

# Using Cosmological Simulations to Understand Massive Black Hole and Galaxy Formation

**Joe McCaffrey B.Sc.**

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Department head  
Dr Neil Trappe

Doctoral Supervisor  
Dr John Regan





*For my parents and Orla*

# Declaration

This thesis has not been submitted in whole, or in part, to this or any other university for any other degree and is, except where otherwise stated, the original work of the author. Those parts of the thesis which have been published or submitted for publication are as follows:

- The work presented in Chapter 2 has been completed in collaboration with J.A. Regan, B. Smith, J. Wise, B. O’Shea, M. Norman and has been published as: McCaffrey, J. et al. A Heavy Seed Black Hole Mass Function at High Redshift – Prospects for LISA. *The Open Journal of Astrophysics* 8, (2025).  
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- The work presented in chapter 3 has been completed in collaboration with S. Hardin, J. Wise, J.A. Regan and has been published as: McCaffrey, J., Hardin, S., Wise, J. Regan, J. No Tension: JWST Galaxies at  $z > 10$  Consistent with Cosmological Simulations. *The Open Journal of Astrophysics* 6, 10.21105/astro.2304.13755 (2023).
- The work presented in chapter 4 has been completed in collaboration with S. Hardin, J. Wise, J.A. Regan and has been submitted to the Open Journal of Astrophysics for review. The preprint can be found at

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## Abstract

This thesis aims to address some of the current mysteries in early Universe astrophysics. These include the high- $z$  galaxies that have been discovered by the James Webb Space Telescope (JWST) and the population of early Universe black holes that exhibit higher mass and accretion rates than previously expected. We use the high resolution, high- $z$  **Renaissance** simulations, built using the adaptive mesh-refinement code ENZO, to achieve this. First we apply post-processing methods to the simulations to investigate the formation and evolution of heavy seed black holes in rapidly assembling halos in the early Universe. We find that these black holes struggle to grow in high- $z$  environments, while also investigating the potential for future Gravitational Wave detectors like LISA, to detect mergers of black holes similar to those simulated here. We also use the **Renaissance** simulations to investigate the validity of standard cosmology in light of the discovery of very high- $z$  galaxies with JWST. Apparent tensions between observations and the limits to how stellar matter which forms from baryonic matter, whose abundance is dictated by  $\Lambda$ CDM, are starting to arise. This provides the perfect opportunity to use high- $z$  simulations, like **Renaissance**, to test these theories directly. We find that **Renaissance** is largely able to explain the existence of these galaxies, while more recently discovered outliers could possibly be explained due to the lack of resolution on small areas of bursty star formation. The work in this thesis emphasises the importance of high- $z$  simulations as we start to uncover the early Universe in incredible detail.



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# Chapter 1

## Introduction

Our Universe is very large, impossibly large. At the same time, it is also incredibly detailed. From details concerning the chemical processes that lead to formation of stars on parsec scales to gravity weaving together the cosmic web on Gigaparsec scales. Astrophysicists have been set the challenge of modelling this large range of phenomena using nothing more in their toolkit other than the language of mathematics. However, trying to model the entire Universe on a blackboard obviously presents a near impossible problem. The mechanisms that, for example, dictate the movement of vast stellar systems, control the rate at which stars and black holes are born and die and the curvature of spacetime itself are far too complex to be single handedly calculated by mere analytical formulae. Therefore we need to apply more hardware in the form of computers to this great task. Computers allow us to perform the millions of the calculations that are required to model the large range of processes that are needed to fully understand the origins of the present-day Universe.

In particular, this thesis focuses on the formation and growth of the most massive black holes that exist in the Universe and also the origins of the galaxies that these

black holes lie at the heart of. In fact it is unwise to approach one of these mysteries without considering the other. They play an important part in each other's lives (see [1] and also the  $M_{\bullet} - \sigma$  plot in Fig.1.1, where  $M_{\bullet}$  is the black hole mass and  $\sigma$  is the stellar velocity dispersion of the host galaxy) that must be examined simultaneously in order to fully grasp the mechanism that govern these behemoths. To start our study of these massive objects, we need to lay out the physical rules that they must follow and establish the conditions and environments which allows galaxies and black holes to form in the first place. The rules will be outlined in the following sections and will give an overview on how overdensities in the Universe lead to the seeds of our galaxies. The amount of dark energy, dark and baryonic matter in the Universe will determine the cosmological parameters, which will be used for cosmological simulations. This baryonic matter (or observable matter) then becomes the basis for forming and fueling our stars that inhabit the newly formed galaxies. We will discuss the first generation of stars, the most massive early stars (Population III or Pop III) that form the ancestors of the more familiar Pop I stars like our very own Sun. We then move on to the topic of the end product of the stars that exceed masses of  $20 M_{\odot}$  – black holes. More specifically, the more massive population of these black holes that form in the early Universe. We know about the existence of black holes from local observations of stellar mass black holes, whether from electromagnetic (EM) signatures via X-ray binaries [2] or gravitational wave (GW) observations from Laser Interferometer Gravitational-Wave Observatory (LIGO) [3] and massive black holes from their Active Galactic Nuclei (AGN) signatures [4, 5] and also possibly their mark on the gravitational wave spectrum [6, 7].

However, the presence of stellar mass black holes alone are not enough to explain the existence of the gigantic supermassive black holes that exist at the heart of the

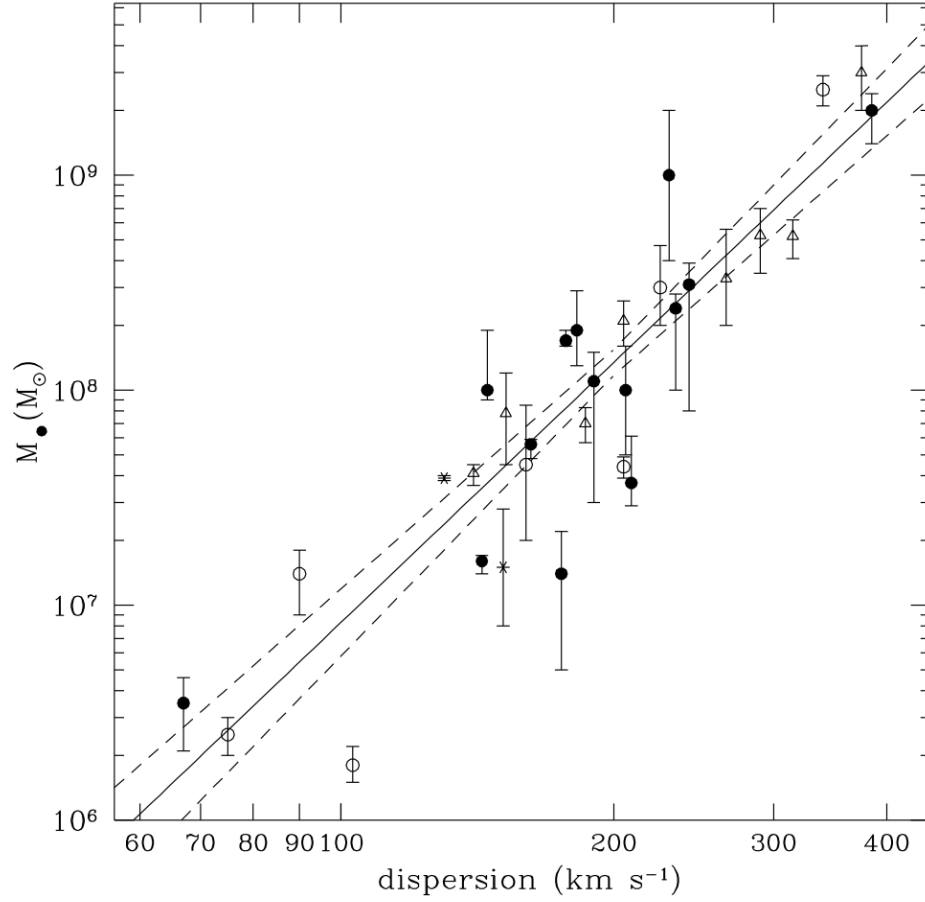


Figure 1.1: Plot showing the mass of black holes in galactic nuclei versus the stellar velocity dispersion of the galaxies they occupy – displaying the intrinsic relationship between black holes and their host galaxies. Figure credit: [8]

majority of galaxies in the Universe [9]. So we will explore possible formation pathways for massive black holes in the early Universe, from light seeds ( $10^2 - 10^3 M_\odot$ ) that form from the remnants of the first generation of stars to heavier seeds ( $> 10^3 M_\odot$ ) that form from more complex pathways that require specific conditions unique to high redshifts. Once these massive black holes form there is still an immense amount of mass for them to gain in order to reach the status of supermassive black holes. Vast amounts of accretion of the surrounding material must be achieved along with mergers between black holes in a cluster or between more massive black holes migrating in from galactic mergers, all within the relatively short age of the Universe of 13.8 billion years.

A question that is commonly asked by the average person is “How do we know that black holes exist?”. Since these objects are so small and do not let any light escape from inside the event horizon, it can be unclear about how they make themselves known to us. We will discuss how signatures can be detected in the form of light emitted from the hot accretion disks around the black holes that constitute some of the brightest objects in the Universe. We will also examine how waves not just in the electromagnetic spectrum provide evidence for the existence of not only black holes, but merging black holes. The discovery of these gravitational waves have opened a new window into black hole physics and we will discuss in the following sections about how future experiments are being devised to measure gravitational waves from even more massive black holes far earlier in the Universe to help build a better picture of how these black holes grow and which seeding models provide an answer to their formation.

In future chapters, we will discuss how we use state-of-the-art cosmological simulations, specifically **Renaissance** [10, 11, 12, 13, 14], to model heavy seed (seeds with a mass  $> 10^4 M_\odot$ ) formation of black holes from rapidly assembling dark matter halos in the early Universe. We will see if these black holes are able to form efficiently and

grow fast enough to reach masses that are comparable to supermassive black holes that we are discovering at early epochs in the Universe. We will also see if these black holes could possibly be part of the population that future GW detectors such as the Laser Interferometer Space Antenna (LISA) will be able to detect. With the hope that if these black holes are too small to be detected in the EM spectrum, then perhaps GW signals can test our theoretical models instead. We also look at the subject of newly discovered massive, high-redshift galaxies by the James Webb Space Telescope (JWST), which seem to be testing the limits constrained by our most accepted model for cosmology, the  $\Lambda$ CDM model, a theory which assumes hierarchical growth of galaxies in an expanding Universe. We again use **Renaissance** as before, which were designed to examine early galaxy formation, to validate the existence of these galaxies and ease the prevailing tension between observations and theoretical expectations in the galaxy formation community.

