (e.g. Alvarez et al. 2009). By the end of the 3D simulations in the zoom setup ($z = 4$), the average (median) values of the accreted mass ratio $M_{\text{acc}}/M_{\text{BH}}$ are $1.8 (1.3) \times 10^{-3}$ for Lseed and $5.2 (4.1) \times 10^{-3}$ for Hseed. Even without Pop II II heating and SN-driven winds (NSFDBK), the average/median value of $M_{\text{acc}}/M_{\text{BH}}$ is still less than 0.01, and the maximum accreted ratio is $\sim 0.04$ across all simulation snapshots, indicating that accretion is usually unimportant. Our results agree with those in previous studies based on 3D cosmological simulations, showing that Pop III seeds can hardly grow via accretion at high redshifts (e.g. Johnson & Bromm 2007; Alvarez et al. 2009; Hirano et al. 2014; Smith et al. 2018). However, semi-analytical models and simulations have found that it is possible for Pop III seeds to grow sufficiently by super-Eddington accretion under peculiar conditions (e.g. Madau et al. 2014; Volonteri et al. 2015; Pezzulli et al. 2016; Inayoshi et al. 2016a; Toyouchi et al. 2019). Our simulations did not capture this scenario, possibly due to different treatments of BH and stellar feedback and limited resolution. The mass spectrum of BH particles at $z = 4$ from FDBox\_Lseed is shown in Fig. 7, which reflects the initial distribution of Pop III seed masses (see Fig. 4) and combinations of BH particles into binary/multiple systems.

Regarding global properties, Fig. 8 shows the redshift evolution of the total (co-moving) accreted mass density $\rho_{\text{acc}}$ for BHs in FDzoom\_Lseed and FDzoom\_Hseed. By the end of the simulation ($z = 4$), the total accreted mass only makes up a small fraction ($1.6 - 5.5 \times 10^{-3}$) of the total BH mass. Besides, we have $\rho_{\text{acc}}(z = 4) \simeq 20 (200) M_{\odot} \text{Mpc}^{-3}$ for Lseed (Hseed), much lower than the upper limit $\sim 10^4 M_{\odot} \text{Mpc}^{-3}$ placed by the unresolved cosmic X-ray background (Salvaterra et al. 2012). Actually, the values of $\rho_{\text{acc}}$ in our simulations are always below the observational upper limit by at least one order of magnitude, even in the
GWs from Pop III-seeded BBHs

(a) Total

(b) Pop III

Figure 5. Star formation histories from FDBbox_Lseed. Left panel: total (co-moving) SFRD, in comparison with the simulation results from Jaacks et al. 2019 (JJ19), semi-analytical models in Hartwig et al. 2016 (HT16) and Mirocha & Furlanetto 2019 (MJ19, based on the observed 21-cm absorption signal), and (extrapolated) observations from Wei et al. 2014 (WJ14), Madau & Dickinson 2014 (MP14) and Finkelstein 2016 (SF16). Right panel: Pop III SFRD, in comparison with the JJ19 simulation, as well as semi-analytical models from HT16 and de Souza et al. 2011 (deS11). For deS11, we have rescaled their most optimistic SFRD by a factor of 0.5 to be consistent with the recent Planck measurement of the optical depth to electron scattering (Inayoshi et al. 2016b). Our simulated SFRD is fitted to the form $\rho_\star,_{\text{PopIII}}(z) = a(1 + z)^b(1 + [z + c]/d)^c$. For FDBbox_Lseed, the best-fitting parameters are $a = 765.7$, $b = -5.9$, $c = 12.8$, and $d = -8.5$ (thick blue curve). The total density of Pop III stars formed across cosmic time inferred from this best-fitting formula is $\approx 7 \times 10^4 M_\odot$ Mpc$^{-3}$, consistent with the constraints in Visbal et al. (2015) set by Planck data.

Figure 6. Distribution of Eddington ratio $\dot{M}_{\text{acc}}/\dot{M}_{\text{Edd}}$ in FDBbox_Lseed at $z = 4$. This log-normal-like distribution peaks at $\dot{M}_{\text{acc}}/\dot{M}_{\text{Edd}} \approx 10^{-5}$, consistent with the results in high-resolution simulations with detailed BH feedback (e.g. Alvarez et al. 2009). This also corresponds to the typical Bondi accretion rate (dashed vertical line, from Equ. 14) for Pop III-seeded BHs embedded in the ISM of typical haloes ($M_{\text{halo}} \approx 10^8 - 10^9 M_\odot$) at $z = 4$, given $M_{\text{BH}} = 125 M_\odot$, $n_{\text{H}} = 1$ cm$^{-3}$, $T = 10^4$ K and $v_\text{esc} = 30$ km s$^{-1}$.

Figure 7. Distribution of BH particle masses in FDBbox_Lseed at $z = 4$ (purple histograms). The majority of BH particles follows the seed mass distribution (black contour), and a group of more massive BH particles with $M_{\text{BH}} \sim 200 - 500 M_\odot$ (which denote binary/multiple BH systems) have been formed from combinations of BH particles. A tiny fraction ($\sim 2 \times 10^{-4}$) of BH particles with $M_{\text{BH}} \approx 10^4 M_\odot$ represent DCBH candidates.

zoom setup for Fseed without Pop II stellar feedback. This implies that BH accretion is dominated by more massive haloes ($M_{\text{halo}} \gtrsim 10^{11} M_\odot$), missing in our simulations with limited volumes, especially in the Pop II-dominated regime ($z \leq 18$). Note that our simulations do not include high-mass X-ray binaries (HMXBs), consisting of Pop III stars and BHs, which can significantly boost BH accretion (e.g. Jeon et al. 2014). Furthermore, our sub-grid model for BH
accretion may underestimate rates due to insufficient resolution, as small (\(<10^5 M_\odot\)) cold gas clumps in the ISM are not resolved.

