Population synthesis of black hole mergers with B-POP: the impact of dynamics, natal spins, and intermediate-mass black holes on the population of gravitational wave sources

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ABSTRACT

The current interpretation of LIGO–Virgo–KAGRA data suggests that the primary mass function of merging binary black holes (BBHs) at redshift $z \lesssim 1$ contains multiples structures and is likely truncated beyond $M_1 > 100M_\odot$, while spins are relatively low. Theoretical models of BBH formation in different environments can provide a key to interpret the population of observed mergers, but they require the simultaneous treatment of stellar evolution and dynamics, galaxy evolution, and general relativity. Here, we present B-POP, a tool enabling population synthesis of BBH mergers originating either via isolated binary stellar evolution or dynamical interactions in young, globular, and nuclear clusters. Using B-POP, we show that observed BBHs can be interpreted as members of a mixed population comprised of $\sim 34\%$ (66\%) isolated (dynamical) BBHs. Our models suggest that the overall primary mass distribution of merging BBHs extends beyond $M_1 \simeq 200M_\odot$. We explore the impact of BH natal spins, showing that the effective spin parameter distribution might hint at different natal spins for single and binary black holes. Hierarchical mergers represent $4.6 - 7.9\%$ of mock mergers in our reference model and dominate the primary mass distribution beyond $M_1 > 65M_\odot$. Taking into account observational biases, we found that around $2.7 - 7.5\%$ of BBH mergers might involve intermediate-mass black hole (IMBH) seeds formed via stellar collisions and accretion in dense clusters. Comparing this percentage with the observed value might help us to constrain the impact of IMBHs on the formation of BBH mergers.

Key words: black holes – gravitational waves – stellar evolution – star clusters – globular clusters – galactic nuclei

1 INTRODUCTION

The LIGO-Virgo-Kagra collaboration (LVK) has recently released an updated catalogue of gravitational wave (GW) events, named GWTC-2.1 (Abbott et al. 2021a). This catalogue contains the properties of 55 candidate black hole binary (BBH) mergers, featuring asymmetric mergers like GW190412 (Abbott et al. 2020c) and several peculiar systems, such as GW190814 (Abbott et al. 2020e), whose companion falls in the so-called lower mass-gap and might be the lightest BH to date, and GW190521 (Abbott et al. 2020d,a), the first BBH merger that produced a remnant with a mass of $\sim 140M_\odot$, i.e. in the mass range of the elusive intermediate-mass black holes (IMBHs). Although still relatively low, the number of BBH mergers detected so far permitted to place some constraints on the BBH population at redshift $z < 1 - 2$. In particular, Abbott et al. (2021b) suggest that the mass distribution of primary black holes (BHs) is characterised by a complex structure, likely described by a power-law with two peaks at $M_1 \sim 20M_\odot$ and $M_1 \sim 40M_\odot$ and a sharp truncation at values $M_1 > 100M_\odot$ (Abbott et al. 2021b). Such a complex distribution is likely the result of different BBH formation channels.

A BBH can form through a variety of branches, but at the first order we can distinguish two broad ensembles: isolated binaries, which form from the evolution of stars paired together at birth, and dynamical binaries, whose formation is mediated by strong stellar encounters in young (YCs), globular (GCs), and nuclear clusters (NCs). According to the field triple channel, which is one of the possible sub-branches of the isolated binary scenario, three stars already bound at birth undergo a complex stellar and dynamical evolution that cul-

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minates in the formation of a merging BBH. Similarly, triples and higher order multiples can form in dense star clusters; in this case the three objects can become a bound system via dynamical interactions. With regards to galactic nuclei, we can distinguish three different sub-branches: i) BBH pairing in NCs without a supermassive BH (SMBH), ii) BBH pairing in NCs with a central SMBH, iii) BBH pairing in active galactic nuclei (AGN) discs. In the first case, BBH formation is regulated by dynamical encounters (Antonini et al. 2016, 2019; Arca Sedda 2020) and is directly linked to the formation history of the NC (Arca Sedda 2020). In the second case, the presence of an SMBH can efficiently affect the long-term evolution of the binary, potentially driving secular effects like Kozai-Lidov resonances (Kozai 1962; Lidov 1962), which can shorten the BBH lifetime and thus contribute to the formation of merging BBHs (Antonini & Perets 2012; Hoang et al. 2018; Fragione et al. 2019; Arca Sedda 2020). In the latter case, the BH pairing is facilitated by the drag force of the AGN disc (e.g. McKernan et al. 2018; Tagawa et al. 2021). While theoretical estimates derived for different channels and sub-channels suggest that they all might contribute to the cosmic population of BBHs, it is still unclear whether it is possible to discern fingerprints of different formation channels from observed mergers, mostly owing to the degeneracies that characterise different formation channels. Several studies suggest that a mixed population of BBHs is the most likely scenario to explain LVK sources (e.g., Arca Sedda & Benacquista 2019; Arca Sedda et al. 2020; Bavera et al. 2020; Zevin et al. 2021; Bouffanais et al. 2021, but see Roulet et al. 2021 and Rodriguez et al. 2021 for a different interpretation).

Different formation channels can leave fingerprints on the distribution of remnant mass and spins, impact the properties of the merging BHs, and determine the merger rate per BH mass. BH spin magnitudes are still far from being understood. Several BHs in high-mass X-ray binaries seem to be nearly maximally spinning (see e.g. Qiu et al. 2019; Reynolds 2021), while LVK BHs support evidence for relatively low spins ($\chi < 0.1 - 0.2$) (Abbott et al. 2021b). This might imply that different formation channels are characterised by different BH spin distributions.

In this work, we present the results of B-POP, a tool capable of creating large samples of BBH mergers formed either in isolation or in dynamical environments, which takes into account state-of-the-art stellar evolution recipes for single and binary stars, a semi-analytic treatment for the formation of dynamical mergers, a flexible treatment for BH natal spins, and implements numerical relativity fitting formulae to calculate remnant masses, spins, and GW recoil kicks. Moreover, B-POP exploits prescriptions for observational biases of second-generation ground-based GW detectors, and prescriptions for BH formation across cosmic time.

Varying the relative amount of BBH mergers forming in one channel or another, the BH natal spin distribution, and stellar evolution, we show that the observed GW sources can be interpreted as a part of a global population equally contributed by isolated and dynamical mergers. Such population exhibits a primary mass distribution characterised by a long tail extending beyond $M_1 > 100 - 200 M_\odot$ which might be particularly difficult to access with ground-based detectors due to observational selection effects.

The paper is organised as follows: in Section 2 we describe the main features and improvements of B-POP and the main properties of our models; Section 3 introduces the main results of our work in terms of primary and total BBH merger mass, spin, and effective spin parameter; Section 4 discusses the implications of our results in terms of hierarchical mergers and massive BH seeds; whilst in Section 5 we summarize our conclusions.

2 THE B-POP CODE

In this work, we exploit an improved version of a semi-analytic tool that combines stellar evolution prescriptions for single and binary stars, a treatment for formation of dynamical and isolated BBH mergers, a treatment for relativistic kicks, and numerical relativity fitting formulae to estimate the properties of the remnant (Arca Sedda & Benacquista 2019; Arca Sedda et al. 2020). This method enables us to explore how different BBH formation channels can affect the properties of mergers observed from ground-based detectors like LIGO and Virgo.