## 1.1 Fundamental Cosmology & $\Lambda$ CDM

When working with our Universe, it is closely modeled as having a Friedmann-Lemaître-Robertson-Walker (FLRW) metric [15, 16] with a line element given by

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu \tag{1.1}$$

where the coordinate system used is  $x^\mu = (ct, r, \theta, \phi)$  and the metric is given by

$$g_{\mu\nu} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & \frac{R^2(t)}{1-kr^2} & 0 & 0 \\ 0 & 0 & R^2(t)r^2 & 0 \\ 0 & 0 & 0 & R^2(t)r^2 \sin \theta \end{pmatrix}. \quad (1.2)$$

For a flat Universe, which is what our Universe closely resembles, the curvature parameter  $k = 0$ . The scale factor  $R(t)$  represents how big the Universe is compared to today with the present time value being  $R(t = t_0) = 1$ . From this point on, we will differentiate epochs of the Universe with the redshift,  $z$ , parameter. Redshift is a consequence of the Universe's expansion, with light waves being stretched as they travel through the Universe and being observed to be having a longer wavelength compared to the same EM-waves being emitted in the rest frame:

$$z = \frac{\lambda_o - \lambda_e}{\lambda_e}. \quad (1.3)$$

This redshift can be related to the scale factor via the following:

$$1 + z = \frac{R(t_0)}{R(t)}. \quad (1.4)$$

In 1915, Einstein derived the field equations [17] which related the curvature of space-time to the matter-energy content inside it. He found that the equations can be written in the form of

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} + \Lambda g_{\mu\nu} = \frac{8\pi G}{c^4}T_{\mu\nu}, \quad (1.5)$$

with  $R_{\mu\nu}$  and  $R$  being the Ricci Tensor and Ricci scalar, respectively, quantities which relate to the curvature of spacetime. The cosmological parameter  $\Lambda$ , originally used to make the Universe static according to Einstein, has since been used to account for the more recently discovered dark energy content of the Universe [18, 19]. The tensor on the right hand side of the equation  $T_{\mu\nu}$  denotes the matter-energy content of the Universe. If we substitute the metric from 1.2, one can derive the Friedmann equations which describe the evolution of the scale factor of the Universe, with the first equation (derived from the time component of the Einstein equations) being

$$\frac{\ddot{R}}{R} = \frac{\Lambda}{3} - \frac{4\pi G}{3}(\rho + 3p), \quad (1.6)$$

where  $\rho$  and  $p$  denote the density and pressure of the Universe respectively. The second equation (derived from the spatial components of the Einstein equations) is then

$$\left(\frac{\dot{R}}{R}\right)^2 = \frac{8\pi G}{3}\rho + \frac{\Lambda c^2}{3} - \frac{kc^2}{R^2}. \quad (1.7)$$

This equation uses the previously mentioned curvature parameter  $k$  and cosmological parameter  $\Lambda$ . The equation also depends on the density of the Universe  $\rho$ . This density takes into account density from radiation, baryonic matter, dark matter and dark energy. These densities can also be written in the form of a density parameter  $\Omega$ , which is calculated from

$$\Omega = \frac{\rho}{\rho_c}, \quad (1.8)$$

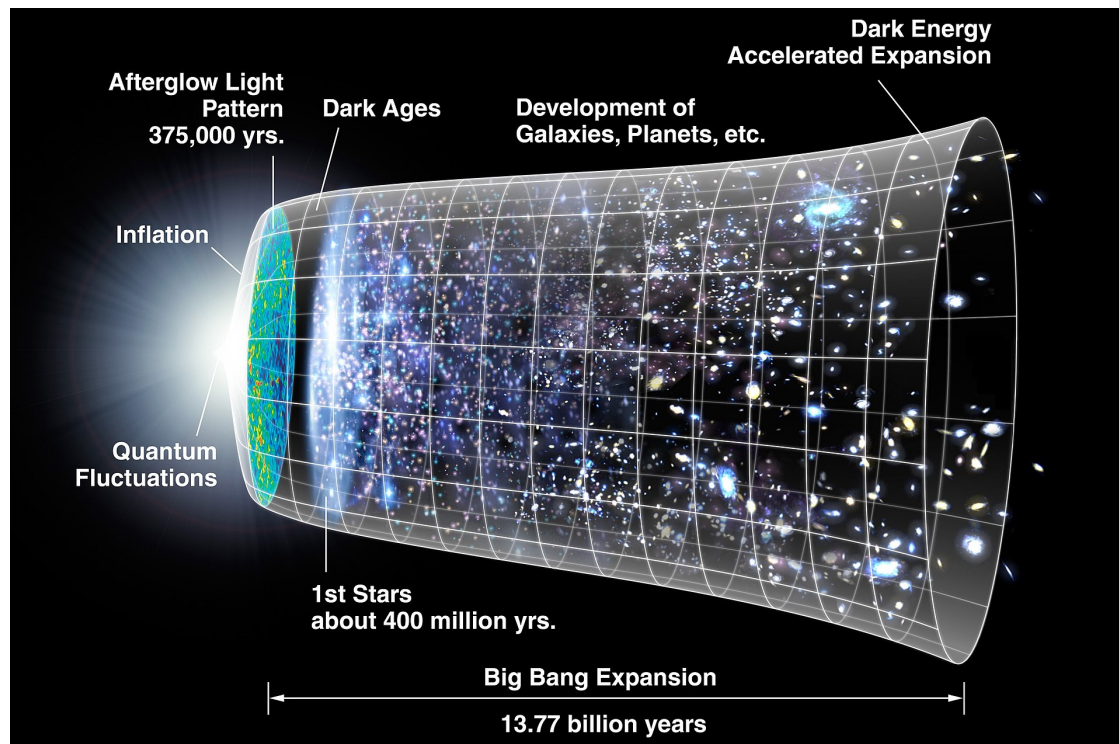


Figure 1.2: Image showing the evolution of the Universe in a  $\Lambda$ CDM framework from the Big Bang all the way up to the present time, with different epochs labeled throughout. In particular, this thesis is largely concerned with the period of about 400 million years after the Big Bang, when the first stars and galaxies formed, which is what JWST is starting to uncover. Image Credit: NASA/ LAMBDA Archive / WMAP Science Team

where  $\rho_c$  is the critical density of the Universe and is obtained from

$$\rho_c = \frac{3H^2}{8\pi G}, \quad (1.9)$$

where  $H(t) = \dot{R}(t)/R(t)$  is the Hubble parameter. Writing the density like this allows us to split it into density parameters representing the proportional content of the Universe [20],

$$\Omega = \Omega_M + \Omega_r + \Omega_\Lambda + \Omega_k, \quad (1.10)$$

where  $\Omega_M$ ,  $\Omega_r$ ,  $\Omega_\Lambda$  and  $\Omega_k$  represent the matter, radiation, dark energy and spatial curvature densities respectively. These quantities are constantly being further constrained with cosmological surveys like the Wilkinson Microwave Anisotropy Probe (WMAP) [21] or the Planck observatory [22]. With accurate measurements for these quantities we are able to make models and perform simulations of universes that closely resemble our own.

The model of the Universe that we will be working with is the  $\Lambda$ -Cold Dark Matter ( $\Lambda$ CDM) model [23, 19, 24]. It is our most accepted model for the Universe as it accounts for the large scale structure of galaxies and also accounts for the existence of an expanding Universe, with the rate of this expansion being measured to be increasing with time. A simple model of the  $\Lambda$ CDM Universe is shown in Fig.1.2, where the Universe starts off as a singularity point, rapidly expands from that point in what is known as the Big Bang. From this point the Universe expands more due to inflation. Baryonic matter arises from pair production and the Universe starts to cool down. Cold dark matter allows for the hierarchical formation of structure in the Universe, with galaxies starting small and building up mass by merging with other smaller galaxies

over time. In the next section we will discuss how galaxies form in this framework and in future chapters we will also discuss how recent measurements by current galaxy surveys have put the validity of the  $\Lambda$ CDM model into question.

## 1.2 Galaxies and the Formation of the First Stars

After the Universe started to cool down a few hundred thousand years after the Big Bang, and protons were allowed to combine with electrons to produce hydrogen, the path towards galaxy formation commenced. Although the Universe at this time was largely homogenous, fluctuations existed in the matter density field, which we can measure from the temperature field in the Cosmic Microwave Background (CMB) using surveys such as WMAP and Planck. The Cosmic Microwave Background is a constant background radiation which was found to be the remnants of Recombination – when the Universe had cooled sufficiently enough (around 400,000 years after the Big Bang) such that free protons and electrons combined to form hydrogen, thus making the Universe transparent [25]. The temperature fluctuations in the CMB directly correlates to the density of the matter fields, due to thermodynamical relations. The first stars are believed to have formed in minihalos ( $M \sim 10^6 M_\odot$ ) at redshifts  $z \sim 20 - 30$  [26]. In a  $\Lambda$ CDM Universe, gas inside these dark matter minihalos, grow and contract adiabatically under gravity, since no energy is transferred with the surrounding system, the gas will heat up. This happens until the gas becomes sufficiently dense enough to form  $H_2$  molecules, after which, the gas begins to cool from  $H_2$  line cooling (as seen in Fig.1.3). The gas cloud continues to grow and becomes denser until it reaches the

Jeans mass which is given by [27, 28]

$$M_J \approx 500 \left( \frac{T}{200 \text{ K}} \right)^{3/2} \left( \frac{n}{10^4 \text{ cm}^{-3}} \right)^{-1/2} M_\odot. \quad (1.11)$$

After which, collapse occurs and will continue to occur until a protostar is able to form, and will then accrete the surrounding matter to become a massive star. These first stars are known as PopulationIII (PopIII) stars. We will differentiate the different epochs of star formation in the Universe using the following notation – PopulationIII stars denote the first generation of metal free stars, PopulationII (PopII) stars refer to the following generation of metal poor stars and PopulationI (PopI) stars denote the modern era, metal rich stars like our Sun. An initial mass function for the first stars (PopIII) is still unconstrained, but the distribution is thought to allow masses reaching around  $\sim 10^2 M_\odot$  [29, 26, 30, 31, 32]. It is thought that they form in small numbers in gas clouds [33]. They radiate incredible amounts of  $H_2$  destroying radiation (Lyman Werner radiation of energy  $E = 11.2 - 13.6 \text{ eV}$  as discussed in §1.3.2) which prevents the host halo and possible surrounding halos from forming additional stars until the PopIII stars end their lives [34, 35, 36, 37, 38]. PopIII stars will end their lives via supernova and inject a small amount of metallicity into the environment, of the order of  $10^{-6} - 10^{-3} Z_\odot$  [39, 40, 41]. It may take a few hundred million years for the next generation of stars (PopII) to form due to the effects of Supernovae (SNe) Feedback from the PopIII stars [42]. Once PopII star formation commences, they can form in much more numbers compared to PopIII stars and make up what we know as the first galaxies, due to more efficient fragmentation in the presence of metal cooling [41].