### 3.3 Mass scaling relations

To evaluate the halo-stellar-BH mass scaling relations in our simulations, we identify DM haloes and their (central/satellite) galaxies using the standard friends-of-friends (FOF) method within the CAESAR code (Thompson 2014). The linkage parameter is \(b = 0.2\) for DM and gas particles, and \(b = 0.02\) for stellar particles. For simplicity, we define the central BH mass as the total mass of all BHs within \(0.5R_{1/2}\) from the galaxy center, where \(R_{1/2}\) is the galaxy’s half mass radius for baryons.

Fig. 9 shows the stellar-halo mass relation for atomic-cooling haloes, with \(M_{\text{halo}} > 2.5 \times 10^7 M_\odot[(1 + z)/10]^{-3/2}\) (Yoshida et al. 2003; Trenti & Stiavelli 2009), hosting resolved galaxies (with \(M_\star > 32 m_\odot \approx 2 \times 10^4 M_\odot\)) at \(z = 4\) in \textit{FDzoom_Lseed}, where the baryon fraction \(M_{\text{baryon}}/f_{\text{baryon}}M_{\text{halo}}\) with respect to the cosmic mean \(f_{\text{baryon}} = \Omega_\text{b}/\Omega_\text{m}\) is color coded. We find that the median stellar mass fraction \(M_\star/M_{\text{baryon}}\) is \(\sim 3\%), and the maximum is \(\sim 20\%), consistent with abundance matching results for low-mass galaxies where stellar feedback is efficient. It is also evident that galaxies with higher stellar mass fractions tend to have lower gas fractions, which is a signature of outflows driven by strong stellar feedback. Similar trends exist for \textit{Hseed}, under fiducial stellar feedback.

Fig. 10 shows the BH-stellar mass relation at \(z = 4\) in \textit{FDzoom_Lseed} for all resolved galaxies (including satellites), in comparison with the extrapolated relations derived from local observations for high-stellar mass ellipticals and bulges, \(\log M_{\text{BH}} = 1.4 \log M_\star - 6.45\), as well as for moderate-luminosity AGNs in low-mass haloes, \(\log M_{\text{BH}} = 1.05 \log M_\star - 4.1\) (with \(M_\star \gtrsim 3 \times 10^9 M_\odot\) and \(z < 0.055\); Reines & Volonteri 2015), where all masses are in \(M_\odot\). It turns out that our simulations tend to overpredict the BH mass in the low-mass regime (\(M_\star \lesssim 10^8 M_\odot\)), while underestimating the BH mass at the high-mass end (\(M_\star \gtrsim 10^9 M_\odot\)). The former trend will be particularly obvious for galaxies hosting DCBHs, in which the BH mass may even exceed the stellar mass (e.g. Agarwal et al. 2013).

The best-fitting power-law relation for \textit{FDzoom_Lseed} at \(z = 4\) is \(\log M_{\text{BH}} = 0.13 \log M_\star + 1.4\). This indicates that the correlation between BH and stellar masses is much weaker in the simulated low-mass systems (\(M_\star \lesssim 10^8 M_\odot\)) at high redshifts (\(z > 4\)) than observed in the nearby Universe. Interestingly, we find that the correlation strength (i.e. the power-law index) slightly decreases with redshift, or in general increases when BH accretion and halo mergers proceed. This outcome implies that sufficient BH accretion and structure formation at \(z \lesssim 4\) are necessary to explain the observed BH-stellar mass scaling relation, relevant only for massive haloes (\(M_{\text{halo}} \gtrsim 10^{11} M_\odot\)) at redshifts (\(z \lesssim 4\)). Actually, the recent work by Delvecchio et al. (2019) predicts that a tight super-linear stellar-BH mass relation only applies at \(z \lesssim 2\) for galaxies with \(M_\star \gtrsim 10^9 M_\odot\), based on the star-forming ‘main-sequence’ and stellar mass dependent ratio between BH accretion rate and star formation rate. Compared with the representative case of \textit{FD} and \textit{Lseed} discussed here, the BH-stellar mass scaling relations for \textit{NSFDBK} and/or \textit{Hseed} runs are only different in terms of normalization, while the evolution of the slope (i.e. correlation strength) is almost identical, so that the above trends also apply.

### 4 GRAVITATIONAL WAVE SIGNALS

#### 4.1 BH binary evolution

As mentioned in Section 2.3.2, combinations of BH particles in our simulations represent formation of \textit{ex-situ} BH binaries or multiple systems (by dynamical capture), whose subsequent evolution is beyond our resolution. Actually, the dynamics of coalescence is rather complex, involving various astrophysical aspects such as a clumpy ISM, DM distribution, and the presence of nuclear star clusters (Roškar et al. 2015; Tanfalı et al. 2018; Oguya et al. 2019), many of which are not taken into account in our simulations. As an exploratory approach, we employ semi-analytical models to calculate the lifetimes of BH binaries under simple assumptions and parameterizations, depending on their large-scale environments. In this way, we can investigate a broad range of parameters to estimate the lower and upper bounds for the GW signals of our simulated BBHs.

Figure 8. Total (co-moving) accreted BH mass density vs. redshift in \textit{FDzoom_Lseed} (solid) and \textit{FDzoom_Hseed} (dashed). The shaded region shows the upper limit on \(\rho_{\text{acc}}\) at \(z = 5\), placed by the unresolved cosmic x-ray background, from Salvaterra et al. 2012. Our simulations results are always below this limit (by at least a factor of 50), implying that under stellar feedback, BH accretion is dominated by more massive haloes (\(M_{\text{halo}} \gtrsim 10^{13} M_\odot\)) and/or HMXBs not modelled in our simulations with limited volumes and resolution. For comparison, we also show the results of the zoom-in simulation in Jeon et al. 2014 (MJ14) with (dashed-dotted) and without (dotted) HMXBs, which indicate that including HMXBs can enhance BH accretion by two orders of magnitude. Our simulations do not capture the early BH accretion in MJ14 at \(z \gtrsim 22.5\) due to limited resolution.
4.1.1 Orbital evolution