Hereafter, we refer to the upgraded tool as B-POP (Black hole POPulation synthesis). B-POP implements a multi-stepped procedure that enables us creating populations of BBH mergers forming either via binary stellar evolution (isolated channel) or via gravitational encounters in star clusters (dynamical encounters). The B-POP workflow, which is shown in Figure 1, can be sketched as follows:

(i) Environment selection

- set the relative amount of BBH mergers forming via the isolated or the dynamical channel;
- for the dynamical channel, set the relative amount of mergers forming in YCs, GCs, and NCs;
- set the metallicity distribution of the host environment for dynamical and isolated channels;
- set the host cluster formation time for dynamical mergers and the binary formation time for isolated mergers;

(ii) Binary properties selection

- set the binary component masses according to a stellar initial mass function;
- for dynamical binaries, set the pairing criterion;
- use single/binary stellar evolution to calculate BH natal masses;
- assign to each BH a natal spin and set the level of spin alignment in the binary;
- assign to each merger a formation time inferred from the adopted star formation rate;
- assign to each merger a delay time, which is calculated accordingly to the formation channel as explained in the next sections;

(iii) Merger remnant

- calculate the remnant BH mass, spin, effective spin, and GW recoil using numerical relativity fitting formulae described in Campanelli et al. (2007); Lousto et al. (2012); Jiménez-Forteza et al. (2017);
- in the case of dynamical mergers, the remnant BH recoil is compared to the cluster escape velocity to model hierarchical mergers.
The mass and delay time for isolated BBHs and single BHs are obtained through the MOBSE code (Mapelli et al. 2017; Giacobbo et al. 2018; Mapelli & Giacobbo 2018). As detailed in Section 2.2, we exploit a semi-analytic method to assembly dynamical binaries.

The database of merging BBHs constructed this way is post-processed to take into account the intrinsic observational bias that might affect ground-based GW detectors. This procedure enables us to obtain two different populations: one “raw”, that should reflect the population of mergers formed via dynamics or isolated stellar evolution, and the other “weighted” through the observation bias criteria adopted.

The aforementioned points summarize the main features of B-POP 1. Compared to the previous versions, B-POP implements several upgrades that are described in detail in the following.

2.1 Formation and delay times, metallicity distribution, and BH natal kicks

In B-POP, every BBH merger is characterised by at least two main time scales: the formation time $t_{\rm for}$, namely the time at which the two BH progenitors formed, and the delay time $t_{\rm del}$, namely the time elapsed from the binary formation to the BBH coalescence.

Whilst the sum $t_{\rm for} + t_{\rm del}$ determines the cosmic time at which the merger takes place, the formation time alone represents a crucial quantity to determine the most likely value of the metallicity of the merger host environment.

For isolated binaries and BHs forming in YCs, we extract a formation redshift from the cosmic star formation rate inferred by Madau & Fragos (2017):

$$
\psi(z) = \frac{0.01(1+z)^{2.6}}{1 + [(1+z)/3.2]^{6.2}} \text{ M}_\odot \text{ yr}^{-1} \text{ Mpc}^{-3},
$$

whereas for BHs in GCs and NCs we extract the formation redshift from the GCs formation rate described in Katz & Ricotti (2013), which is nearly flat in the redshift range $z \approx 2 - 6$. We convert the formation redshift into a cosmic time assuming the set of cosmological parameters provided by Ade et al. (2016), namely $H_0 = 67.74 \text{ km/s/Mpc}^2$, $\Omega_m = 0.3089$, $\Omega_\Lambda = 0.6911$.

The delay time is calculated either directly from MOBSE for isolated binaries, or is inferred from the typical timescales of dynamical binary formation and mergers, as detailed in the next section. Following our previous paper (Arca Sedda et al. 2020), we assume that at redshift $z = 2$ the metallicity of GCs and NCs can be described by a lognormal distribution limited between $Z = 0.005 - 0.001$, i.e. the typical range of values observed in Galactic GCs, whilst for galaxies and YCs we adopt the metallicity distribution derived from the SDSS (Gallazzi et al. 2006), which is measured at redshift $z \approx 0$.

To take into account the fact that, on average, the larger is the redshift the lower the metallicity, we shift the metallicity distribution by a redshift-dependent factor, $\delta Z$, defined as (see e.g. Zevin et al. 2021; Bavera et al. 2020)

$$
\log(\delta Z/Z_\odot) = -0.074 z^{\alpha_Z},
$$

with $\alpha_Z = 1.34$ in the case of isolated binaries (Bavera et al. 2020) and $\alpha_Z = 1.2$ for star clusters.

2.2 Dynamical binaries and hierarchical mergers

In B-POP, we extract cluster masses and half-mass radii from the observed distribution of GCs (Harris et al. 2014) and NCs (Georgiev et al. 2016). For YCs, we adopt the same mass distribution used for GCs shifted by two dex toward lower masses (Portegies Zwart et al. 2010). We exploit the Python built-in Gaussian kernel density estimator to reconstruct the mass and half-mass radius distributions for different cluster types, and then we use the cumulative distribution to sample our mock clusters. For GCs and NCs, this procedure preserves the observed distributions and enables us to take into account the low- and high-end tails. For YCs, these choices imply that the mass distribution peaks at around $10^4 \text{ M}_\odot$, with the high-end tail extending up to $10^6 \text{ M}_\odot$. The cumulative distribution of YCs obtained this way implies that the probability to have a YC with a mass $> 10^4 \text{ M}_\odot$ is 50%.

The cluster mass distribution is described by either a Plummer (1911) density profile or a power-law distribution with slope $\gamma$ (Dehnen 1993). This is crucial to determine the cluster central density and escape velocity.

For YCs and GCs, we assume that the cluster has a probability of 50% to be described by a Dehnen (1993) sphere, and in such a case we adopt a value for the inner density slope of $\gamma = 1(1.5)$ for YCs/GCs. This choice enables us to explore how the matter distribution and the presence of a density cusp in the cluster innermost region could affect BBH formation. Otherwise, we adopt a Plummer (1911) sphere to model the cluster.

For YCs, we adopt a Dehnen (1993) model with $\gamma = 1.9$. According to this choice, the central escape velocity is thus determined as:

$$
v_{\rm esc}^2 = \frac{2GM_{\text{c}}}{r_{\text{h}}} \times \left\{ \frac{1.3}{[2^{1/(3-\gamma)} - 1](2 - \gamma)^{-1}} \right\}_{\text{Plummer, Dehnen}}.
$$

We note that in the case of YCs, the choice $\gamma = 1$ leads to an escape velocity in Dehnen (1993) models $\sim 30\%$ smaller than in Plummer (1911) models – at fixed value of $r_h$, while in the case of GCs, where $\gamma = 1.5$, $v_{\text{esc}}$ is practically the same in both models. The choice of a flat (Plummer) or a cusp (Dehnen) density profile aims at capturing the different phases of cluster life, as early evolution, mass segregation, and binary formation can significantly affect cluster matter distribution. If the remnant BH of a dynamical merger receives a kick $v_{\text{kick}} < v_{\text{esc}}$, we check whether the BH remnant can undergo one (or more) further mergers within a Hubble time. In case of multiple generation mergers we follow the evolution of the BH remnant until either: a) $v_{\text{kick}} > v_{\text{esc}}$, b) the number of BHs in the innermost region of the cluster is fully consumed in repeated mergers, c) the total delay time exceeds 14 Gyr.

We assume that the number of BHs participating in one or multiple mergers in star clusters is comparable to the number of dynamical BHs.

1 We refer the reader to Arca Sedda et al. (2020) for further details about the previous version of our tool.

2 It has been shown that Plummer (1911) closely resemble King (1962) models with an adimensional potential well $W_0 \approx 6$ (Aarseth et al. 2008), which have been extensively used to fit the observed properties of Galactic GCs (Harris et al. 2014).
of BHs lurking inside the cluster scale radius, which is directly connected to the cluster half-mass radius:

\[ n_{\text{bhs}} = f_{\text{bh}} f_{\text{reten}} f_{\text{encl}} M_c, \]  

where \( f_{\text{bh}} = 0.0008 \) is the fraction of cluster mass in stellar BHs according to a Kroupa (2001) initial mass function, \( f_{\text{reten}} = 0.5 \) represents the fraction of BHs retained in the cluster (see e.g. Morscher et al. 2015; Arca Sedda et al. 2018), and \( f_{\text{encl}} \) is the fraction of cluster mass enclosed within the cluster typical radius.