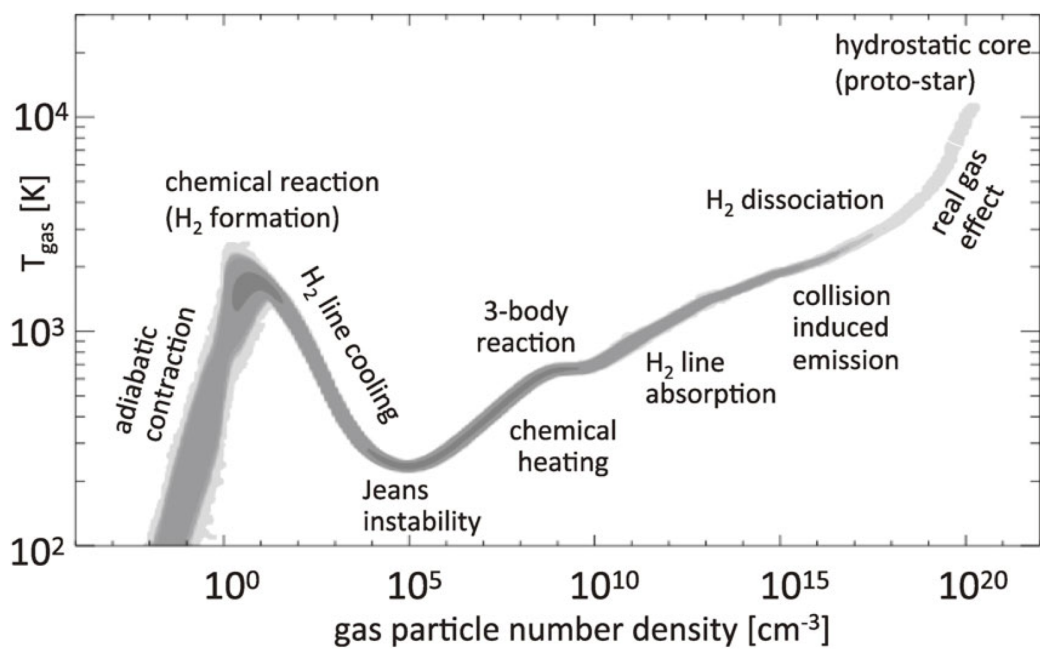


Figure 1.3: Temperature density plot showing how pristine gas in the first dark matter minihalos evolves and eventually collapses to form the first protostellar population. Image credit: [43]

## 1.3 Formation of the first Black Holes

For stellar-mass black holes, their lives begin as the by-product of a core-collapse supernova from a massive (or PopI) star with  $M > 20 M_{\odot}$  [44]. However, these black holes cannot be assumed to be the origin for very massive black holes in the centers of galaxies as they would need to accrete vast amounts of matter in a relatively short period of time to grow up to 8-10 orders of magnitudes to reach supermassive status ( $10^8 - 10^{10} M_{\odot}$ ). This is why we must explore alternative venues for massive black hole formation in the early Universe. As we will discuss in this section, there are multiple venues that can be taken for massive black hole formation, which can be split into two categories: Light Seed ( $\sim 10^2 M_{\odot}$ ) and Heavy Seeds ( $> 10^4 M_{\odot}$ ). More detailed information on these formation paths can be found in [45].

### 1.3.1 Light Seeds

As we discussed in the previous section, the first stars (PopIII) form in pristine, primordial, metal-free environments. Due to the lack of metals, cooling in these gas clouds is largely inefficient, allowing for their monolithic collapse, with little to no fragmentation, to form massive stars of the order of  $10^2 - 10^3 M_{\odot}$  (for a top heavy IMF). These stars do not live for long, expected to die before even a million years after their formation [46]. They are believed to end their lives in a pair instability supernova for masses  $> 100 M_{\odot}$  [47], leaving a remnant in the form of a black hole with a mass that can reach around  $10^2 M_{\odot}$ , though the mass distribution is still highly unconstrained. While these black holes do start their lives with a much higher mass than local stellar mass black holes (which have a characteristic mass of around  $> 3 M_{\odot}$  [20]), there is still a lot of work they need to do in order to resemble local supermassive black holes. In fact, research

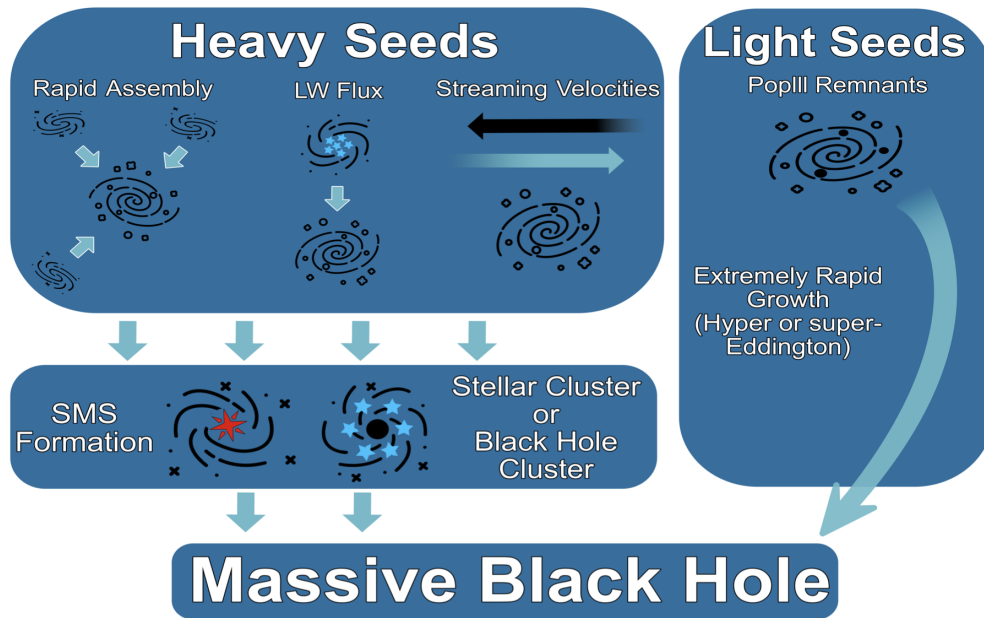


Figure 1.4: Formation pathways of massive black holes in the early Universe. Light seeds are simply the remnants of PopIII stars, whereas heavy seeds have multiple options in which to form, from Rapid Assembly, Lyman-Werner flux and streaming velocities. The pathways either result in the formation of a supermassive star or nuclear stellar cluster which leads to the formation of a heavy seed. Image credit:[45]

shows that these black holes would consistently need to accrete at the Eddington limit in order to achieve this [48, 49]. However, it is shown that these black holes have a hard time accreting mass at high- $z$ , due to the clumpy environments that they are situated in [13]. It is possible that these light seeds can experience bouts of super-Eddington accretion given that conditions allow for radiation feedback to become inefficient due to trapping in the accretion flow [50].

### 1.3.2 Heavy Seeds

While the light seed pathway is mainly constrained to one path (the end remnants of PopIII stars), heavy seeds provide the chance for black holes to begin their lives with masses of the order of  $10^4 M_{\odot}$  through multiple pathways. We will discuss three of them here.

#### Rapid Assembly

The early Universe was full of cold dark matter (as described by  $\Lambda$ CDM) which act as the building blocks for the first halos. The first dark matter halos are allowed to accrete vast amounts of matter which increase the mass of these young halos by orders of magnitude. However due to the constant merging of the halo with smaller clumps of matter, the halo remains largely dynamically heated [51, 14, 52], with this heating rate overcoming the cooling rate from inefficient  $H_2$  cooling, preventing the formation of stars inside the halo, keeping the halo metal-free. As the halo continues to grow, it exceeds the atomic cooling limit, where atomic hydrogen allows the halo to efficiently cool. This large-scale cooling allows for a wide-scale adiabatic collapse, with negligible fragmentation due to the absence of metals, into a single stellar object known as a supermassive star (SMS) [53, 54, 55, 56]. The SMS can accumulate to a mass in excess

of  $10^4 - 10^5 M_\odot$ , providing a large advantage to the black hole seed as it needs to accrete less matter in order to reach supermassive black hole status, in contrast to the light seed model.

## Lyman Werner Radiation

An alternative pathway for stopping the formation of stars and metal pollution, is the presence of a radiation that disassociates any  $H_2$  that exists in the halo [57, 58], halting fragmentation below the atomic cooling limit. This radiation lies in the range of 11.8 – 13.6 eV and is known as Lyman-Werner radiation. This radiation largely comes from neighbouring halos that are experiencing a burst of star formation.

In the synchronised pair scenario[59], while one halo goes through regular star formation, it radiates Lyman Werner radiation such that a neighbouring halo continues to grow while remaining pristine until it reaches the atomic cooling limit, where they halo will then collapse to produce an SMS like the Rapid Assembly pathway [60, 51].

## Nuclear Stellar Cluster Mergers

A pathway that avoids the formation of a singular supermassive star, is that of heavy seeds being formed from the runaway collapse of a nuclear stellar cluster (NSC) [61]. In the early Universe, as halos accreted large amounts of pristine, metal-free matter, gas fragments less efficiently, allowing the formation of massive stars (as discussed in the previous sections). In the densest parts of these high- $z$  redshift halos, a nuclear stellar cluster made from these massive stars can form, where gravitational interactions between the stellar components of the cluster can cause the NSC to collapse on a timescale less than the lifetime of the stars. The massive star that results from the collapse of the NSC ends its life in the form of a black hole with a mass much greater

than that of a singular PopIII star. In the case where the NSC is embedded in a rich reservoir of gas, as would be expected in the early Universe, the stars in the clusters would accrete this gas before merging into a singular massive star which can then end its life as a black hole with a possible mass of  $10^{4-5} M_{\odot}$  [62, 63, 64].

## 1.4 Eddington Limit & AGN

On face value, black holes have the ability to accrete vast amounts of matter at an unbounded rate. However, as with most things, there is a limit to how much material a black hole can consume in a given time interval. As matter falls into the gravitational well of a black hole, it begins to speed up, the environment around it becomes more dense and the medium heats up due to the effects of friction. This increase in energy allows for the emission of electromagnetic radiation, which then applies an outward pressure to the incoming material, reducing the amount of matter being accreted by the black hole. In a spherically symmetric situation, the limit on the accretion rate is given by

$$\dot{M}_{\text{edd}} = \frac{4\pi GMm_p}{\epsilon\sigma_T c}, \quad (1.12)$$

where  $M$  is the mass of the black hole,  $m_p$  is the proton mass,  $\epsilon$  is the radiative efficiency and  $\sigma_T$  is the Thompson cross-section [65, 66]. Assuming a radiative feedback efficiency of  $\epsilon = 0.1$ , the above formula can be simplified to

$$\dot{M}_{\text{edd}} \sim 10^{-8} \left( \frac{M}{M_{\odot}} \right) M_{\odot}/\text{yr}. \quad (1.13)$$

There are cases in which the black hole can exceed the Eddington limit, due to non-symmetrical effects, in which the incoming material forms a disc along the plane of the black hole and radiation pressure is largely directed from the poles due to effects from its strong magnetic field, thus largely avoiding this pressure having an impact on inflowing material [67, 68]. There are also effects due to photon trapping, in which radiation becomes trapped by the optically thick inflow rate [69].