Assuming that the orbital evolution of BBHs is driven mostly by surrounding stars (in 'dry' galaxy mergers)\textsuperscript{19} and GW emission, the evolution of the semimajor axis takes the form (Sesana & Khan 2015)

\[
\frac{da}{dt} = \frac{da}{dt}_{3b} + \frac{da}{dt}_{GW} = -Aa^2 - \frac{B}{a^3}.
\]

The first term denotes the effect of interactions with surrounding stars (i.e. three-body hardening), while the second term corresponds to the energy and angular momentum loss via GWs. Here

\[
A = \frac{GH\rho_{\text{inf}}}{\sigma_{\text{inf}}} , \quad B = \beta F(e) , \quad \beta = \frac{64G^3M_1M_2M}{5\pi^2} ,
\]

where $M_1$ and $M_2$ are the masses of the primary and secondary BHs, $M = M_1 + M_2$, $\sigma_{\text{inf}}$ and $\rho_{\text{inf}}$ are the velocity dispersion and stellar density at the radius of influence $r_{\text{inf}}$ of the BH binary, $F(e) = (1 - e^2)^{-7/2}(1 + (73/24)e^2 + (37/96)e^4)$ given the eccentricity $e$, and $H \sim 15 - 20$ is a dimensionless parameter.

The binary system spends most of its lifetime in a phase with a characteristic semimajor axis that can be estimated by imposing $(da/dt)_{3b} = (da/dt)_{GW}$:

\[
a_{\ast/GW} = \left( \frac{B}{\beta} \right)^{1/5} = \left( \frac{64G^3\sigma_{\text{inf}}M_1M_2M^2F(e)}{5\pi^2H\rho_{\text{inf}}} \right)^{1/5} .
\]

The binary hardening time, i.e. the time taken for $a$ to reach $a_{\ast/GW}$, can be estimated with

\[
t_{\text{HD}} \simeq \frac{1}{Aa_{\ast/GW}} = \left( \frac{1}{4\pi^2} \right)^{1/5} .
\]

For typical parameters $e = 0.09$, $M_1 = M_2 \sim 100 M_\odot$, $\sigma_{\text{inf}} \sim 10$ km s$^{-1}$, $\rho_{\text{inf}} \sim 10^3 M_\odot$ pc$^{-3}$ and $H = 17.5$ (see the next subsection for details), we have $a_{\ast/GW} \sim 5 \times 10^7$ pc and $t_{\text{HD}} \sim 2.4$ Gyr. Given such small $a_{\ast/GW}$ and large $t_{\text{HD}}$, it is very challenging to fully simulate the binary hardening process in cosmological simulations.

We assume that the eccentricity is fixed to the initial value in the three-body hardening stage. The contribution from GW emission to hardening is comparable to that from the surrounding stars when $a$ is close to $a_{\ast/GW}$. In other words, the system only emits strong GW signals at $a \lesssim a_{\ast/GW}$, when actual coalescence is about to happen. The time spent in the subsequent GW dominated phase ($a < a_{\ast/GW}$) can be estimated with\textsuperscript{20}

\[
t_{\text{col}} = \frac{12 \epsilon_{\text{GW}}^3}{19} \frac{1}{\beta} \int_0^1 dx \frac{x^{29/10}(1 + (121/304)x^2)^{1181/2299}}{\ln(1 - x^{3/2})} ,
\]

\[
\epsilon_{\text{GW}} = \left( \frac{a_{\ast/GW} - (1 - e^2)}{e^{12/19}} \right) \left( \frac{1 + 21}{304} \right)^{870/2299} ,
\]

assuming that the effect of surrounding stars is negligible.

\textsuperscript{19} It is a reasonable approximation to ignore the effect of gas on binary evolution, since Pop III stars are typically massive with strong PI and SN feedback which leads to low gas density around the newly-born BHs. Besides, considering the uncertainties in the density profiles of stars around BBHs, the additional friction by gas can be captured with steep stellar density profiles.

\textsuperscript{20} http://www.physics.usu.edu/Wheeler/GenRel2013/Notes/GravitationalWaves.pdf
In our model, $t_{\text{col}}$ and $t_{\text{BH}}$ are comparable, and the ratio $t_{\text{col}}/t_{\text{BH}}$ increases with $e$, covering the range $1/4 - 2$.

For simplicity, we set $H = 17.5$, and the only unknowns in the above formulas are $\sigma_{\text{inf}}$ and $\rho_{\text{inf}}$. However, for Pop III-seeded BHs with $M_{\text{BH}} \lesssim 10^3 M_\odot$, the influence radii are typically sub-parsec, far beyond our spatial resolution. Besides, $\sigma_{\text{inf}}$ and $\rho_{\text{inf}}$ are defined for the long-term (Gyr-scale) quasi-steady state of the background stellar system, unavailable from our simulations designed for high redshifts ($z \gtrsim 4$). In light of this, as in Sesana & Khan (2015), we estimate $\sigma_{\text{inf}}$ and $\rho_{\text{inf}}$ with BH-bulge scaling relations, as described below.

### 4.1.2 Environments around BBHs

We assume that the stars surrounding a BBH follow the Dehnen density profile (Dehnen 1993)

$$\rho_*(r) = \frac{(3 - \gamma)M_\star}{4\pi r^2 (r + r_0)^{\gamma - 1}},$$  \hspace{1cm} (25)

where $\gamma$ is the inner slope, $M_\star$ is the bulge mass, and $r_0$ is the core size, which is related to the bulge effective radius $R_{\text{eff}}$, as well as $r_{\text{inf}}$:

$$R_{\text{eff}} = \frac{3r_0}{4[2^{1/3} - 1]},$$  \hspace{1cm} (26)

$$r_{\text{inf}} = \frac{M_\star}{(2M_\star)^{1/3} - 1}.$$  \hspace{1cm} (27)

To estimate the bulge mass $M_\star$, we consider two models. The first model \textit{(obs-based)} extrapolates the observed scaling relation $M_\star \sim M_{BH}^{10.11} M_\odot (M_{BH}/0.49)^{1/1.16}$ (Kormendy & Ho 2013) to our low-mass regime, where $M_\star \equiv M/(10^6 M_\odot)$.