At the lowest level of approximation, to assign the BBH component masses we assume a simple single stellar BH mass spectrum (SSBH). However, as pointed out in the recent literature, the actual mass spectrum of BHs participating in dynamical interactions can be much more complex, especially in clusters harboring a large population of primordial binaries (Di Carlo et al. 2019, 2021; González et al. 2021; Rizzuto et al. 2021b,a; Rastello et al. 2021).

Some BHs can form out of collisions or mergers of massive stars initially paired in close binaries, while others can be former members of soft binaries that have been ionized via repeated interactions with other stars or compact objects (see e.g. Spera et al. 2019; Di Carlo et al. 2019; Rizzuto et al. 2021b,a). In the following, we will refer to this mass spectrum, associated with BHs formed from stellar collisions and former

Figure 1. B-POP workflow.
components of isolated binaries, as mixed single BH mass spectrum (MSBH).

When selecting BH masses from both SSBH and MSBH mass spectra, we only consider BHs with a natal kick, which is provided by MOBSE, smaller than the host cluster escape velocity.

Heavy NCs (LogM/M⊙ > 7.5) can give rise to “cascades” of BH mergers, leading to massive BHs with mass as large as 10^4−5 M⊙. However, given the rarity of such dense and massive star clusters, these “oversized” BHs are expected to be extremely rare (see also Mapelli et al. 2021; Fragione & Silk 2020). We leave the investigation of such massive seeds to a follow-up study.

One additional pathway that can contribute to BH formation in star clusters is via stellar collisions and stellar accretion onto “normal” BHs, a process that can trigger the formation of IMBH seeds as massive as 100−500 M⊙ (Di Carlo et al. 2019; Arca Sedda et al. 2021b; Rizzuto et al. 2021b; González et al. 2021). Hereafter, we label the mass spectrum associated to IMBH seeds as heavy BH mass spectrum (HSBH).

Although many efforts have been made toward a better comprehension of how BHs develop in star clusters, it is still unclear whether typical BH populations in stellar systems are mostly dominated by a SSBH mass spectrum, or if the MSBH and HSBH spectra play a significant role in determining BH pairing and merger. Following a rather agnostic approach, we regulate the amount of BHs extracted from the SSBH, MSBH, or HSBH mass spectra via two parameters: the mixing fraction (f_max) and the seed formation probability (f_seed). In practice, we assume that the whole population of BHs is composed of 1 − f_max − f_seed BHs from the standard single BH mass spectrum, f_max from processed primordial binaries, and f_seed BHs byproduct of repeated stellar collisions.

In B-POP, the evolutionary timescales of dynamical BHs are linked to the cluster evolution as follows. For each BBH, we select a cluster formation time (t_cluster) as explained in the previous section, and sum it up to the BH formation time (t_form), which is provided directly by MOBSE. The two BHs are assumed to reach the centre of the host cluster in a dynamical friction timescale t_dynamical (see e.g. Binney & Tremaine 2008)

\[ t_{\text{dynamical}} = 0.42 \text{Gyr} \left( \frac{10 m_\ast}{m_{\text{CO}}} \right) \left( \frac{r}{r_h} \right)^{1.76} \left( \frac{t_{\text{rel}}}{4.2 \text{ Gyr}} \right), \]

where m_\ast is the average mass of stars in the environment, m_{\text{CO}} is the mass of the heavy object (either single or binary), r is its position, and t_{\text{rel}} is the relaxation time.

\[ t_{\text{rel}} = 4.2 \text{ Gyr} \left( \frac{15}{\log \Lambda} \right) \left( \frac{r_h}{4} \right)^{3/2} \sqrt{\frac{M_\ast}{10^7 M_\odot}}, \]

with log Λ the Coulomb logarithm.

Once the BHs reach the core, the time needed for the BH pairing will be given by the minimum between the typical three-body interaction timescale t_3body (Lee 1995)

\[ t_{\text{3body}} = 4 \text{ Gyr} \left( \frac{10^6 M_\odot}{\rho_c} \right)^2 \left( \frac{\sigma_c}{30 \text{ km/s}} \right)^9 \times \left( \frac{m_\ast}{m_{\text{CO}}} \right)^{9/2} \left( \frac{10}{m_{\text{CO}}} \right)^{-5}, \]

and the binary-single capture process t_bs (Miller & Lauberg 2009)

\[ t_{\text{bs}} = 3 \text{ Gyr} \left( \frac{0.01}{f_b} \right) \left( \frac{10^6 \text{ pc}^{-3}}{n_\ast} \right) \times \left( \frac{\sigma_c}{30 \text{ km/s}} \right) \left( \frac{10M_\odot}{a_h (M_1 + M_2 + m_p)} \right)^2. \]

In the equations above, ρ_c and σ_c represent the cluster density and velocity dispersion, ζ ≤ 1 is a parameter representing the level of energy equipartition among the heavy and light population of stars − we assume ζ = 1 in our calculations, f_b is the binary fraction, m_p is the typical mass of stellar perturbers, and

\[ a_h \approx 50 \text{AU} \left( \frac{M_1 + M_2}{30 M_\odot} \right) \left( \frac{30 \text{ km/s}}{\sigma_c} \right)^2 \]

is the hard binary separation.

The actual value of each timescale has been selected from a Gaussian distribution peaking at the nominal value and assuming a dispersion of 10%. This choice takes into account the uncertainties in cluster mass and half-mass radius, the cosmic star formation history, and the small scale physics regulating star formation in the galactic field.

We assume that a hard BBH is formed after a total time t_{form} + t_{birth} + t_{dynamical} + min(t_3body, t_bs). The further evolution of the binary is regulated through the binary-single interaction timescale t_{1-2} (Gültekin et al. 2004; Antonini et al. 2016)

\[ t_{1-2} = \frac{0.02 \text{ Gyr}}{\zeta} \left( \frac{10^6 \text{ pc}^{-3}}{n_\ast} \right) \left( \frac{\sigma_c}{30 \text{ km/s}} \right) \times \sqrt{\frac{10 m_\ast}{M_1 + M_2}} \left( \frac{0.05 \text{AU}}{a_h} \right) \left( \frac{20}{M_1 + M_2} \right), \]

which is the typical timescale in which the binary spends most of its lifetime.

At this stage, we calculate two critical values of the BBH semi-major axis (a), namely the maximum value below which the binary gets ejected via further interactions (a_{ej}) and the maximum value below which GW emission dominates the evolution (a_{gw}) (Antonini et al. 2016):

\[ a_{ej} = 0.07 \text{AU} \left( \frac{M_1 + M_2}{M_1 + M_2 + m_p} \right) \left( \frac{v_{esc}}{50 \text{ km/s}} \right)^{-2}, \]

\[ a_{gw} = 0.05 \text{AU} \left( \frac{M_1 + M_2}{20M_\odot} \right)^{3/5} \left( \frac{M_2/M_1}{1 + M_2/M_1} \right)^{1/5} \times \left( \frac{\sigma_c}{30 \text{ km/s}} \right)^{1/5} \left( \frac{10^6 M_\odot}{\rho_c} \right)^{1/5}, \]

where μ = M_1 M_2/(M_1 + M_2) is the reduced mass of the binary system. If the BBH has a_{ej} > a_{gw}, the binary will be ejected and merge outside the cluster over a GW timescale (t_{GW}), calculated according to Peters (1964). Otherwise, the BBH merger will be mediated by three-body encounters over a timescale t_{GW3} ≃ 5(M_1 + M_2)/m_p t_{1-2} (Miller & Hamilton 2002; Antonini & Rasio 2016).