Active Galactic Nuclei (AGN) are actively accreting supermassive black holes at the centre of active galaxies [20, 70, 71]. The AGN system comprises the central supermassive black hole and accretion disk, surrounded by a thick torus of gas and dust. Seyfert galaxies are a type of AGN, with two types existing that differ by their respective observation angle. Type I Seyfert galaxies are defined as the core being directly visible to an observer, whereas with Type II Seyfert galaxies, the core is largely obscured by the surrounding torus. In spectroscopy, Type I Seyfert galaxies possess both broad and narrow emission lines. The broad lines are due to doppler shift occurring from the rapid motion surrounding the black hole at the heart of the galaxy. In Type II Seyfert galaxies, because the area surrounding the black hole is obscured, this doppler shift is not observed and only the narrow lines are spectroscopically observed. There also exist quasars, which are objects that differ from Seyfert galaxies, in that their host galaxies aren't easily observable, and their spectra show a significant non-thermal continuum [72]. The jets powered by the central supermassive black holes are extremely energetic, constituting some of the brightest objects in the Universe. Lastly, blazars are

quasars which are orientated in a way in which our viewing angle is directly parallel to the emitted jets. AGN's provide electromagnetic evidence for the existence of rapidly accreting black holes. A diagram showing the structure of AGN and the viewing angles that distinguish Type I, II Seyfert galaxies and blazars from each other is shown in Fig.1.5.

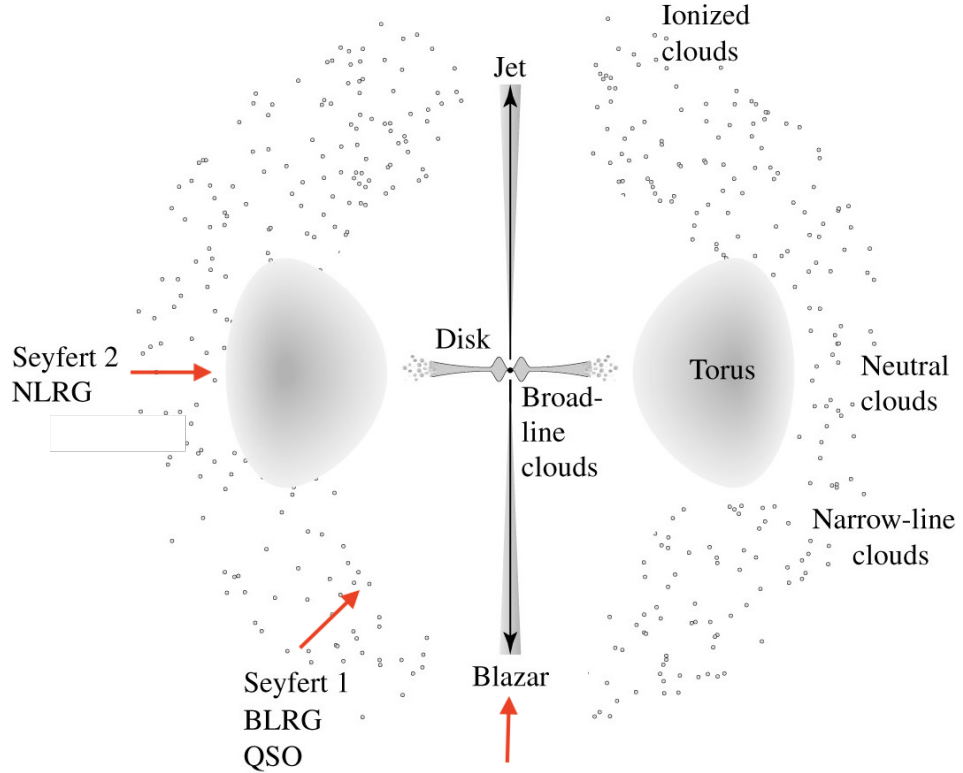


Figure 1.5: Schematic obtained from [20] showing the structure of an AGN, with red arrows indicating the viewing angles that distinguish Seyfert I, II galaxies and blazars from each other. The dot in the middle indicates the supermassive black hole at the hearts of AGN. NLRG refers to a Narrow Line Region Galaxy, BLRG refers to a Broad Line Region Galaxy and QSO is a Quasi-Stellar Object, also known as a quasar.

## 1.5 Black Hole Mergers and Gravitational Waves

Once our seeds have formed and a population of black holes has been established, they are then allowed to grow either via gas accretion or merging with other black holes. Accretion onto black holes can be observed via EM signatures [73, 2], as material entering the black hole heats up in a surrounding accretion disc due to friction. Observing mergers of black holes requires a different method from studying the EM spectrum. Thankfully merging black holes can leave a signature in the form of an imprint on spacetime itself, gravitational waves, which were first hypothesised to exist by Albert Einstein [74].

If we take a flat Minkowski metric in a weak field limit, meaning  $T_{\mu\nu} \rightarrow 0$  for all  $\mu$  and  $\nu$ , and add a perturbation to the field in the form of [75]

$$g_{\mu\nu} = \eta_{\mu\nu} + h_{\mu\nu}, \quad (1.14)$$

where  $h_{\mu\nu} \ll 1$ , one can show that by inserting 1.14 into the Einstein Field equations 1.5 that the perturbation obeys the wave equation in a vacuum

$$\square h_{\mu\nu} = 0, \quad (1.15)$$

thus showing that spacetime can ripple in the form of what we now call gravitational waves. Here,  $\square$  refers to the d'Alembert operator which is the equivalent of

$$\square = \partial^\mu \partial_\mu = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2. \quad (1.16)$$

Gravitational waves have been hypothesised to exist for decades, with their first

direct detection only being made in 2015 with the first-light of the LIGO observatory in the US [76]. The two interferometers, situated in Washington and Louisiana, detected the gravitational wave signal from the merger of two stellar mass black holes with masses of  $36 M_{\odot}$  and  $29 M_{\odot}$ . As the black holes orbit each other, their orbits decrease due to the emission of gravitational waves, resulting in a loss of orbital energy [77]. These black hole binaries usually form from the remnants of stellar binaries, or even black holes that get caught in each others orbit in dense stellar clusters [78]. However when we move to possible black hole binaries in the intermediate to supermassive regime, their path to coalescence is a little more complicated. Massive black holes are thought to occupy the nuclei of most galaxies. As galaxies merge, the black holes that they contain go through a series of phases that can occur over billions of years in order to reach compact binary status and the commencement of gravitational wave emission. The first thing that occurs is that the black hole from the satellite halo, slowly experiences a drag from the background stellar, gas and dark matter medium, where the change in velocity is given by the following equation [79, 80]

$$\frac{d\mathbf{v}}{dt} = -16\pi^2 (\ln \Lambda) G^2 m (M + m) \frac{1}{v_M^3} \int_0^{v_M} v^2 f(v) dv \mathbf{v}_M, \quad (1.17)$$

where  $\ln(\Lambda)$  is the Coulomb logarithm,  $M$  is the mass of the black hole,  $m$  is the mass of each star in the stellar velocity distribution,  $v$  represents the velocities given by the distribution and  $f(v)$  represents the velocity distribution where a Maxwellian distribution is commonly given in the case where we assume a uniform density field. One can estimate the time taken for the satellite black hole to reach coalescence with the black hole of the main halo by assuming a stellar background given by an isothermal sphere and the satellite black hole moving in a circular orbit around the center of the

host halo. Thus the delay due to dynamical friction can be estimated by [81, 82]

$$t_{DF} \sim \frac{8}{\ln(\Lambda)} \left( \frac{r}{\text{kpc}} \right)^2 \frac{\sigma}{200 \text{ km/s}} \frac{10^7 M_\odot}{M} \text{ Gyr}, \quad (1.18)$$

where  $\sigma$  gives the stellar velocity dispersion of the host halo. We can see from Fig. 1.6 that dynamical friction covers a large portion of the distance covered from galaxy merger to black hole coalescence and plays arguably the most important part in bringing the two black holes together. After this stage, it is three-body interactions with stellar objects that causes the black hole to further lose orbital momentum and fall further into the gravitational well. The satellite black hole will then form a binary with the host halo's black hole. Further loss of orbital energy can be established due to the presence of a circumbinary disk, surrounding the black hole binary [83]. The main cause for coalescence at this point is the loss of kinetic energy due to the emission of gravitational waves [77]. As the black holes sink faster and faster towards each other, the energy emission in the form of GWs increases, thus speeding up the merger time. As the black holes reach each other and merge, there will be a final ringdown signal and a final singular black hole will be produced. The mass of this black hole is less than the sum of the progenitors, due to the mass lost being converted into energy for gravitational waves.

## 1.6 Cosmological Simulations & Renaissance

Due to the complex nature of the Universe, it is necessary to make use of simulations to model the wide scale of physics within it. There are simulations which utilise general relativity to simulate the environment around a black hole in detail (e.g. [84, 85, 86]), simulations which focus on stellar and planetary formation at small scales [87] and

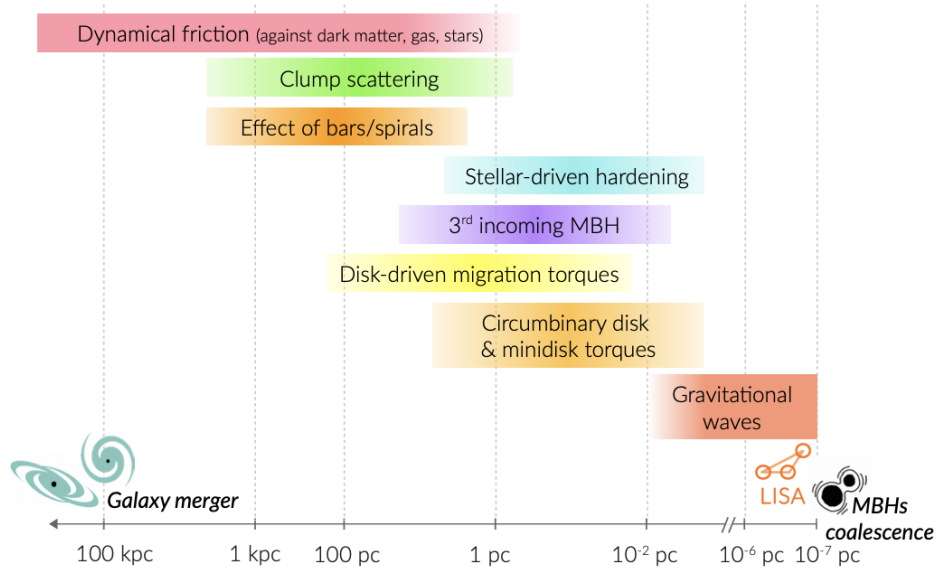


Figure 1.6: Plot showing the mechanisms by which two massive black holes are brought together following a galactic merger, while also denoting the length scales at which these mechanisms dominate. Dynamical friction can be seen to be operating at large separation scales, stellar hardening and circumbinary disks further bring the two black holes together, while at small scales, GW's dominate the hardening process at smaller scales and cause the massive black hole binary to coalesce. Image credit: Elisa Bortolas [82]

simulations which model how nuclear stellar clusters collapse to form black holes [88]. However, if we wish to study large scale black hole and galaxy formation and growth, we need to make use of cosmological simulations. Many complex processes need to be accounted for in these simulations, including chemical evolution, morphology of galaxies, fluid and N-body dynamics and various feedback mechanisms from stars and AGN. Due to the large scale complex nature of these simulations, there may come a cost to how low the masses of “particles” or spatial regions can be resolved in such simulations. This lack of supreme resolution can lead to a loss of information, so a careful tuning of parameters needs to be performed in order to get the best out of cosmological simulations. There are a number of large scale cosmological simulations that exist including EAGLE [89], Illustris [90], TNG100 [91], RomulusC [92], OBELISK [93] and Simba [94]. For the following chapters we will focus on the **Renaissance** simulations which are focused on early galaxy formation and were built using the adaptive mesh refinement code ENZO [95, 96].