In the second model \textit{(sim-based)}, we estimate the bulge mass with the best-fitting BH-stellar mass relation measured at the last snapshot in the corresponding simulation ($z = 4$, see Fig. 10 for an example): $M_{\star\text{, sim}}(M) = f_{\text{bulge}} M_{\star\text{, sim}}(M)$, where $M_{\star\text{, sim}}(M)$ is the best-fitting formula for \textit{total} stellar mass versus BH mass, and $f_{\text{bulge}}$ is the bulge mass fraction, which we treat as an adjustable parameter in the range $f_{\text{bulge}} \sim 0.2 - 1$. In principle, the scaling relation evolves with redshift such that the simulation results should converge to the observed results at $z \sim 0$. However, limited by computational resources, we can only run our simulations down to $z = 4$, which is only 11% of the age of the Universe, so that we cannot take into account the entire cosmic evolution of the scaling relations self-consistently. The \textit{obs-based} and \textit{sim-based} models adopted here with parameters $\gamma$ and $f_{\text{bulge}}$ are meant to explore the range of GW rates under uncertainties in the environments of BBHs embodied by the scaling relations.

Once $M_\star$ is known, the bulge effective radius is given by (Dabringhausen et al. 2008)

$$R_{\text{eff}} = \max(2.95 M^{0.596}_\star, 34.8 M^{0.399}_\star) \text{ pc},$$  \hspace{1cm} (28)

where $M_{\star, 6} \equiv M_\star/(10^6 M_\odot)$. The first term in the bracket is for ultracompact objects (such as ultracompact dwarfs, globular and nuclear star clusters), whereas the second is for regular elliptical galaxies. In our case with $M_{BH} \sim 100 - 1000 M_\odot$, we have $M_\star \sim 10^5 - 10^6 M_\odot \ll 10^8 M_\odot$, such that the second term always applies, i.e., $R_{\text{eff}} = 34.8 M^{0.399}_\star \text{ pc}$, leading to conservative estimations of $\rho_{\text{inf}}$. Finally, we obtain $\rho_{\text{inf}}$ by evaluating the density profile (25) at $r_{\text{inf}}$, which is derived from equations (26)-(28) for the estimated $M_\star$.

![Figure 11. Distribution of initial eccentricity for ex-situ BBHs formed at $z_{\text{BH}} > 4$ in FDBbox.Lseed.](image-url)
GWs from Pop III-seeded BBHs

4.2 Intrinsic rate density of GW events

Here and in the following subsection, we discuss the GW signals from the simulated ex-situ BBHs, mainly showing results for the most representative (fiducial) case of FDbox_Lseed. The results for Baseed are similar. The effects of stellar feedback and resolution are explored in Appendices A and B. We focus on the intrinsic and detection rates of GW events. It is also interesting to explore the statistics of detectable sources, such as distributions of masses, spins and eccentricity. However, given the uncertainties in the simulated GW events from our idealized treatment of BBH evolution, we defer such discussions to future work.

Fig. 12 shows the intrinsic GW rate densities of ex-situ BBH-BH merger events at zBBH > 4 in FDbox_Lseed, vs. zGW for γ = 1.5, 1.0, 0.5 and 0, with the obs-based scaling relations. The results for sim-based scaling relations are similar, and thus not shown. The main difference between the obs-based and sim-based models is that GW events tend to occur at higher redshifts in the sim-based model compared with the case of obs-based scaling relations. For the sim-based model, the local rate density is insensitive to f_bulge for f_bulge ~ 0.2 – 1. In both models, the local (zGW ≲ 0.3) rate density generally increases with γ (see Fig. 13), and resides in the range ~ 10^{-3} – 0.04 yr^{-1} Gpc^{-3} for γ ~ 0 – 1.5. Actually, the intrinsic GW rate density is a convolution of the distribution of tGW and the formation rate density of BBHs. The former will be a ‘redshifted’ version of the latter when the delay time tGW is non-negligible (compared with tBH). In our case, tGW ~ 1 Gyr typically for γ < 1.5, such that GW events only occur at zGW ≲ 10, even though BBH formation starts at zBBH ~ 18 and has a rate density of ~ 0.1 – 1 yr^{-1} Gpc^{-3} for zBBH = 4 – 18.

Interestingly, the rate density of ex-situ Pop III BBHs is comparable to the predictions for in-situ Pop III BBHs in some previous studies at the level of ~ 0.01 – 0.1 yr^{-1} Gpc^{-3} (Belczynski et al. 2017; Hartwig et al. 2016), especially when their results are rescaled to our simulated total density of Pop III stars formed across cosmic time ≈ 7 × 10^{4} M_{⊙} Mpc^{-3}, as shown with the thin curves.

Figure 12. Co-moving rest-frame rate densities of GW events from ex-situ BBHs formed at zBBH > 4 in FDbox_Lseed, for γ = 1.5 (triangle), 1 (circle) 0.5 (square) and 0 (diamond), measured with a bin size ∆zGW = 0.3, where the obs-based scaling relations are used. Error bars denote 1σ uncertainties assuming that the number of GW events in each redshift bin follows a Poisson distribution such that σ_i = nGW,i/√N_i for bin i which contains N_i events. For comparison, we show the original results for in-situ BBHs from Belczynski et al. 2017 (BK17, for different scenarios of Pop III star-forming clouds: FS1 and FS2, see their Fig. 12) and Hartwig et al. 2016 (HT16, with a IMF mass range 1 – 100 M_{⊙}, see their Fig. 2). We also rescale the results of BK17, calibrated to our total Pop III stellar mass density ∼ 7 × 10^{4} M_{⊙} Mpc^{-3}, as shown with the thin curves.