If the sum of all timescales above is smaller than a Hubble time, the BBH is labelled as a merger and the associated GW recoil kick is calculated. If the BBH merges inside the cluster and the GW kick is larger than v_{esc}, the remnant is ejected from the cluster and the merger chain is halted, otherwise the remnant is displaced from the centre to a maximum distance \[ t_d = r_h \sqrt{v_{esc}/(v_{esc} - v_{gw})} - 1 \] (see e.g. Antonini et al.
In the latter case, the remnant is assumed to come back to the cluster centre over a dynamical friction time \( t_{df} \), and to form a hard binary over a \( t_{ba} \) timescale. The whole procedure is repeated until either the reservoir of stellar BHs in the cluster centre is emptied, or the remnant is ejected from the cluster, via dynamical interactions if \( a_{ej} > a_{gw} \) or GW kick if \( v_{kick} > v_{esc} \).

### 2.3 Black hole natal spins

One of the most debated aspects of stellar BH formation and pairing is the actual distribution of natal spins. Observations of BHs in low- and high-mass X-ray binaries suggest that BHs have large natal spin, up to 0.9 (see e.g. Qin et al. 2019), whilst Fuller & Ma (2019) suggest that efficient angular momentum transport triggered by the Tayler-Spruit dynamo (Spruit 2002) can lead to spins as low as 0.01 in BHs born from single stars. In this framework, the population of detected BBH mergers hints at a spin distribution for merging BHs attaining relatively low values, \( \chi_{1,2} \approx 0.02 \) (Abbott et al. 2021b).

Given these uncertainties, in B-POP we allow for different choices. Throughout the paper, we extract spins in the range \( 0 \rightarrow 1 \) and explore four different cases:

- Spins are drawn from a Gaussian distribution centered on \( \chi_{1,2} = 0.5 \) with dispersion 0.1 (high spin model, denoted with GSS and letter H);
- Spins are drawn from a Gaussian distribution centered on \( \chi_{1,2} = 0.2 \) with dispersion 0.1 (low spin model, denoted with GSS and letter L);
- Spins are drawn from a Maxwellian with dispersion 0.2 (model denoted with MXL);
- Spins are set to 0.01 according to Fuller & Ma (2019) (model denoted with FM19);
- Spins are set to 0.01 for dynamical BHs whilst extracted from a Maxwellian, with dispersion 0.2, or a Gaussian centered on \( \chi_{1,2} = 0.5 \) for BHs in isolated mergers (model denoted with FM19+MXL and FM19+GSS).

### 2.4 Observational biases

Several parameters can affect the probability to detect BBH mergers. Among others, the distance at which the merger takes place, the direction of the GW that hits the detector, and the binary orbital parameters. For ground-based detectors like LIGO and Virgo, the accessible cosmological volume \( V_T \) depends on the primary mass via a power-law \( \propto M_1^{-2} \), at least in the \( 10 < M_1/M_\odot < 100 \) mass range, and increases for increasing binary mass ratio (Fishbach & Holz 2017). The volume-mass ratio dependence can also be described by a power-law in the form \( \propto M_1^\beta \), with \( \beta = 0.47 \pm 0.72 \) depending on the primary mass (see Figure 7 in Arca Sedda 2021).

In B-POP, we first create a sample of BBH mergers following the method described in the previous sections, and then we sample “mock” observations of BBHs exploiting the \( V_T = M_1 \) and \( V_T = q \) relations as selection criteria (see also Arca Sedda 2020).

Additionally, we require that mock BBHs happen at a redshift \( z < 2 \), i.e. close to the maximum distance reachable with LIGO at design sensitivity (Abbott et al. 2020b).

Although rather crude, this approach enables us to study both the overall population of mergers forming in isolation or dynamically, and the sub-population of mergers that might be accessible with second-generation GW detectors.

### 2.5 The reference model

Our reference model has the following features:

- Fraction of dynamical mergers (compared to the total): \( f_{dyn} = 0.5 \);
- Fraction of mergers coming from YCs, GCs, NCs: \( f_{YC,GC,NC} = 1/3 \);
- BBH merger formation time selected according to:
  - the cosmic SFR from Madau & Fragos (2017) for isolated binaries and dynamical binaries in YCs,
  - the cluster formation rate from Katz & Ricotti (2013) for GCs and NCs;
- Galaxy and YC metallicity distribution adapted from Gallazzi et al. (2006);
- GC and NC metallicity distribution is assumed flat in logarithmic values as discussed in our previous work (Arca Sedda et al. 2020) and similar approaches (see e.g. Bavera et al. 2020; Zevin et al. 2021);
- As detailed in Section 2.1 above, the metallicity distribution is conveniently rescaled via the redshift-dependent factor shown in Equation 2;
- We weight the metallicity distribution with the probability for a BBH to merge in an environment with a given metallicity, assuming a power-law with slope \( -1.5 \);
- Dynamical BBH masses are extracted from SSBH and MSBH mass spectra assuming a mixing fraction of \( f_{max} = 0.5 \), whilst we neglect the contribution of IMBH seeds (thus \( f_{seed} = 0 \));
- BH spins are extracted from a Gaussian distribution centred on \( \chi_{1,2} = 0.2 \) with dispersion 0.1 truncated between 0 and 1;
- The polar angle \( \theta \) between BH spins and the BBH angular momentum is extracted from:
  - a uniform distribution in \( \cos \theta \) in the case of dynamical binaries,
  - the cumulative distribution \( P_\theta = [(\cos \theta + 1)/2]^{\alpha_\theta + 1} \) (Arca Sedda & Benacquista 2019) for isolated binaries. In this case we adopt \( \alpha_\theta = 8 \), which implies 20(55)% of binaries having \( \theta_{1,2} \) values that differ by less than 5(20)%;
- The angle \( \phi \) between the BH spin vectors is assigned assuming a uniform distribution in \( \cos \phi \).

To explore the parameter space, we create different models varying the BH spin distribution, the fraction of dynamical mergers, the impact of the single BH mass spectrum adopted, and the role of IMBH seeds in determining the observed BH mass spectrum, as detailed in the next sections. For each model, we create a database of 100,000 BBH mergers from which we select mergers happening at a redshift \( z < 2 \) according to the adopted observational selection criteria. The choice of a power-law with slope \( -1.5 \) returns results consistent with results from isolated binaries (e.g. Giacobbo et al. 2018) and star cluster simulations (e.g. Askar et al. 2017), as shown in our previous paper (Arca Sedda et al. 2020)
3 RESULTS

In this section we present the main features of BBH mergers from the reference model and discuss how they compare with LVK data in terms of global properties, primary mass distribution, and effective spin parameters.

The adopted selection criteria and the requirement that mergers must occur at $z < 2$ clearly impact the actual fraction of mergers coming from one formation channel or another. Compared to the initial assumptions, i.e. $f_{\text{iso}} = f_{\text{dyn}}$, we find that the actual fraction of mock BBHs coming from the isolated (dynamical) channel is $f_{\text{iso}}(\text{dyn})_{\text{mock}} \simeq 34\% (66\%)$. Similarly, the selection affects the amount of BBHs forming in YCs, GCs, and NCs, leading to $f_{\text{VC,GC,NC}}$, mock $\sim (29, 53, 18\%)$, with a difference of $< 1\% - 2\%$ from one models set to another. Note that this owes entirely to the selection criteria.