## ENZO & Renaissance

ENZO [95, 96] is an adaptive mesh refinement [97] code that uses cartesian coordinates to simulate volumes of astrophysical fluid dynamics. It uses this adaptive mesh refinement to resolve regions of high density, such that the physics of active formation and feedback environments can be resolved while also minimising the computational cost. A number of physical phenomena can be simulated with ENZO, including magneto-hydrodynamics, N-body mechanics, the chemical evolution of primordial gas, heating and cooling mechanisms and the code also accounts for the cosmological expansion to allow for large-scale modelling.

The **Renaissance** simulations [10, 11, 12, 13, 14], constructed using the ENZO code,

are a suite of N-body, hydrodynamic simulations focussed on early Universe galaxy formation (see Fig.1.7). They consist of three regions: Rarepeak (RP), Normal and Void, labeled by their respective level of overdensity. These regions sit in a parent box with a side length of 40 cMpc, with the RP region having dimensions of  $(3.8 \times 5.4 \times 6.6)$  cMpc<sup>3</sup> and both the Normal and Void regions both simulating comoving volumes of  $(6.0 \times 6.0 \times 6.125)$  cMpc<sup>3</sup>. The cosmology that the simulations are based on uses parameters measured by the 7-year data release of the WMAP data with  $\Omega_M = 0.266$ ,  $\Omega_b = 0.0449$  and  $\Omega_\Lambda = 0.734$ . The simulations account for the modelling of PopIII and PopII star formation and feedback, with a dark matter mass resolution of  $2 \times 10^4 M_\odot$  and a maximal spatial resolution within the adaptive mesh of 19 comoving pc. This allows for the evolutionary tracking of massive galaxies from the hierarchical build-up of small building blocks. Due to the computational complexity of *Renaissance*, the RP region is run to a redshift of  $z = 15$ , the Normal region to  $z = 11.6$  and the Void region run to  $z = 8$ . A plot of the renaissance simulations and its regions is shown in Fig.1.7.

## 1.7 JWST & Electromagnetic Signatures

On the 25<sup>th</sup> of December 2021, the James Webb Space Telescope [99] was launched from French Guiana with the ESA Ariane 5 rocket. After a weeks long journey to the L2 lagrange point, it required 5 months of commissioning to deploy and calibrate the instruments occupying JWST. On board JWST is a primary mirror with a diameter of 6.5 m and a focal length of  $\sim 130$  m, composed up of 18 tessellating, beryllium-coated, hexagonal mirrors. The main instruments that JWST is equipped with are the Near InfraRed Camera (NIRCam)[100, 101], Near Infrared Spectrometer (NIRSpec)[102, 103], Mid InfraRed Instrument (MIRI)[104, 105] and Near Infrared Imager and Slitless Spec-

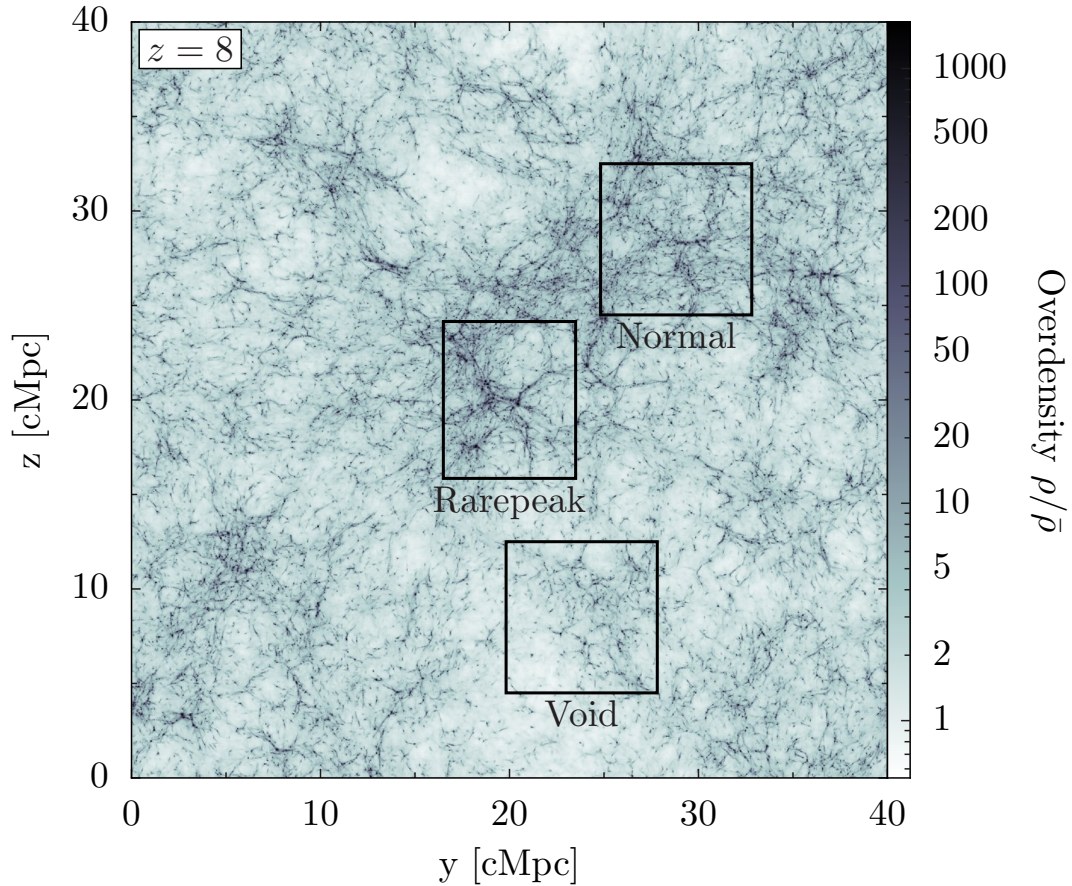


Figure 1.7: Mass-weighted density projection of the  $(40 \text{ comoving Mpc})^3$  exploratory dark matter simulations at redshift  $z = 8$  used in the **Renaissance** suite. The survey volumes of the Rarepeak, Normal and Void regions are outlined. The Rarepeak region is centered on the most massive halo at  $z = 6$ , and resimulated at a higher resolution up to  $z = 15$ . Due to projection effects, the Normal region appears as dense as the Rarepeak region. However, the average overdensity of the Normal region is only 9% higher than the mean matter density. This visualisation is originally published in [98].

trograph (NIRISS)[106, 107] so that JWST can probe the red-end of the optical and infrared parts of the EM spectrum. This crucially samples optical and UV emission originating in the early Universe which have been redshifted into the IR range due to cosmological expansion. Since its launch, JWST has made numerous advancements in the fields of exoplanets, planet formation and high redshift galaxies. For the purposes of this thesis, we will focus on some of the discoveries that have been made by JWST with respect to the high- $z$  galaxy and black hole population, and also discuss some of the questions that have been raised because of said discoveries.

## High redshift Galaxies

In 2023 a number of high- $z$  galaxies were discovered by JWST, with spectroscopically confirmed redshifts of  $z > 10$  [108, 109, 110, 111]. The masses and star formation rates (SFRs) of these galaxies were then constrained using spectral fitting models (e.g. [112]), which concluded that these galaxies displayed very high stellar masses and star formation rate (SFR) values for this epoch of the Universe. So much so, that there are concerns that these galaxies are testing the limits of the  $\Lambda$ CDM model, in that they seem to be exceeding the limits of how much baryonic matter is available to convert into stellar matter, with star formation efficiencies approaching  $f_* \sim 100\%$  [113, 114, 115, 116, 117, 118, 119]. There have been studies to alleviate this prevailing tension by using cosmological simulations to see whether or not such high mass, high- $z$  galaxies can exist like in [120]. While they found that such high mass galaxies can exist, these cosmological simulations were not designed to probe such high redshifts, and so additional research was needed. In Chapters 3 & 4 (derived from [121, 122]), we will utilise the high- $z$  nature of the **Renaissance** simulations in an attempt to answer whether or not these curious JWST galaxies can indeed exist in the standard  $\Lambda$ CDM framework.

## Early Overmassive Black Holes

As JWST gained access to this high- $z$  population of galaxies in the Universe, we also gained knowledge on the early population of black holes that existed in these galaxies. In particular, [123] have discovered that a population of black holes are displaying an uncharacteristically high ratio between the mass of these black holes and the stellar masses of their host galaxies in the redshift era of  $z \sim 4 - 7$ . These ratios in the range of  $M/M_* \sim 0.01 - 0.1$ , suggesting a redshift evolution of the black hole/stellar mass relationship throughout cosmic time. Such high mass black holes existing in the early Universe also suggests that these black holes are growing at a considerable rate in the time not long after their formation. There is additional research [124] however which suggests there is a sampling bias in the selection of these overmassive black holes, given that they would be the brightest objects that JWST will be able to detect, and in fact there may be an undetected population of lower mass black holes which would bring the black hole/stellar mass relation down to the local measurements.

## 1.8 LISA and future GW detectors

So far we have shown that the existence of GWs has been proven with LIGO, through detections of signals from merging stellar mass black holes. With this new area of astronomy unlocked, we can start to look for evidence of more elusive objects in the Universe. In fact, we have already started to uncover the low frequency end of the GW spectrum in pulsar timing array observations with the NanoGrav research collaboration [6] and the European Pulsar Timing Array (EPTA) [7]. A Pulsar Timing array is a type of gravitational wave observatory that uses the distances to pulsars as arm lengths for a GW detector, analogous to the arms of LIGO. Data from NanoGrav

and EPTA has revealed that there is a stochastic background signal in the Universe corresponding to low frequency GWs, likely caused by supermassive black holes binaries or SMBH interactions with their local environments.

If we want to make direct detections of merging massive black holes, we need a detector with arm lengths much larger than what LIGO has. In fact, we need arm length larger than the size of the Earth. For this reason, we need to look to space to situate our desired GW detector. This is where LISA takes the spotlight. LISA, due to be completed in the late 2030's, is an ESA-led space based mission for a GW detector with arm lengths of 2.5 million km. It consists of three satellites set in a heliocentric orbit, with an orbital phase offset of  $20^\circ$  separation between the detector and Earth.

The main scientific goals of LISA are the detection of gravitational waves from massive black hole binaries, Extreme Mass Ratio Inspirals and from compact binaries in our own galaxy [125]. For this work, we mainly focus on LISA's ability to open the window on massive black hole mergers. LISA's primary sensitivity range lies in the black hole mass range of  $10^3 - 10^7 M_\odot$  up to a possible redshift of  $z \sim 20$  as can be seen in Fig.1.9. This makes it an ideal instrument to probe early Universe black hole populations and identify the formation pathways in which massive black holes are born.