Figure 13. Local (zGW ≲ 0.3) rate density of GW events from ex-situ BBHs formed at zBBH > 4 in FDbox_Lseed, with the obs-based scaling relations, as a function of the inner slope γ.

21 For γ > 1.25 in the sim-based model, almost all BBHs merge at zGW ≲ 0.3, leading to a zero local rate density of GW events.
more metal-enriched progenitors (Pop II and Pop I stars). Note that, the highest local rate density \( \simeq 0.04 \, \text{yr}^{-1} \, \text{Gpc}^{-3} \) achieved in \textsc{FDBox} \textsc{Lseed} with \( \gamma \sim 1.5 \) is lower than the upper limit \( 0.36 \, \text{yr}^{-1} \, \text{Gpc}^{-3} \) for IMBH binaries of \( M = 210 \, M_\odot \) (similar to the mass scale of Pop III-seeded BBHs in the \textsc{Lseed} scenario) inferred from the first advanced LIGO observing run (Chandra et al. 2020).

### 4.3 Effects of binary identification

As described in Section 2.3.2, we form BBHs as bound systems at our force resolution limit of \( \epsilon_e \sim 8 \, \text{pc} \), which may not be small enough to ensure that the resulting BBHs are hard binaries, especially for BBHs with highly eccentric orbits which can be easily disrupted at apocenters. Since only hard binaries will be hardened to emit GWs, the GW rates may be overestimated by our optimistic binary identification scheme. In this subsection, we evaluate the relevant effects with semi-analytical post-processing and test simulations.

For each BBH in the fiducial run \textsc{FDBox} \textsc{Lseed}, we estimate the unresolved true initial semi-major axis \( a_{\text{true}} \) by a random draw from a logarithmically flat distribution, which is observed in binary-stars (Abt 1983). Similar distributions (dominated by close binaries) are also obtained in N-body simulations of Pop III star clusters (see fig. 8 of Belczynski et al. 2017), where close binaries dominate. Therefore, we expect it to be a good approximation to the case of dynamically formed BBHs. Actually, as long as the distribution of \( a_{\text{true}} \) is dominated by close binaries, the fraction of hard binaries is more sensitive to the lower bound \( a_{\text{min}} \) than the detailed shape of the distribution. In our case, we set \( a_{\text{min}} = 0.1 \, \text{pc} \), which is the typical size of Pop III star clusters (e.g. Susa et al. 2014; Sugimura et al. 2020a). Beyond this scale, the two Pop III clusters from which the two BHs originate should be regarded as one initially, and governed by the in-situ channel. We adopt \( 2\epsilon_e/(1 - e) \) as the upper bound, since \( (1 - e)a_{\text{true}} < 2\epsilon_e \) is required for the binary to be identified in the simulation (at the pericenter). Given \( a_{\text{true}} \), only hard binaries are preserved for GW calculations, which satisfy \( K_{\text{ap}} > (1/3)(\sigma^2_{\text{M}_*}) \), where \( K_{\text{ap}} = \left[ (1 - e)/(1 + e) \right] E_0 = \left[ (1 - e)/(1 + e) \right] Gm_{\text{BH}}/(2a_{\text{true}}) \) is the kinetic energy at the apocenter, and \( (\sigma^2_{\text{M}_*}) = (10 \, \text{km} \, \text{s}^{-1})^2 \, M_\odot \) is assumed for typical surrounding (Pop II/I) stars. In this way, the efficiency of BH-BH mergers drops by a factor of \( \sim 4 \), for the \textit{obs-based} scaling relations given \( \gamma = 1.5 \), with removal of most highly eccentric binaries (\( e > 0.8 \)). The resulting all-sky detection rates are reduced by a factor of \( \sim 4 - 17 \) (see the next subsection for details)\(^{23}\). Note that if the distribution of \( a_{\text{true}} \) is instead dominated by wide binaries, the reduction of GW rates will be larger.

To verify the above results, we run test simulations under the same setup and feedback model as those for \textsc{FDBoom} runs. In the test runs, \( \epsilon_e \simeq 3 \, \text{pc} \), and only hard BH binaries are considered with \( [(1 - e)/(1 + e)] E_0 > (1/3)(\sigma^2_{\text{M}_*}) \), where the binding energy \( E_0 \) is measured on-the-fly. We find similar trends as those seen in analytical calculations: When the simulation only identifies hard binaries, the efficiency of BH-BH mergers is reduced by a factor of \( \sim 4 \) (3), compared with the optimistic case of \textsc{FDBoom} \textsc{Lseed} (\textsc{FDBoom} \textsc{Lseed}), with up to a factor of \( \sim 22 \) (16) suppression in detection rates, for the \textit{obs-based} scaling relations with \( \gamma = 1.5 \).

### 4.4 Detectability

To evaluate the detectability for our simulated GW sources, we adopt the phenomenological model ‘PhenomC’ from Santamaria et al. (2010) to calculate the waveform of the GW signal in the frequency domain \( [h(f)|M_1, M_2, D_L, z_{GW}] \), under the simplifying assumption that the two BHs before merger are non-spinning in circular orbits, and where \( D_L \) is the luminosity distance to the source. This assumption of zero spin and circular orbit, as well as the intrinsic waveform uncertainties may lead to uncertainties in the resulting signal-to-noise ratio (SNR) of a few tens of percent. We consider several GW detectors covering the frequency range \( 10^{-4} - 10^3 \, \text{Hz} \): LIGO O2 (Abbott et al. 2019a, for the instrument at Livingston as an example), advanced LIGO by design (AdLIGO; Martynov et al. 2016), ET under xylophone configuration (ETxylophone; Hild et al. 2009), DO with optimal performance (DOoptimal; Arca Sedda et al. 2019) and LISA (Robson et al. 2019). For each source, given \( [h(f)] \), the SNR for an instrument with a noise power spectral density (PSD) function \( S(f) \) is obtained by integrating in the \textit{observer-frame} frequency domain:

\[
\text{SNR}^2 = 4 \int_{f_{\text{min}}}^{f_{\text{max}}} \frac{|h(f)|^2}{S(f)} df,
\]

assuming that the noise is stationary and Gaussian with zero mean. Here we set\(^{24}\) \( f_{\text{min}} = 10^{-4} \, \text{Hz} \) and \( f_{\text{max}} = 2 f_{\text{RD}}/(1 + z_{GW}) \), where \( f_{\text{RD}} \) marks the beginning of the ringdown phase (see equation (5.5) in Santamaria et al. 2010).