3.1 Component masses, effective spin parameter, and mass ratios of merging BBHs

In order to determine whether the BBH merger population in the reference model is representative of the GWTC-2 data, Figure 2 compares mock data and observations in terms of combined distribution of component mass, mass-ratio, and effective spin parameter for both the low- and high-spin reference models.

The combined mass distribution of BBH components lies in the same region as LVK detections in the $3 - 60 M_\odot$ mass range, with the contour plot enclosing the 100% of mock binaries fully embracing the observed population of BBH mergers.

Despite an apparent overlap between the distribution of different channels, it is possible to recognize in the parameter space some regions where one channel clearly dominates.

For instance, isolated BBHs have higher mass-ratio and lower masses, on average, compared to dynamical BBHs. Given this, in the reference model we found a sweet spot in the component mass range $M_1 > 40 M_\odot$ and $M_2 < 30 M_\odot$ where $\sim 98.3\%$ of mergers have a dynamical origin.

Therefore, upon our main assumptions, mergers with masses in the aforementioned ranges could be characterized by a high probability to have formed in a star cluster.

A few sources appear to be outliers in our distribution. The heaviest source detected so far, GW190521, sits in the region of the $M_1 - M_2$ plane containing only 1% of our BBHs, populated by dynamical mergers that underwent multiple merger events. This suggests for GW190521 a dynamical origin triggered by a series of hierarchical mergers. Another interesting source is GW190517, a BBH merger with $M_1 = 36.4^{+14.8}_{-7.8} M_\odot$ and $\chi_{\text{eff}} = 0.53^{\pm 0.19}$. The large value of $\chi_{\text{eff}}$ brings this source in the region dominated by isolated binaries in the high-spin model (ID0H), despite the observational uncertainties, whilst it lies in the region containing $\leq 1\%$ BBHs in the low-spin model (ID0L).

The choice of $n_\theta = 8$ in the reference model implies that $\sim 55\%$ of the isolated mergers have the spin-orbital angular momentum angles differing by less than 20%. As shown in the right panel of Figure 2, in the high-spin reference model (ID0H), the $n_\theta$ value adopted coupled with the overall high mass-ratio of isolated binaries, causes a clear overdensity in the $q - \chi_{\text{eff}}$ plane around $q \simeq 0.9$ and $0.3 < \chi_{\text{eff}} < 0.5$. Compared to the high-spin model, low spins lead to i) a richer population of mergers with $M_1 > 80 - 100 M_\odot$, ii) a dearth of mergers with $|\chi_{\text{eff}}| > 0.3$.

In order to better highlight the properties of the two formation channels explored here, Figure 3 shows the $M_1 - M_2$ and $q - \chi_{\text{eff}}$ planes for models in which the BBH population is either only isolated (panels in the upper row) or dynamical; in the latter case the BBH masses are extracted either from the SSBH (panels in the central row) or the MSBH (panels in the lower row) mass spectra. For clarity’s sake, here we refer to models with high-spins (all denoted with letter H).

In the case of isolated BBHs, which are shown in the top row panels of Figure 3, the spin distribution peaking around $\chi_{\text{eff}} = 0.5$ owes to a combination of factors: first, the choice $n_\theta = 8$ implies $\sim 55\%$ BBHs having $\theta_1, 2$ that differ by less than 20%; second, isolated mergers have similar-mass BBHs on average; third, the choice of a Gaussian distribution peaked over $\chi_{1,2} = 0.5$ for BH natal spins.

For nearly equal mass BBHs and spins $\chi_{1,2} \sim 0.5$, the condition $\chi_{\text{eff}} > 0.25$ requires $\cos \theta_1 > 0.5$. This condition is satisfied in the $P_{\chi_{\text{eff}} > 0.25} = 5, 33, 58, 85\%$ for $n_\theta = 0, 2, 4, 8$. Decreasing the value of $n_\theta$ would bring the peak of the $\chi_{\text{eff}}$ toward smaller values, but the clear tendency of isolated BBHs to feature mass ratio values $q > 0.9$ would still cause a clear difference between observations and models, despite the large uncertainties associated with the observed mass ratios.

Focusing on BBHs with a mass ratio $q > 0.9$, we find that around 61% of mergers in the reference model are isolated BBHs. Around 70% of these isolated mergers have total masses $M = 50 - 90 M_\odot$, whilst 90% of them have masses in the range $M = 25 - 100 M_\odot$.

Figure 3 compares the total mass–effective spin parameter distribution for isolated and dynamical mergers. Regarding dynamical BBHs, we find that a simple single mass spectrum (SSBH) seems to match the observed data in terms of component masses, mass ratio, and $\chi_{\text{eff}}$. In the case of BBHs with component masses extracted from a mixed mass spectrum (MSBH), instead, we see that the $M_1 - M_2$ distribution deviates significantly from the SSBH model, favouring the formation of small mass ratios ($q \lesssim 0.1 - 0.2$) and filling efficiently the region $M_1 < 40 M_\odot$ and $M_2 < 20 M_\odot$, which is poorly covered by the SSBH. The peculiar mass distribution obtained for dynamical binaries likely owes to a combination of factors, among which the request that BHs have natal kicks smaller than the cluster escape velocity and the fact that, on average, heavier BHs are characterised by smaller kicks.

As discussed in the next section, adopting a complex mass spectrum for BHs in dynamical mergers might be the key to understand the likely complex mass distribution of observed BBH mergers.

3.2 The primary mass distribution

One of the main insights that can be inferred from the LVK database is the distribution of primary masses ($M_1$) in merging BBHs. As inferred from GWTC-2 data, the primary mass distribution is expected to be well described by a broken power-law characterised by a peak at masses $M_1 \sim 40 M_\odot$.
that truncates around $M_1 \gtrsim 100M_\odot$ (Abbott et al. 2021b). In our analysis, we reconstruct the overall population of merging BBHs first and then we derive the distribution of mergers sampled according to the observation selection criteria described in Section 2. In the following, we will refer to the overall population of BH primaries as “global primaries” and to BHs sampled through the selection criteria as “mock primaries”. Since the choice of BH natal spins does not critically impact the $M_1$ distribution, in the following we show results for high-spin models only.

The upper panels of Figure 4 show the mass distribution of global primaries. The reference model matches the power law + peak model inferred by LVK at masses $< 100 M_\odot$. Our model is characterised by a long tail extending beyond $300 M_\odot$, mostly dominated by hierarchical merger products developed in dense clusters. In the reference model with high spins (IDOH), mergers with $M_1 > 50 M_\odot$ constitute the $f_{>50} = 4\%$ of the overall BBH population, with $f_{\text{hier}} \sim 18\%$ of them being hierarchical mergers. Similarly, the model with low spins (IDOL) is characterised by $f_{>50} = 4.4\%$ and $f_{\text{hier}} \sim 33\%$.

The lower panels of Figure 4, instead, compare our mock primaries with the median primary masses of GWTC-2 mergers (Abbott et al. 2021b). For the reference model, we find that the observation biases lead to a primary mass distribution truncated at $M_1 < 150 - 170 M_\odot$. This happens because the highest primary masses are generally associated with lower mass ratios, leading to a lower detection probability given the $VT - q$ relation. Therefore, our analysis suggests that there is a population of unseen BHs with primary masses as high as $M_1 = 150 - 200 M_\odot$ (around 0.47% of all BHs in the reference model) that escape LVK detection due to the $VT - M_1$ and $VT - q$ selection effects. Among mock sources, we find around $0.2\%$ mergers with a primary mass $> 100 M_\odot$, and (2 - 3)% BBHs with a total mass $100 < M_{\text{bin}} / M_\odot < 170$.