Additional proposed instruments include the Einstein Telescope (ET) [126] and the Cosmic Explorer (CE) [127]. These are ground based interferometers that are designed to look at stellar-mass to low end massive black hole mergers at extremely high redshifts. While these observatories are still in the proposal stage, it would be beneficial for a synergy between these interferometers and LISA to cover a broad mass spectrum of black hole mergers and be able to constrain black hole formation models from these detections [128]. A plot showing the characteristic strains of LISA, ET and CE is shown in Fig.1.8, while a Signal-to-Noise Ratio plot for LISA and ET as a function of merger

primary mass is shown in Fig.1.9

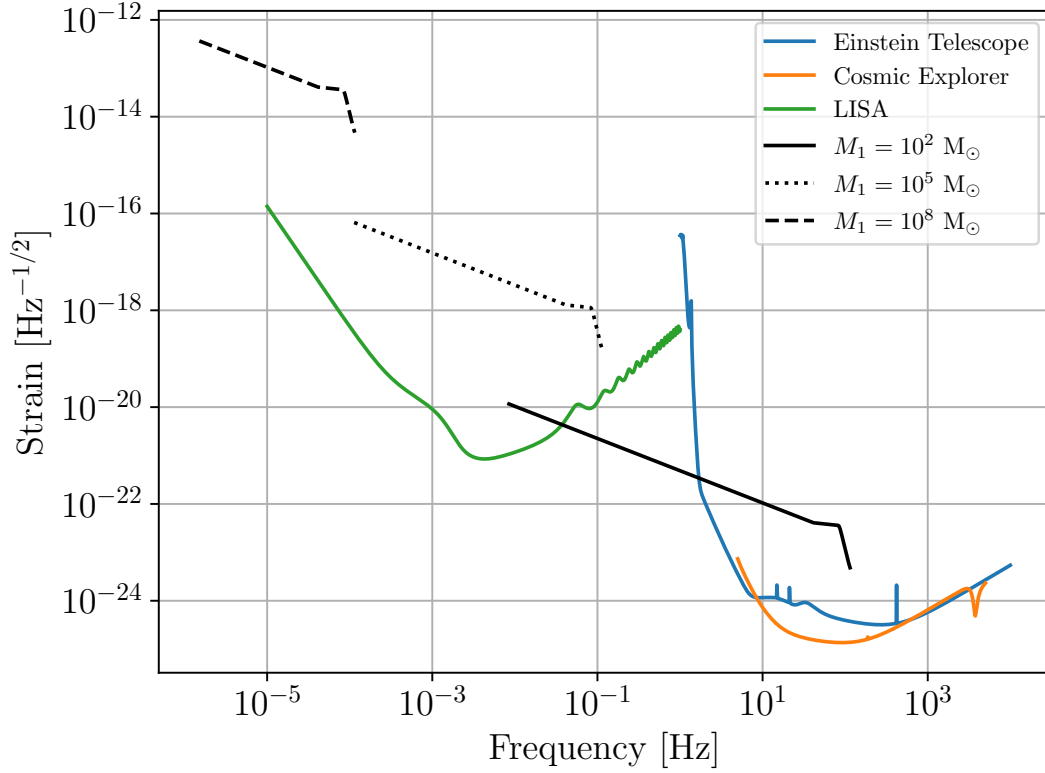


Figure 1.8: Characteristic Strains of the future LISA and the proposed Einstein Telescope and Cosmic Explorer instruments. Data for the sensitivity curve of LISA was obtained from [129]. ET’s curves are from [130] and CE’s curves are from [131]. Also plotted, are merger signals of black holes binaries with a mass ratio of 1, with primary masses of 10<sup>2</sup>(high stellar mass BH), 10<sup>5</sup>(IMBH) and 10<sup>8</sup> M<sub>⊙</sub>(SMBH) at  $z = 1$  on the figure.

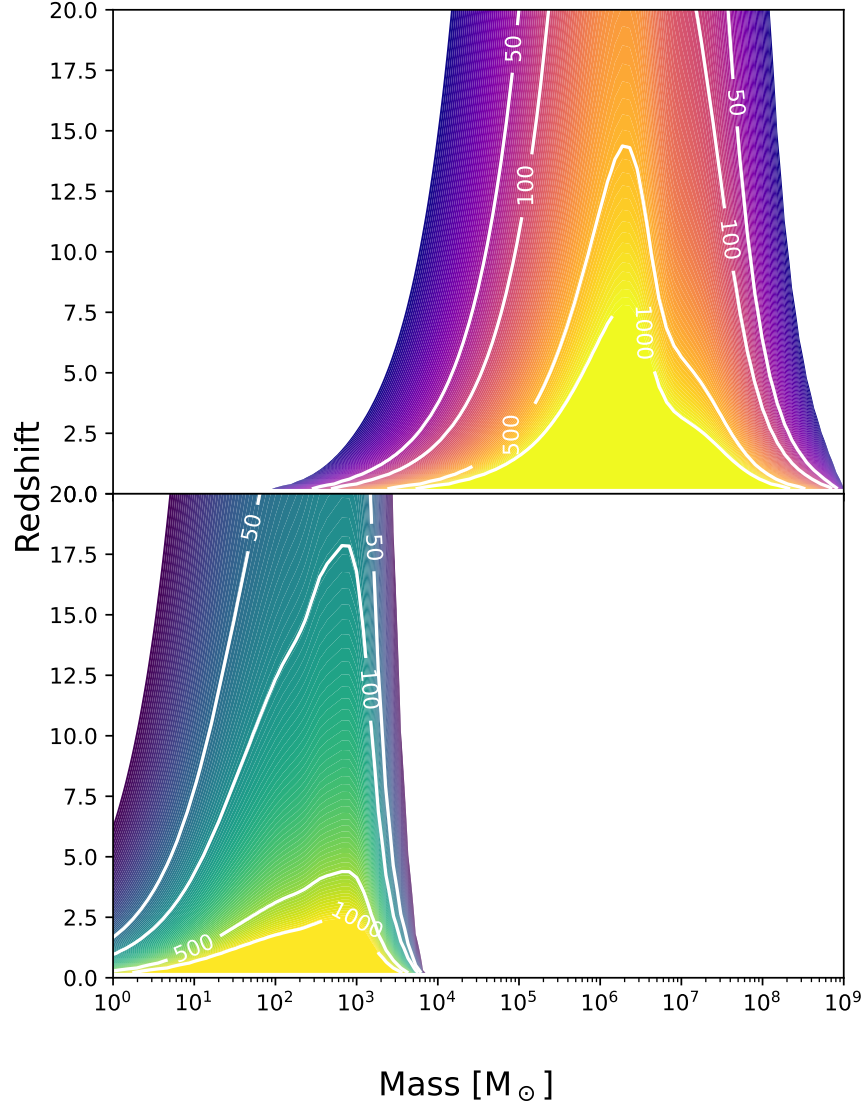


Figure 1.9: Waterfall plots showing the signal-to-noise ratio of re LISA (top) and the Einstein Telescope (bottom). We have left out the Cosmic Explorer from this plot due to the fact that its and the Einstein Telescope’s sensitivity curves largely overlap. The x-axis denotes the mass of the primary black hole in the merger, where the merger has a mass ratio of  $M_1/M_2 = 1$ . The SNR values are denoted on the waterfall plots as contour lines. SNR calculations are based on code built by [129].



# Chapter 2

## Modelling Massive Black Hole Formation in Renaissance

### 2.1 Introduction

Massive Black Holes (MBHs) are a common feature in almost every galactic center in the Universe [e.g. [132](#), [133](#), [134](#), [135](#)]. These central MBHs can have masses that range from millions to billions of times the mass of the Sun and exist at epochs from the present day Universe back to, at least, only several hundred million years after the Big Bang [[136](#), [137](#), [138](#), [139](#), [140](#)]. The very existence of MBHs in the very early Universe places a severe challenge to our understanding of compact object formation, growth and evolution at early times [[141](#)]. An outstanding challenge in astrophysics and cosmology is, therefore, how did the first seed black holes grow to the masses we observe in galaxy centres, like for example the case of the UHZ1 black hole, which has an observed mass of  $10^7 - 10^8 M_{\odot}$ , existing around 400-500 million years after the Big Bang [e.g. [142](#), [143](#), [144](#)].

To this end models have focused on trying to explain how MBHs can form and ultimately end up powering the quasars in galactic nuclei. There are a number of potential pathways that can lead to a MBH [e.g. 145]. In broad terms the pathways can be broken into the light seed pathway and the heavy seed pathway. The light seed pathway [e.g. 146] relies on the remnants of Population III (Pop III) stars, the first generations of stars in the Universe. The black holes formed from these stars would have an upper limit of at most  $10^3 M_{\odot}$  [147, 148, 149]. In order for these black holes to reach the masses that we observe at high- $z$ , they would need to undergo accretion at the Eddington rate for extended periods and for the high- $z$  quasar population, in particular, accretion at, or beyond, the Eddington rate with a duty cycle of very close to unity would be required. This may be physically unlikely as the black hole would need a consistent supply of matter to accrete from and would need to stay at the centre of a dense accretion flow [150, 151, 152].

The dynamics of black hole accretion has turned out to be one of the main bottlenecks to efficient accretion onto light seed black holes with numerous studies showing that light seed black holes are unable to efficiently sink to the high-density centre of galaxies [e.g. 153, 154]. While dynamics, without doubt, does provide a strong bottleneck to efficient growth, growth within more favourable environment may be possible [e.g. 155, 156, 157, 158, 159, 160, 161, 162, 163]. The question is how frequently this efficient (possibly via bursts of super/hyper-Eddington) accretion occurs and what is the parameter space that allows it to occur? If the probability of growth in the light seed scenario is too low then perhaps another seed formation pathway is required.

The heavy seed pathway emerges as an attractive scenario in this case. For the heavy seed pathway the initial mass of the black holes is expected to be in the range  $10^3 - 10^5 M_{\odot}$ . The actual formation of the heavy seed can occur via two, potentially

overlapping, pathways. On the one hand we have formation via a supermassive star (SMS) in the nucleus of the halo [e.g. 164, 165, 166, 167, 168, 169], or else a heavy seed may form via dynamical runaway within a dense stellar cluster or dense black hole cluster [170, 171, 172, 173, 174, 175, 176, 177, 178, 179]. Both of these scenarios have been thoroughly investigated via analytic, semi-analytic and numerical modeling over the last decade. While convergence of models is certainly lacking it is also true that heavy seed formation has been shown to be viable and with number density values shown to be potentially compatible with the observed population of high- $z$  MBHs [139]. More exotic channels for black hole formation include the formation of massive protostars that are fueled by the annihilation of dark matter particles instead of nuclear fusion [180].

Over the last two decades a number of channels have been explored which can in principle lead to environments capable of supporting heavy seed formation. These are i) formation of heavy seeds in haloes exposed to large Lyman-Werner (LW) fields, ii) baryonic streaming velocities leading to heavy seed formation and iii) rapid halo assembly leading to heavy seed formation. In this paper we focus exclusively on the rapid-assembly channel. Further details on the other channels can be found in the review by [143]. The rapid-assembly channel potentially leads to a much greater number density of MBHs at high- $z$  being only dependent on the assembly history of the halo up to the atomic cooling limit. Recent numerical simulations by [181], [182], [183] and [52] shown that inflow rates of approximately  $0.1 \text{ M}_{\odot} \text{ yr}^{-1}$  into the halo centre (i.e. down to scales of order 1 - 50 pc) is sufficient to suppress the cooling effect of  $\text{H}_2$  allowing larger Jeans masses to develop. In turn this allows the formation of massive proto-stars [182, 184]. It is this pathway we explore in this paper and from this model we quantify the expected number density of heavy seeds.