The waveforms of all simulated GW events (at \( z_{GW} \geq 0 \)) with the \textit{obs-based} scaling relations under \( \gamma = 1.5 \) from \textsc{FDBox} \textsc{Lseed} are shown in Fig. 14 (in terms of the frequency evolution of the characteristic strain \( 2|h(f)| \)), on top of the sensitivity curves of the detectors considered here. Due to the rarity of DCBH candidates, we only found events involving Pop III-seeded BBHs (BBHPopIII). Under \textsc{Lseed}, the median total mass of detectable sources is \( \approx 250 \, M_\odot \) for all the instruments considered here, while the median redshifts are \( \approx 0.55 \) for AdLIGO (by design), 0.69 for ETxylophone and DOoptimal (whose typical waveforms overlap), and 0.45 for LISA and LIGO O2. The integrated all-sky detection rates (with SNR > 10) as functions of \( \gamma \) are shown in Fig. 15, under the \textit{obs-based} scaling relations. The results in the \textit{sim-based} model is similar, where the detection rates are insensitive to \( f_{\text{hulge}} \) (within a factor of 2 variations for \( f_{\text{hulge}} \sim 0.2 - 1 \)). The detection rate generally increases with

\(^{23}\) The detection rates are suppressed more for GW detectors more sensitive to high-z events (\( z \gtrsim 2 \)) such as ET and DO when the analysis is restricted to hard binaries. The reason is that high-z events are dominated by highly eccentric BBHs with shorter delay times, whose number is significantly reduced when the hard binary criterion is imposed.

\(^{24}\) Note that a GW event only resides at \( (1 + z_{GW}) \times f = f_{\text{RD}} > f_{GW,0} = \pi^{-1}\sqrt{GM/(1 + e)^{1.954}/|\nu_{GW}(1 - e^2)|} \) in the frequency domain, where \( f_{GW,0} \) is the peak frequency at the onset of the GW-driven inspiral. In our case, \( f_{GW,0}/(1 + z_{GW}) \lesssim 10^{-5} \, \text{Hz} \), such that \( f_{\text{min}} = 10^{-4} \, \text{Hz} \) for \( f_{GW,0}/(1 + z_{GW}) \) always holds.

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The BH masses involved in our simulated GW events are typically \( M \gtrsim 100 \, M_\odot \), higher than the estimated BH masses from most detected sources. However, this could be an artifact of our BH seeding models, as we only track the most massive BHs in each Pop III population even in our BH seeding models, as we only track the most massive BHs.

The BH masses involved in our simulated GW events are typically \( M \gtrsim 100 \, M_\odot \), higher than the estimated BH masses from most detected sources. However, this could be an artifact of our BH seeding models, as we only track the most massive BHs in each Pop III population even in our BH seeding models, as we only track the most massive BHs. In principle, low-mass Pop III-seeded BHs of \( \sim 40 - 50 \, M_\odot \) can also form ex-situ BH binaries and merge at \( z \lesssim 1 \) to be detected by LIGO O2.

### Figure 14

Waveforms (\( 2f(h(f)) \)) of all simulated GW events with the obs-based scaling relations under \( \gamma = 1.5 \) from FDBox_Lseed, together with sensitivity curves (\( \sqrt{f} \times S(f) \)) for selected GW detectors. The simulated BH mergers involving two Pop III seeds are plotted with faint gray curves. For illustration, we also label the transition point from inspiral to ringdown for each event. The labels are color coded by \( z_{GW} \). The sensitivity curves for LIGO O2, AdLIGO (by design), ETxylophone, DOoptimal and LISA are shown in thick and normal solid, dashed, dashed-dotted and dotted, respectively (see the text of Sec. 4.4 for descriptions of the detectors). For illustration, we also plot the typical waveforms of DCBH-DCBH mergers (\( M_1 = M_2 \sim 10^5 \, M_\odot \)) and DCBH-BH_{Pop III} mergers (\( M_1 \sim 10^4 \, M_\odot, M_2 \sim 100 \, M_\odot \)) at \( z_{GW} \sim 7 \) with the red dashed and orange dashed-dotted curves.

### Figure 15

All-sky detection rates (with SNR > 10) of GW events from ex-situ BHs formed at \( Z_{BH} > 4 \) in FDBox_{Lseed}, for AdLIGO by design (solid), ET’s xylophone configuration (dashed), the optimal performance of DO (dashed-dotted) and LISA (dotted), as functions of \( \gamma \), where the stellar environments are characterized with the obs-based scaling relations.
spins (e.g. Safarzadeh 2020. Last but not least, one salient feature of ex-situ BBHs formed by dynamical capture, are their high initial orbital eccentricities (see Fig. 11). However, as GW emissions circularize binary orbits, such that even with the highest initial eccentricity found in our simulations $(1 − e ∼ 10^{-5})$, the eccentricity drops to $\leq 0.1$ for $f_{\text{rest}} \gtrsim 10^{-2} \text{ Hz}$, making it difficult to measure with ground-based GW detectors (see Fig. 14), given the parameter-estimation degeneracy between BH spins and orbital eccentricity (Huerta et al. 2018). Nevertheless, it is possible to make robust eccentricity measurements for nearby sources with future planned space-based instruments sensitive at low frequencies, such as LISA and DOs.