Figures 4 and 5 show the $M_1$ distribution for global and mock BBHs for other models. Adopting a Maxwellian distribution peaked over $\chi_{1,2} = 0.2$ rather than a Gaussian peaked over $\chi_{1,2} = 0.5$ implies that merger remnant can get, statistically, lower kicks. This in turn can imply a larger fraction of hierarchical mergers. As a result, the $M_1$ distribution for the Maxwellian distribution case (ID 5) exhibits a slightly longer tail at $M_1 > 100 M_\odot$ that declines less sharply than the reference model ID0. This leads the percentage of primaries heavier than $100 M_\odot$ to $\sim 0.6\%$, slightly larger than the reference model.

In the case of isolated mergers (ID1), the global distri-
bution of the primary mass is sharply truncated at $M_1 \lesssim 50M_\odot$. This is a clear consequence of binary evolution models adopted in Mjobse. Nonetheless, our analysis suggests that sources with a primary mass $M_1 > 50M_\odot$ are easy to explain with a dynamical origin.4

In the "mock" sample, we find that around 2.4% of BBHs are hierarchical mergers. Comparing them to the overall distribution of mock mergers, we find that hierarchical mergers dominate completely the range $M_1 > 60M_\odot$, owing to the SSBH and MSBH mass spectra adopted.

4 We note that $\sim 9$ sources in GWTC-2.1 have a median primary mass above $M_1 > 50M_\odot$, and 5 exceeds the this threshold at 90% credibility level.

3.3 To spin or not to spin?

As the number of detected BBHs increases, the constraints on the properties of BBH mergers become more robust. The current sample of detected BBH mergers suggests that merging BBHs are characterised by relatively low spins, with a possible peak of the distribution around $\chi_1 \sim 0.2 - 0.3$ (Abbott et al. 2020a, 2021b), and effective spin parameters narrowly distributed around zero (Abbott et al. 2020a), with a tail extending to positive values.

To quantify the impact of BH spins on our mock population, we create a series of variations of the reference model assuming that BBH mergers are characterised by either a Gaussian distribution centered on $\chi_1 = 0.5$, or $0.2$ (ID0H/L), a Maxwellian with dispersion 0.2 (ID5), or a fixed value of $\chi_{1,2} = 0.01$ (ID10). Additionally we vary the $n_\theta$ parameter, which regulates the amount of BBHs with aligned spins, set-

Figure 2. Surface maps showing the combined distribution of component masses (left-hand panel) and of mass ratios and effective spin parameter (right-hand panel). In top (bottom) row panels, we draw BH spins from a Gaussian distribution centered on $\chi_{1,2} = 0.5(0.2)$. The surface maps are compared to GWTC-2.1 data (Abbott et al. 2021b,a). Contour lines encompass $70 - 90 - 99 - 100\%$ of the simulated BBH population. Marginal histograms show the contribution of isolated (straight line steps) and dynamical (dashed steps) BBHs. Both panels show to the reference model. The BBH sample is weighted through the $VT - M_1$ and $VT - q$ relations to account for the main observational biases.
Figure 3. Same as Figure 2, but here we show a model that includes only isolated BBHs (top panels), or only dynamical BBHs with masses taken either from the SSBH (central panels) or the MSBH mass spectrum (bottom panels). All models are characterised by natal spins following a Gaussian distribution peaked over $\chi_{1,2} = 0.5$. 

$\chi_{eff}$
Figure 4. Upper panels: primary mass ($M_1$) distribution of the overall BBH merger population in the reference model (global primaries, blue filled step) compared to the power law + peak model from Abbott et al. (2021b) (dashed line). Lower panels: same as above, but here we consider a BBH sub-population sampled through the $VT - M_1$ and $VT - q$ relation (mock primaries, red filled step) as compared to the median primary masses from GWTC-2.1 (open black steps) and GWTC-2 data (dotted black steps). Here, for each GW event we use only the median value without considering the uncertainties. The distribution for hierarchical mergers in the sample is highlighted (dashed grey open steps). The two panels show the reference model assuming for BH natal spin a Gaussian peaked on $\chi = 0.5$ (left) or a Maxwellian with dispersion 0.2 (right).

The high spin model matches the \(|\chi_{\text{eff}}| > 0.3\) range, which instead is poorly populated by low-spin models. This has several implications for BH natal spins in single and binary systems.

High-spin (e.g. ID0H) and Maxwellian spin models (e.g. ID5) are characterised by a wide distribution that extends beyond \(|\chi_{\text{eff}}| > 0.3 - 0.5\), whilst low- and non-spinning scenarios (e.g. ID0L or ID10) exhibit a narrower distribution peaking around 0.

The shallower distribution of mergers with $\chi_{\text{eff}} < 0$ and the detection of sources having $\chi_{\text{eff}} > 0.3$ could hint to differences in the distribution of natal spins for BHs in isolated and dynamical mergers, although the current observational uncertainties and the low statistics significantly affect the interpretation of observed sources.

As recently suggested by Fuller & Ma (2019), efficient angular momentum transport driven by magnetic fields can lead to stellar BHs with natal spin as small as $\chi_{1,2} \sim 0.01$ for both single and binary stars, although in the latter case binary processes can spin-up the BH to large spin values. To test this idea, we build two further models, ID13 and 14, in which we assign to dynamical mergers a fixed spin $\chi_{1,2} = 0.01$ following Fuller & Ma (2019), whilst we assign to isolated mergers a natal spin either drawn from a Maxwellian peaked over 0.2 (ID13) or from a Gaussian peaked over 0.5 (ID14), and we adopt $n_\theta = 8$ in both cases\(^5\).

As shown in Figure 6, adopting different distributions for BHs in isolated and dynamical mergers clearly affects the overall $\chi_{\text{eff}}$ distribution, possibly explaining both a dearth of mergers with $\chi_{\text{eff}} < -0.3$ and a population of mergers with $\chi_{\text{eff}} > 0.3$. These models suggest that BH merging in isolated or dynamical binaries might be characterised by different natal spin distributions, likely owing to the underlying different physical processes that contribute to the formation of mergers in each channel. In these regards, population synthesis tools like B-POP can readily serve as rapid and flexible parameter-space explorers, and can be exploited to compare models against the crescent number of observations. For instance, the detection of a few sources with negative $\chi_{\text{eff}}$ could significantly help constraining the natal spin distribution of BHs in isolated and dynamical mergers.

4 DISCUSSION

4.1 Hierarchical mergers: a route to form massive BH seeds in extremely dense environments

When mergers take place in star clusters, sufficiently large escape velocities can favour the retention of the merger products and the development of multiple generation (hierarchical) mergers. As expected, we find that the vast majority of multiple generation mergers occur in dense GCs and NCs.

Figure 7 shows the mass distribution of single and recycled mergers in YCs, GCs, and NCs for the low-spin reference model (ID0L). The mass spectrum of first-generation mergers is characterised by a well defined distribution that poorly depends on the cluster type, showing two clear peaks at $15M_\odot$ and $\sim 60M_\odot$. The mass distribution of hierarchical mergers, instead, depends crucially on the environment, with clusters characterised by higher densities and masses favoring the formation of heavier BH remnants, on average. YSCs host a handful of repeated mergers with total mass $\sim 100M_\odot$. GCs exhibit a peak around $70M_\odot$ with a large

\(^5\) This choice implies a $\sim 55\%$ probability to draw the angles between the spin directions and orbital angular momentum differing by less than 20%.
the mixed one (MSBH, lower panel).

Figure 5. Same as in Figure 4, but here we show only isolated (upper panel) and dynamical mergers assuming for BH natal mass either the simple single mass spectrum (SSBH, central panel) or the mixed one (MSBH, lower panel).

dispersion in the range $40 - 200\,M_\odot$ and a sharp truncation at masses $> 200\,M_\odot$. For NCs, instead, the mass distribution peaks at $100\,M_\odot$ and slowly decreases down to $500\,M_\odot$.