The larger mass of heavy seeds compared to light seeds gives heavy seeds distinct advantages over light seeds. The larger initial masses contribute directly to a larger sphere of influence which can be represented by the Bondi-Hoyle radius [185]. The Bondi-Hoyle radius scales as the black hole mass squared giving the heavy seed mass black hole a significantly larger probability of accreting material. Additionally, dynamical friction scales with  $M_{\text{BH}}^2$  again meaning that heavy seed black holes are more likely to experience efficient sinking towards higher density regions compared to lighter seeds [186].

On the observational side it is still beyond the reach of modern telescopes to observe the seed formation epoch. Recent measurements by JWST of MBHs in very early galaxies has led some authors to conclude that these measurements are inline with expectations from a heavy seed pathway [187, 123, 188]. This is because the MBH population that JWST has thus far revealed at high- $z$  does appear to reflect an over-massive population with respect to the host galaxy stellar mass, albeit selection bias may yet be at play [124]. While the weight of evidence now likely points to heavy seeds being the origin for at least some of the MBHs being detected by JWST, periods of super-Eddington accretion onto a light seed cannot be ruled out [e.g. 155, 160, 163, 189].

## 2.2 Methodology

### 2.2.1 The Renaissance Simulations

The **Renaissance** simulations<sup>1</sup> [10, 190, 191, 192] are a suite of three zoom-in regions of cosmological N-body, hydrodynamical simulations using the adaptive mesh refinement

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<sup>1</sup><https://rensimlab.github.io/>

code Enzo [95, 96]. The zoom-in regions originate from a parent box with a comoving volume of 40 cMpc on the side. The *Renaissance* simulation setup is briefly described here but we refer the reader to the previous papers for more detailed discussion.

The goal of the *Renaissance* simulation suite was to model early galaxy formation, including Pop III and Pop II star formation and feedback. In order to accomplish this, high resolution was required to allow us to resolve (mini-)halos of masses  $\sim 10^6 M_\odot$  and then track their growth through accretion and mergers with other halos. More details on the parameters concerning the three zoom-in regions (RP, Normal and Void) can be found in 1.6. As the goal of this study is to constrain the number density of heavy seed black holes we choose to study only the Normal and Rarepeak regions here as the Void region has been previously found to support only very few, if any, heavy seeds [193].

The *Renaissance* simulations contain models for metal free (Population III) and metal-poor (Population II) to allow for self consistent (early) star formation. Crucially the simulations, however, do not contain a prescription for black hole formation [see also 194]. We will use the information that the *Renaissance* simulation snapshots supply to predict regions in which massive black hole (MBH) formation is likely to occur. We then use that same information to predict the accretion and merger rates for MBHs in the early Universe. The resolution for the dark matter particles in *Renaissance* is  $2.4 \times 10^4 M_\odot$  while the gravitational softening length is resolved down as far as 19pc.

### 2.2.2 Seeding the Massive Black Hole Population

To identify regions of MBH formation, we analyse each halo, from its starting point within the merger trees (built by Rockstar [195] and consistent-trees [196]) and work our way forward to identify the earliest point at which each halo satisfies the conditions needed for seed formation. The filters we use to identify MBHs within haloes inside the

simulation volumes are determined by the following conditions:

- $T_{\text{vir}} > \text{Atomic Cooling Limit } (\sim 10^4 \text{ K})$
- Metallicity,  $Z < 10^{-3} Z_{\odot}$
- Compactness,  $\gamma > 0.5$
- Inflow rate,  $\dot{M} > 0.1 \text{ M}_{\odot}/\text{yr}$

We now discuss each of these criteria in turn.

We only consider haloes that exceed the atomic cooling threshold. Atomic cooling haloes are characterised by reaching a virial temperature at which atomic line emission cooling becomes effective. The virial temperature at which this occurs is  $T_{\text{vir}} \approx 10^4 \text{ K}$ , where

$$T_{\text{vir}} = 0.75 \times 1800 \left( \frac{M_{\text{vir}}}{10^6 \text{ M}_{\odot}} \right)^{2/3} \frac{(1+z)}{21} \text{ K}, \quad (2.1)$$

[197]. This presents us with a mass limit that we use to identify the atomic cooling halos,

$$M_{\text{crit}} = 10^{12} \left[ 0.75 \times 1800 \left( \frac{(z+1)}{21} \right) \right]^{-3/2} \text{ M}_{\odot} \quad (2.2)$$

As the halos collapse, due to radiative cooling, the density increases and the opportunity for massive stars and subsequent black hole formation presents itself. In the absence of metals (discussed below) and thus fragmentation, a single supermassive star can form [14, 198] and thus end its life in a higher mass MBH compared to black holes formed from the Pop III stars in the light seed pathway [199].

In addition to the atomic cooling limit mass threshold, we also impose a minimum metallicity threshold of  $Z < 10^{-3} Z_{\odot}$ . We require the halo to have low metallicity as the

presence of metals adds an additional and very efficient coolant lowering the Jeans mass substantially, thus causing fragmentation to occur [29, 200, 199]. The fragments that will form in metal enriched gas would form Pop II stars and perhaps a proto-globular cluster depending on the environmental conditions. Our criteria of filtering out all haloes with a metallicity  $Z > 10^{-3} Z_{\odot}$  allows for the formation of both supermassive seeds, through a near monolithic collapse, and potentially also fragmentation into massive star clusters [179, 201, 202], allowing for multiple methods in which a heavy seed can form. In this way we are combining the dynamical runaway collapse model [e.g. 203, 204, 205, 206, 207, 208] and the super-massive star model into a single pathway - the formation of a heavy seed [209, 210, 211, 212, 213, 214, 215]. For the purposes of this study we are agnostic to the emergence of the heavy seed black hole at scales we cannot resolve.

The third criteria for every MBH seed halo to meet concerns the distribution of the mass inside the halo. We consider a parameter we label as ‘compactness’, which is defined as the ratio of mass inside a sphere of half the virial radius centered on the highest density point, over the total mass of the halo. A compactness,  $\gamma$ , threshold of  $\gamma > 0.5$  is used to identify halos that are sufficiently compact for seed formation to occur. Mathematically we define  $\gamma$  as:

$$\gamma = \frac{M(r < 0.5R_{\text{vir}})}{M(r < R_{\text{vir}})}, \quad (2.3)$$

where  $\gamma = 0.5$  for a singular isothermal sphere.

By identifying compact galaxies, as given by  $\gamma$ , we are selecting galaxies which are likely to provide a rich environment for both initial MBH seed formation and potentially also early growth.

Finally, we consider only halos with a mass inflow rate exceeding  $0.1 \text{ M}_\odot \text{ yr}^{-1}$  which is needed to generate the conditions thought necessary to allow for (super-)massive stars to form [216, 168, 14, 217], thus resulting in a heavy seed. The gas mass inflow rate is directly connected to the growth rate of the halo [see e.g. 217] with higher growth rates leading to higher dynamical heating within the halo [218]

The mass inflow rate, which is defined as

$$\frac{\partial M}{\partial t} = \int_{\sigma} \rho \vec{v} \cdot d\vec{\sigma} \quad (2.4)$$

$$= 4\pi R^2 \rho v_r \quad (2.5)$$

where  $\sigma$  is the sphere of virial radius  $R_{vir}$  centered on the highest density point of the halo in question,  $\vec{v}$  is the velocity of the gas flowing through an infinitesimal area element on  $\sigma$  [219, 182]. The inflow is calculated on a sphere of 20 pc radius centered on the highest density point. We choose the highest density point as the centre due to the clumpy nature of the halo.

Once all of the heavy seed halo conditions are met, we assume the formation of a heavy seed MBH. In reality the heavy seed MBH will be preceded by phase of stellar evolution either via a supermassive star, a dense stellar cluster or some combination. In either case the lifetime of the stellar phase of the heavy seed is expected to be of order  $10^6$  years [220, 168]. Due to the fact that the time between snapshots in **Renaissance** is on the order of a few million years, we can assume that our heavy seeds can immediately be identified as MBHs. It is noted that because we allow heavy seeds to form in halos that reach atomic cooling limit ( $\sim 10^6 \text{ M}_\odot$ , along with the other criteria for seeding), this allows for black holes to form in earlier times compared to other simulations that seed at  $10^{10} \text{ M}_\odot$  (EAGLE [89], FABLE [221] and SIMBA [222]). Thus, giving the black

holes in this model extra time to grow in comparison to other cosmological simulation.

Some of our choices for the seeding prescription are open to investigation (as is almost universally true for all subgrid models). In particular our choice of the Inflow Rate threshold ( $0.1 \text{ M}_{\odot} \text{ yr}^{-1}$ ) and the compactness parameter are valid avenues for further exploration. The inflow rate threshold is the parameter that ultimately dictates the number density (see Figure 2.3). The value chosen is based on the high resolution studies of [182] and [217] which show that MBH seeds can form in haloes experiencing inflow rates at or above this threshold. As such we believe our choice to be robust.

### 2.2.3 Assigning Masses to the Seeds

After the halos have been identified, we need to assign a black hole mass to the seeds. Since there is no constrained initial mass function (IMF) for MBH seeds, we will instead rely on observationally derived scaling relations to build our initial black hole population. In this work we make use of two stellar mass versus black hole mass relations, the first is using data from the local Universe [223, using the local AGN relation, rather than the relation used for inactive elliptical and spiral galaxies] while the second is derived from high- $z$  JWST galaxies [123]. The second relationship suggests that central MBHs are “over-massive” with respect to their host galaxy stellar masses.

We also need to consider the possibility that these massive black holes can form in halos with no or negligible stellar matter. Therefore, we derive an additional relation for the black hole mass as a function of the stellar mass for halos with a stellar mass of  $< 10^3 \text{ M}_{\odot}$  directly from the *Renaissance* datasets.