To demonstrate the dependence of detection rates on BH seeding models, we show the results for selected detectors from \textsc{FD Zoom Lseed} and \textsc{FD Zoom Hseed} in Table 2, under the optimistic conditions of \textit{obs-based} scaling relations with $\gamma = 1.5$ and \textit{sim-based} scalings with $\gamma = 1.5$ and $f_{\text{bulge}} = 1.0$. Generally speaking, the detection rates for AdLIGO (by design), ETXylophone and DOoptimal are not very sensitive according to our IMF, such that the BBH formation rate can be as important as the in-situ channel for Pop III-seeded BBHs and deserves further investigation. However, given the large uncertainties (up to 2 orders of magnitude) for both the in-situ and ex-situ pathways (see below), the (relative) contributions to Pop-III BH-BH merger events from the two channels are still uncertain, to be revealed by future observations and more advanced theoretical models.

Since cosmological hydrodynamic simulations are always limited in resolution, volume and redshift range, we cannot self-consistently model the small-scale (sub-parsec) physics of BH seeding, as well as formation and evolution of BBHs. Instead, we use idealized sub-grid models whose parameter spaces are explored to estimate the range of GW rates. There are several caveats in our methodology, which may significantly impact the results:

- On the one hand, we only keep track of at most one BH from one Pop III stellar population that typically includes a few BHs, leading to possible underestimation of the BBH formation rate. Actually, the average number of BHs is 6 according to our IMF, such that the BBH formation rate can be boosted by up to a factor of 36 (for \textit{Lseed}) if multiple BHs are considered from each Pop III stellar population.
- On the other hand, we form BBHs as bound systems at our force resolution limit $\epsilon_R \sim 8 \text{ pc}$, which may not be small enough to ensure that the resulting BBHs are hard binaries, especially for BBHs with high eccentric orbits which can be easily disrupted at apocenters. Since only hard binaries will be hardened to emit GWs, we may have underestimated the GW rates. With analytical calculations and test simulations, we estimate the overestimation to be up to a factor of $\sim 4$ and $\sim 20$ in the efficiency of BH-BH mergers and detection rates of GW events, respectively, under the optimistic condition of BBH evolution (see Sec. 3.1).

We also rely on semi-analytical post-processing to calculate BBH evolution, based on parameterized BH-stellar mass scaling relations and stellar density profile. We found that the predicted GW rates are highly sensitive to the environments around high-z BBHs, which are captured by the inner slope $\gamma$ of stellar density profile in our model (see Fig. 12 and 15). Generally speaking, denser environments
(i.e. larger $\gamma$) lead to more rapid binary hardening by three-body encounters, such that more BBHs can merge within the Hubble time, resulting in higher GW rates. The realistic long-term environments around Pop III-seeded BBHs are still unknown, which can be more complex than the cases covered by our simple parameterized model.

To arrive at more robust predictions for the GWs from high-$z$ ex-situ BBHs, one must design more realistic sub-grid models addressing the following aspects:

- The mass and phase space distributions of BH systems (including single BHs, in-situ BBHs and X-ray binaries) as the end products of Pop III star-forming clouds, which, involving the initial mass function, star cluster evolution (over at least a few Myr) and supernova explosion/direct collapse mechanisms, may not be universal.
- The (erratic) dynamics of Pop III-seeded BHs ($M_{BH} \sim 100$ – $1000 M_\odot$) in galaxies, which is crucial for dynamical capture (and BH accretion), but challenging for cosmological simulations with limited mass resolution.
- The stellar and gas environments around BBHs that drive binary evolution across cosmic time, which is non-trivial as their host systems undergo mergers and accretion.

Actually, such considerations are general for the ex-situ channel of BBH formation by dynamical capture, from any generations of progenitor stars in the Universe. Moreover, it is generally interesting and crucial to evaluate the relative contributions of the ex-situ and in-situ channels, if we were to derive useful information (on the evolution of single and binary stars, BH seeding, dynamics and growth, cosmic structure formation) from the GW signals of coalescing compact objects.

In future work, we will use small-scale simulations (for individual minihaloes/dwarf galaxies) to develop more physically-justified sub-grid models for BH seeding, dynamics, as well as binary formation and evolution. For instance, we can derive the fractions of ejected and remaining BHs from N-body simulations of Pop III stellar groups (e.g. Ryu et al. 2015), and allow Pop III stellar particles to spawn multiple BH particles. In this way, we can also identify X-ray binaries among BH seeds whose accretion and feedback will be included (Jean et al. 2014). It is also interesting to study the GW signals from Pop III seeded BBHs in high-$z$ dense star clusters (dominated by Pop II stars), such as nuclear star clusters and globular clusters, by combining models of their formation and evolution (e.g. Devecchi & Volonteri 2009; Devecchi et al. 2010, 2012; Lupi et al. 2014; Kim et al. 2018; El-Badry et al. 2019) with direct N-body and Monte Carlo simulations of dense star clusters (e.g. O’Leary et al. 2016; Rodriguez et al. 2016a, 2018; Hoang et al. 2018).

The ultimate goal is to predict the distributions of GW events involving Pop III-seeded BBHs from both the ex-situ and in-situ channels in the GW parameter space (mass, redshift, eccentricity and spins), in comparison with the results of the events from other origins (e.g. Pop II and I stars). In this way, we may be able to identify a region in the parameter space dominated by Pop III-seeded BBHs, that can provide guidance for future GW instruments and insights on extracting information of early structure formation from GW observations. In the next decades, this region can be populated by hundreds to thousands of GW events, from which new constraints can be derived, e.g. for the Pop III binary statistics and stellar evolution models (for the in-situ channel), as well as typical environments of BBH evolution and BH mass function (for the ex-situ channel).

It is only by considering both the ex-situ and in-situ channels of binary formation that the power of the GW window can be fully realized in the era of GW astrophysics. With more advanced GW detectors coming into operation over the next decades, it is timely for the fields of star and galaxy formation to address the theoretical challenges involved in understanding binary remnants from the first stars.