Moreover, the mass function of hierarchical mergers in NCs displays a clear rise beyond $M_{\text{tot}} > 10^4\,M_\odot$, owing to the population of heavy BHs forming in high-density NCs. Clusters with mass $0.5 < M_c/10^7\,M_\odot < 3.5$ and half-mass radius $0.2 < r_h/<pc < 1$ have sufficiently high density ($>10^7\,M_\odot\,pc^{-3}$) and velocity dispersion ($400 < v_{\text{esc}}/\text{km s}^{-1} < 2000$) to harbour a merger avalanche that builds up BHs $>> (0.5 - 1) \times 10^4\,M_\odot$ over timescales $< 5 - 10$ Gyr. In our reference model, we find the formation of such massive BHs in $\sim 12\%$ NCs.

Figure 8 compares the combined distribution of primary mass and spin for single and repeated mergers in the case of spins drawn from a Gaussian centered on $\chi_{\text{eff}} = 0.5$ or $0.2$ (ID0H/L) or a Maxwellian (ID5) distribution. The mass distribution for repeated mergers is nearly flat in the range $M_1 < 75\,M_\odot$ in the case of high spins, while it shows a more pronounced peak at around $M_1 \simeq 60\,M_\odot$ in low-spin models, with the ID0L model being characterised by a narrower $\chi_{\text{eff}}$ distribution. This happens because lower spins imply smaller GW recoil and, thus, a larger probability for hierarchical mergers.

In the high-spin model ID0H, $\sim 23\%$ of repeated mergers have a primary $M_1 > 50\,M_\odot$ and $\chi_1 > 0.6$, while only $2\%$ of first-generation mergers have such high mass and spins. Changing the value of $\alpha_m$, thus the amount of nearly aligned isolated mergers, does not affect appreciably the distribution. The percentage of high mass and spin hierarchical mergers remain almost the same adopting a low-spin model, but the amount of single generation mergers with such properties drops to $0.4\%$. Therefore, in the framework of low natal spins for merging BHs, the detection of mergers with $\chi_{\text{eff}} > 0.6$ and masses $M_1 > 40\,M_\odot$ could represent a strong indication of a dynamical origin (but see also Gerosa et al. 2021). In the semi-plane $45 < M_1/M_\odot < 85$ and $\chi_1 > 0.3$, hierarchical mergers are the $14\%$, $61\%$, and $22\%$ of the population in the high-spin reference model (ID0H), in the ID0L model and in the Maxwellian spins model (ID5), respectively.

### 4.2 The role of massive IMBH seeds

The initial evolutionary phases of dense clusters can favour the growth of an IMBH seed with a mass in the range $100 - 500\,M_\odot$ (Portegies Zwart & McMillan 2002; Giersz et al. 2015; Mapelli 2016; Di Carlo et al. 2019, 2021; Rizzuto et al. 2021b; González et al. 2021; Arca Sedda et al. 2021a). If retained in the parent cluster, these seeds can capture a BH companion (Di Carlo et al. 2021; Rizzuto et al. 2021b) and undergo coalescence (e.g. Arca Sedda et al. 2021b; Rizzuto et al. 2021b; Arca Sedda et al. 2021a).

To explore the impact of such IMBH seeds onto the population of BBH mergers, we explore two further models, assuming that a certain fraction of dynamical BBHs have a primary with mass falling in the range $100 - 500\,M_\odot$, i.e. in the IMBH mass range. For these IMBH seeds, we adopt a power-law mass spectrum with slope $-2$. This choice implicitly assumes that the IMBH mass scales linearly with the cluster mass, as happens for supermassive BHs and galactic nuclei, and that the overall cluster mass function follows a power-law with slope $-2$ (Lada & Lada 2003). Nonetheless, we note that the IMBH mass spectrum is highly uncertain,
We do not show the population of BBH remnants with mass (ID0L). The histograms refer to the overall population of mergers. As derived from the Default (GAUSSIAN) LVK models (Abbott et al. 2021b). The shadowed gray areas are the corresponding 90% credible intervals.

Figure 7. Mass distribution of first generation (filled steps) and multiple generation (open steps) dynamical mergers for different cluster types and assuming the reference model with low spins (IDOL). The histograms refer to the overall population of mergers. We do not show the population of BBH remnants with mass \( > 10^8 \text{M}_\odot \).

Figure 6. Red solid lines with markers: distribution of \( \chi_{\text{eff}} \) in our reference model assuming: \( n_0 = 8 \) and a Gaussian BH natal spin distribution peaked over \( \chi_{1,2} = 0.5 \), 0.2 (models ID0H/L), a Maxwellian (model ID5), a Gaussian centered over \( \chi_{1,2} = 0.2 \) and \( n_0 = 4 \) (model ID8L), a mixed spin distribution in which single BHs have negligible spins and binary BH spins are taken from a Gaussian centered over \( \chi_{1,2} = 0.5 \) (model ID13) or from a Maxwellian with dispersion 0.2 (ID14). Dashed black (Dotted gray) lines: posterior distribution of \( \chi_{\text{eff}} \) as derived from the Default (GAUSSIAN) LVK models (Abbott et al. 2021b). The shadowed gray areas are the corresponding 90% credible intervals.

Figure 9 shows the primary mass distribution for global and mock BBHs in models ID11 and ID12. The impact of IMBH seeds is apparent from this figure, namely the high-end of the \( M_1 \) distribution is densely populated by these objects. When the observation selection criteria are applied, the mock \( M_1 \) distribution, which is shown in the lower panel of Figure 9, is still characterised by a long tail extending beyond \( 100 - 300 \text{M}_\odot \), which contains \( \gtrsim 10\% \) of the mock BBH population. Comparing the result of this model with the reference one, we see that increasing the amount of detected GW sources is crucial to constrain the formation of IMBH seeds in dense star clusters.

Comparing the primary mass distribution for this high-mass seed models with the reference model, it is clear how owing to the dearth of thorough studies about the formation of these objects in clusters in a wide mass range.

In model ID11, we assume that 40% of dynamical BBH mergers have masses taken from the “standard” BH mass spectrum (SSBH), 40% from the mixed BH mass spectrum (MSBH), and 20% are comprised of IMBH seeds. In model ID12, we assume that 85% of BHs have masses taken from SSBH, 5% from MSBH, and the remaining 10% is composed of IMBH seeds. We do not find appreciable differences between models with high or low BH natal spins.
important it will be to increase the amount of detected BBH mergers with future observations. In fact, increasing the population of detected mergers in the $M_1 > 100 M_\odot$ can be key to quantify the role of IMBH seeds in “polluting” the overall population of BBH mergers.

Figure 10 compares the mass spectrum of first-generation and repeated mergers in the case of model ID11H(12H), i.e. $\sim 20(10)\%$ of mergers involving IMBH seeds and 40(5)$\%$ of BH masses taken from the MSBH spectrum. A substantial population of heavy seeds can significantly impact the mass of hierarchical mergers in all cluster types. The percentage of hierarchical mergers in the overall BBH merger population is $18.7 - 23.7\%$ for models 11H and 11L, and $5.8 - 9.7\%$ in models ID12H and 12L. The larger amount of hierarchical mergers in models denoted with L owes to the fact that lower spins lead generally to lower GW recoils, whilst the larger amount of mergers in models denoted with number 11 owes to the larger amount of IMBH seeds allowed in the overall population.

In YCs, the presence of IMBH seeds triggers the formation of a population of hierarchical mergers with masses in the range $100 - 900 M_\odot$. Most of them are mergers with $M_1 \gg M_2$, whose remnants might receive kicks sufficiently small to be retained inside the parent cluster. The mass distributions of first-generation and repeated mergers in GCs are similar, although the latter is shifted by 0.7 dex toward larger values. NCs, instead, are characterised by a population of mergers with masses $> 500 M_\odot$, with a small sub-population of mergers ($\sim 0.052\%$) reaching masses $M_{\text{tot}} > 10^5 M_\odot$ over a $5 - 10$ Gyr timescale.

Considering the overall population of mock BBHs, we find around $2.7 - 7.5\%$ of mergers with $M_1 > 100 M_\odot$ and $6.6 - 11.0\%$ with $M_1 + M_2 > 100 M_\odot$ in the high-mass seed models (ID11H/L and ID12H/L). For comparison, in the low- and high-spin reference models (ID0H/L) we found $3.7 - 5\%$.

Figure 8. Primary spin and mass surface map distribution for first generation (blue contours and filled steps) and multiple generation BBHs (orange contours and open steps), assuming a BBH population equally contributed by isolated and dynamical BBHs and adopting a Gaussian distribution peaked on either $\chi_1 = 0.5$ (left panel, ID0H) or $\chi_1 = 0.2$ (central panel, ID0L), and a Maxwellian with dispersion $\sigma_1 = 0.2$ (right panel, ID5) for BH natal spins.

Figure 9. Same as in Figure 4 but for high-mass seed models with high spins (ID 11H and 12H). In model ID 11H, 40(40)$\%$ of dynamical mergers have masses taken from SSBH (MSBH) and the remaining masses are taken from the IMBH seed spectrum adopted. In model ID 12H, instead, we assume that 85$\%$ of mergers have masses taken from SSBH, 5$\%$ from MSBH, and 10$\%$ from the IMBH seed mass distribution.
of mergers with $M_1 + M_2 > 100\,M_\odot$. Note that, in general, models with high-spins are characterised by a lower percentage of high-mass mergers, owing to the lower probability for hierarchical mergers to occur. Interestingly, GWTC-2 contains 4 mergers out of 47 detections having a median mass above this threshold and only 1 exceeding $M_1 + M_2 > 100\,M_\odot$ at 90% credible level, corresponding to the 2.1–8.5% of the sample. Increasing the amount of GW sources in this mass range will thus help unveiling the impact of IMBH seeds onto the population of merging BBHs, at least at relatively low redshift.

5 SUMMARY

We presented B-POP, a semi-analytic tool that enables population synthesis for BBH mergers taking place either in isolated binaries or in young, globular, and nuclear clusters. In its current version, B-POP exploits a library of single and binary BHs modelled with MOBSE, though it can be easily fed with other stellar evolution libraries. The code implements a semi-analytic technique to model the dynamical formation of BBHs in star clusters, and a flexible interface to set a wide variety of parameters, like BH natal spins for isolated and dynamical mergers, the amount of IMBH seeds possibly forming in clusters, the relative amount of mergers occurring in different environments, and the star formation history of galaxies and clusters. Additionally, B-POP includes observation selection criteria that filter the modelled population of BBHs and returns a sub-sample of mergers as might be seen with second-generation ground-based GW detectors.

In the following, we summarize our main findings:

- assuming that isolated and dynamical binaries are equally distributed, we find that observation selection criteria lead to a "mock" population of mergers composed of $\sim 34\%$ ($66\%$) of isolated (dynamical) BBHs;
- in our reference model, the primary mass distribution of mock mergers matches GW observations;
- the reference model produces a sub-population of mergers with masses heavier than $100 - 200\,M_\odot$, whose detection might be hindered by observation selection criteria;
- assuming that BHs in isolated binaries have relatively high spins and that single BHs have low or even negligible spins leads to an effective spin distribution of mock mergers characterised by a dearth of mergers with $\chi_{\text{eff}} < -0.3$ and a sub-population of mergers with $\chi_{\text{eff}} > 0.3$;
- in our reference model, around $4.6 - 7.9\%$ of mock mergers are the byproduct of multiple (hierarchical) mergers, mostly developing in GCs and NCs, with total masses extending beyond $10^5\,M_\odot$. In a small fraction of cases ($\sim 0.03 - 0.06\%$), hierarchical merger remnants can reach a mass $> 10^4\,M_\odot$;
- depending on BH natal spins, hierarchical mergers are $20 - 60\%$ of all the detectable BBHs with $\chi_1 > 0.3$ and primary mass $45 < M_1/M_\odot < 85$;
- we explore the impact of IMBH seeds formed out ofstellar collisions on the overall BBH population. If we assume that $10 - 20\%$ of all BBH mergers involve an IMBH seed formed via stellar collisions, around $2.7 - 7.5\%$ of mock mergers have $M_1 > 100\,M_\odot$.

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DATA AVAILABILITY
The data and the code associated with the present study are available upon reasonable request to the corresponding author.

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Answer: The data and the code associated with the present study are available upon reasonable request to the corresponding author. The references are mainly astronomical, covering a range of topics including gravitational waves, black hole binaries, and other astrophysical phenomena. The data and code are available upon request. Appendix A discusses the impact of a mixed single BH mass spectrum on the population of BBH mergers. As discussed in the previous sections, we can draw BH masses for dynamical mergers from three mass spectra: SSBH, MSBH, and HSBH. The first refers to the single BH mass spectrum output by MOBSE, the second represents the population of BHs formed in binary systems modelled with MOBSE that did not end their life in a compact binary merger, whilst the third represent the population of IMBH seeds possibly formed via stellar accretion processes and stellar collisions in dense clusters. In this section we discuss the different outcomes of the SSBH and MSBH mass spectra. Figure A1 shows the surface maps of component masses, remnant mass, and effective spin parameter for models ID2.
and ID4, where we consider dynamical mergers only with masses taken from either SSBH or MSBH, respectively.

The “standard” single BH mass spectrum, SSBH, i.e. model ID2 with low (L) and high (H) spins, is characterised by a 2D distribution of component masses that encompasses the majority of detected BBH mergers, especially in the mass range $15 < M_1/M_\odot < 65$ and $M_2 < 45 M_\odot$. All detected mergers but one fall inside the region of the $M_f - \chi_{\text{eff}}$ plane containing more the 99% of mergers in model ID2L. Nearly half of detected mergers sit in the clear overdensity limited by $25 < M_{\text{rem}}/M_\odot < 100$ and $|\chi_{\text{eff}}| < 0.25$. Conversely, BHs coming from the MSBH mass spectrum have more peculiar component mass distributions, which cover mostly the range $M_1 < 40 M_\odot$ and $M_2 < 20 M_\odot$. The $M_f - \chi_{\text{eff}}$ distribution shows a clear overdensity that overlap quite well with 6 observed mergers which have a remnant mass $M_f \simeq 25 M_\odot$ and $|\chi_{\text{eff}}| < 0.25$.

Interestingly, the mass ratio distribution of SSBH and MSBH are quite different, as shown in Figure 3, with the former being characterised by $q > 0.3$ and the latter showing a clear peak at smaller $q$ values, in the region $|\chi_{\text{eff}}| < 0.25$ and $0.1 < q < 0.45$.

Comparing low- and high-spin models in the bottom panels of Figure 3, we see that whilst L models provide a better representation of the low-end of the $\chi_{\text{eff}}$ distribution, H models are more suited to represent the high-end.

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Figure A1. Component mass distribution (top panels) and remnant mass - effective spin parameter distribution (central and bottom panels) for models with only dynamical BBHs where the BH masses are extracted from either a single mass spectrum (SSBH, left panels) or from a mixed mass spectrum (MSBH, right panels). Top and central panels represent models in which BH spins are drawn from a Gaussian centered on $\chi_{1,2} = 0.2$, whilst bottom panels have BH spins drawn from a Gaussian centered on $\chi_{1,2} = 0.5$. 