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To demonstrate the effect of stellar feedback, we focus on the star formation and BH accretion histories, as well as GW signals, in the zoom setup with the Hseed seeding scenario. Without PI heating and SN-driven winds from Pop II stars, the total SFRD is enhanced by about one order of magnitude at $z \lesssim 14$, becoming much higher than the observational constraints at $z \lesssim 10$, as shown in Fig. A1. This leads to a factor of 10 increase in the Pop II stellar density by $z = 7$. However, the Pop III SFRD remains almost unchanged (thus not shown). This is reasonable as we do not turn off the Pop III feedback and LW field for NSFDBK which play the most important roles in regulating Pop III SF. Another factor is that the LW radiation is enhanced by the increased Pop II stellar density by a factor of $10^{7}$, becoming much higher than observational constraints at $z \lesssim 10$.

**APPENDIX A: EFFECT OF STELLAR FEEDBACK**

To demonstrate the effect of stellar feedback, we focus on the star formation and BH accretion histories, as well as GW signals, in the zoom setup with the Hseed seeding scenario. Without PI heating and SN-driven winds from Pop II stars, the total SFRD is enhanced by about one order of magnitude at $z \lesssim 14$, becoming much higher than the observational constraints at $z \lesssim 10$, as shown in Fig. A1. This leads to a factor of 10 increase in the Pop II stellar density by $z = 7$. However, the Pop III SFRD remains almost unchanged (thus not shown). This is reasonable as we do not turn off the Pop III feedback and LW field for NSFDBK which play
Table A1. Detection rates per year and percentages (in brackets) of simulated GW events with SNR > 10 from ex-situ BBHs formed at $z_{\text{BH}} > 7$ in FD Zoom Hseed and NSFDBK Zoom Hseed, under the obs-based scaling relations with $\gamma = 1.5$ and sim-based scaling relations with $\gamma = 1.5$ and $f_{\text{bulge}} = 1.0$. The detection percentage reflects the ratio of the number of sources with SNR > 10 and the total number of sources (at $z_{\text{GW}} \geq 0$). The first column is the flag FDBKPopII, indicating whether Pop II feedback is included. See Sec. 4.4 for descriptions of the detectors considered here.

| Detector   | obs-based | sim-based |
|------------|-----------|-----------|
|            | $\gamma = 1.5$ | $\gamma = 1.5$ |
| FDBKPopII  | AdLIGO    | ETxylophone | LISA |
|            | $f_{\text{bulge}} = 1.0$ | $f_{\text{bulge}} = 1.0$ |
|            | 5.9 (54%) | 30 (85%) | 30 (85%) |
|            | 7 (43%) | 39 (100%) | 39 (100%) |
|            | 0 | 143 (77%) | 11 (15%) |
|            | 0 | 104 (86%) | 10.1 (14%) |

26 As indicated in equation (9), the wind launching probability is approximately proportional to $m_*/m_{\text{SF}}$. In the BH run, $m_*/m_{\text{SF}}$ is increased by up to a factor of 8, so that wind launching becomes more immediate and efficient.

27 Under the fiducial resolution, the smallest resolved structures with $\sim 32$ DM particles have masses $\sim 2 \times 10^6 \, M_{\odot}$, comparable to the H$_2$ cooling threshold for Pop III SF, which means that some low-mass Pop III-hosting minihaloes are likely unresolved. In the BH run, these haloes will be resolved, leading to additional Pop III star formation.

secondary collapsed gas clumps, such that dynamical fraction from Pop II stars does not play an important role in BBH formation.

**APPENDIX B: NUMERICAL CONVERGENCE**

Similar comparisons as those in appendix A are made for FD Zoom Lseed and FD ZoomHR Lseed to test numerical convergence, as shown in Fig. B1-B3 and Table B1. Generally speaking, the code shows good enough convergence in star formation and BH accretion histories, as well as GW signals. With higher resolution for gas and DM, the total SFRD is reduced by a factor of 2 at $z \lesssim 14$ (see Fig. B1), showing better agreement with observations, while the Pop III SFRD is moderately increased, especially at $z \gtrsim 12$, such that the total density of Pop III stars formed by $z = 7$ is enhanced by a factor of 2 (see Fig. B2). These rather small differences can be explained by more efficient winds, especially at small scales, more resolved minihaloes hosting Pop III stars at the low-mass end and weaker LW feedback due to the reduced Pop II SF. The BH accreted mass density is higher than its low-resolution counterpart by a factor of $\sim 5$ for $z \lesssim 22$ (see Fig. B3), caused by the enhancement in Pop III SF and the nature of sub-grid Bondi accretion.

In the optimistic cases of obs-based scaling relations with $\gamma = 1.5$ and sim-based scaling relations with $\gamma = 1.5$ and $f_{\text{bulge}} = 1.0$, the total number of GW sources in FD ZoomHR Lseed is $N_{\text{merger}, \text{HR}} = 12$, 3 times the number $N_{\text{merger}} = 4$ in FD Zoom Lseed. The detection rates for ETxylophone and DOptimal are also higher by up to a factor of $\sim 3$, which is reasonable since these instruments can reach almost all sources. While for AdLIGO and LISA, the differences can be larger but suffer from large statistical uncertainties. The samples of GW sources are too small to tell whether such differences in detection rates imply poor numerical convergence. The increase of GW events in the high-resolution run can be explained by the enhanced Pop III SF and the better resolved dynamical friction from gas.
Figure B1. Total (co-moving) SFRD from FDzoom_Lseed (solid) and FDzoomHR_Lseed (dashed). We also plot the corresponding results in the literature for comparison, which are described in detail in the caption of Fig. 5. With higher resolution for gas and DM, the total SFRD is reduced by a factor of 2 at \( z \lesssim 14 \).

Figure B2. Pop III (co-moving) SFRD from FDzoom_Lseed (solid) and FDzoomHR_Lseed (dashed). We also plot the corresponding results in the literature for comparison, which are described in detail in the caption of Fig. 5. With higher resolution for gas and DM, the Pop III SFRD is moderately increased, especially at \( z \gtrsim 12 \), such that the total density of Pop III stars formed by \( z = 7 \) is enhanced by a factor of 2.

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