For the stellar mass relations, we use the following relationship when seeding black

holes in haloes with stellar masses in excess of  $10^3 M_\odot$ .

$$\log\left(\frac{M_{\text{BH}}}{M_\odot}\right) = \beta + \alpha \log\left(\frac{M_*}{M_\odot}\right) \quad (2.6)$$

In [123] (the high redshift, overmassive case) the mean value of the parameters were constrained to be  $\alpha = 1.06$  and  $\beta = -2.43$ . For the local relation [223], the mean values are  $\alpha = 1.05$  and  $\beta = 7.45$ . For seeding MBHs in haloes with stellar masses less than  $10^3 M_\odot$  we use the following relation:

$$\log\left(\frac{M_{\text{BH}}}{M_\odot}\right) = \delta + \gamma \log\left(\frac{M_{\text{vir}}}{M_\odot}\right), \quad (2.7)$$

For the [123] relation, the free parameters are set to be  $\gamma = 1.9$  and  $\delta = -11.9$ . While for the [223] relation, the free parameters are set to  $\gamma = 1.9$  and  $\delta = -13.78$ , respectively. We hereafter refer to the seeding method using the relation from [223] as RV15 and to the method using [123] as P23. Finally, we impose a minimum black hole seeding mass of  $M_{\text{BH}} > 100 M_\odot$ . We include black holes with masses less than  $10^3 M_\odot$  to investigate whether light seeds in lower mass galaxies are able to grow enough in order to reach masses comparable to heavy seed black holes. We decided to use a range of black hole seed masses, in contrast to other simulations (e.g. EAGLE [89], FABLE [221] and SIMBA [222]). Using a range of masses will allow us to study the impacts black hole mass will have on the accretion calculations onto the black holes as well as the kind of mass ratios we expect to see in black hole mergers.

## 2.2.4 Growth of the MBH population

We allow the seeded MBHs to grow under accretion from the surrounding gas reservoirs - as derived from the *Renaissance* datasets. To model the growth through accretion we follow the method of [224] where they grow stellar mass black holes in post-processing using the Bondi-Hoyle method [225],

$$\dot{m}_{\text{B-H}} = \frac{\alpha \pi G^2 M_{\text{BH}}^2 \rho}{\max(|\vec{v}|, c_s)^3}, \quad (2.8)$$

where the boost factor  $\alpha$  is included to account for the fact that the *Renaissance* simulations cannot fully resolve the Bondi-Hoyle radius, given by

$$r_b = \frac{2GM_{\text{BH}}}{c_s^2} \quad (2.9)$$

The choice for the value of  $\alpha$  is discussed later in §2.2.5. The mass of the MBH at each timestep is given by

$$M_{i+1} = M_i + \dot{m}_{\text{B-H}} \Delta t \quad (2.10)$$

The next question is where to position our seeded MBHs at each timestep (i.e. at every output dataset). For this we take two different approaches. In the first case we simply place the MBH at the point of maximum (gas) density in each host halo and keep it there at each timestep, the  $\rho_{\text{max}}$  method. The highest density point is recorded independently of the black holes existence via the halo merger tree, so there is no chance of the black hole moving to a nearby galaxy that contains a more dense region than the original halo. Taking the highest density point as the default position of the MBH is clearly a somewhat optimistic approach in this model. Realistically, however, this method may not be the most optimistic approach, due to feedback effects from

star formation in the dense local environment. This stellar feedback may effectively expel a substantial amount of the gas from the local reservoir, that would otherwise be accreted by the massive black hole still in the dense environment [226]. There is also the matter of feedback from the black hole itself during its accretion cycle, which could also impact the surrounding gas density, thus leading to slight inaccuracies in the accretion calculation, see [227, 228, 229, 230, 231]. Due to the relatively low mass of even the most massive galaxies in **Renaissance** ( $M_{*,max} \sim 5 \times 10^7 M_{\odot}$ ) the central nucleus of the halo will be poorly defined and the central potential relatively shallow. Moreover, the mass of the seed black hole ( $M_{seed} < 10^4 M_{\odot}$ ) does not guarantee that it will sink to the center of the halo. In fact, it has been shown from simulations that MBHs with masses below  $10^4 M_{\odot}$  do not sink to the center within a Hubble time [e.g. 153, 154]. This is therefore the most optimistic and simplest approach and almost certainly not wholly realistic. To counter this we also take a second approach.

The **Renaissance** simulations, like other cosmological N-body simulations, consist of dark matter particles which make up the host halos of galaxies. To gain a more realistic view of the accretion onto the MBH, we also use the nearest dark matter particle to the highest density point of the halo, at the time of seeding, as a MBH proxy (the  $DM_{proxy}$  method). We then track this particle, via its unique particle ID as it travels within the central regions of the galaxy. In this way we use the DM particle and in particular its dynamics to create a more realistic position for the MBH seed. An example for the positions of the black holes, corresponding to each accretion method is shown in Figure 2.1.

Over all of our  $DM_{proxy}$  positions and  $\rho_{max}$  positions the median distance from both the  $DM_{proxy}$  and  $\rho_{max}$  positions to the DM centre of mass, as calculated by Rockstar, is approximately  $10^2$  pc. The seeding using both methods is therefore initially consistent

with the centre of mass approach, as used by many subgrid approximations.

Finally, due to the fact that we post-process the accretion rates via the *Renaissance* snapshot data, we assume that the accretion is constant between snapshots. In reality, due to the clumpy nature of the galaxy, the black hole will experience irregular periods of accretion. Our methodology therefore cannot account for the likely episodic nature of accretion between snapshots and is instead a time-averaged rate. The interval between snapshots is  $\Delta z = 0.1$ .

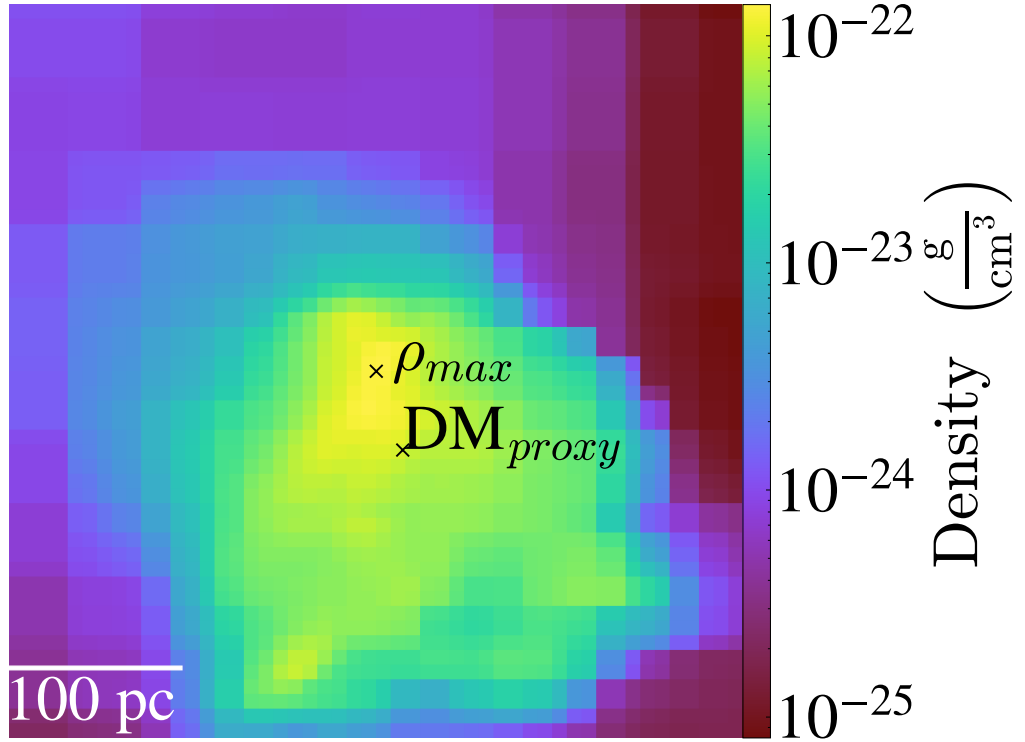


Figure 2.1: An example of the two methods by which the accretion onto the black holes are calculated.  $\rho_{max}$  represents the position of highest density in the halo, the most optimistic case for the accretion. While  $\text{DM}_{proxy}$  represents the position of the black hole proxy particle (a dark matter particle from the simulation), a more realistic situation for the black hole, taking into account the wandering nature of a black hole around its host halo. The stellar mass of this halo is  $7 \times 10^5 M_{\odot}$ . The MBH in this galaxy is of the order of  $10^5 M_{\odot}$ , using the overmassive [123] relationship.

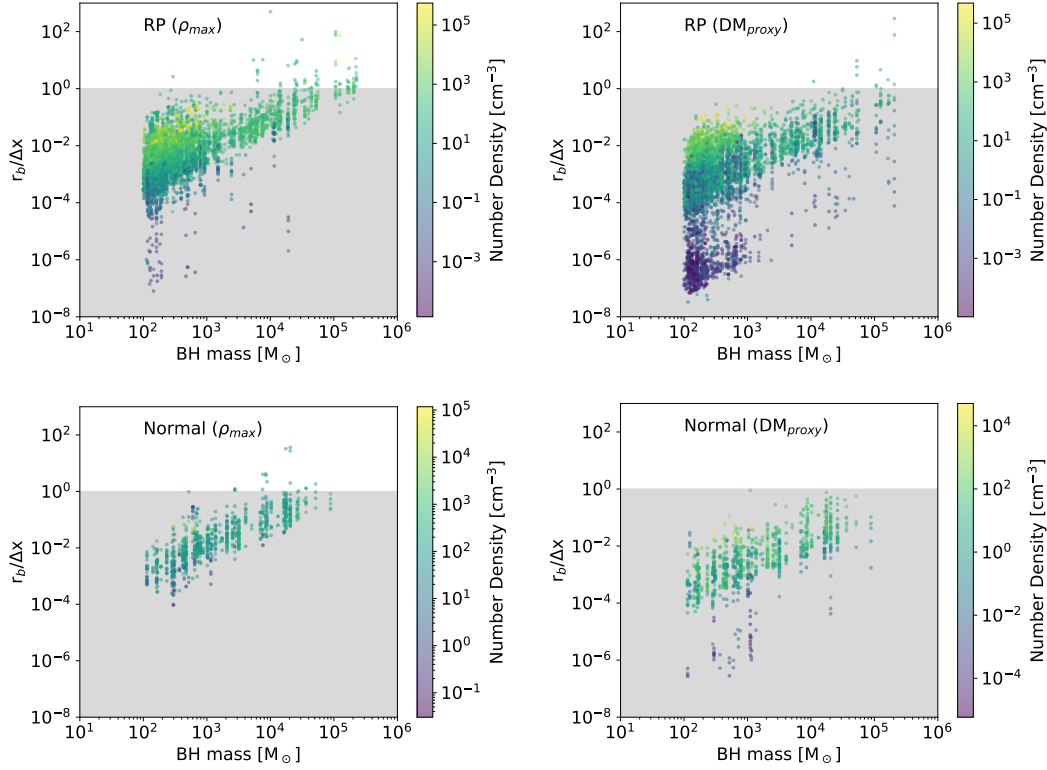


Figure 2.2: The population of Massive Black Holes showing the ratio between the Bondi radius,  $r_b$ , and the cell length,  $\Delta x$ , for the two black hole positions, for each region from **Renaissance**. The masses for the black holes are from P23. Using the RV15 method would only make the Bondi radii less resolved, thus further requiring the boost factor for the accretion calculation. The colorbar represents the number density of gas in the region surrounding the black hole. The grey region represents the black holes where the Bondi radius is unresolved.

### 2.2.5 Boosting the Accretion

As can be seen from eq.2.8, we include a boost factor,  $\alpha$ , to account for the fact that **Renaissance** may underestimate the accretion onto a MBH, in unresolved regions where the cell length is larger than the Bondi radius described by eq.2.9. Only MBHs where the Bondi radius is not resolved are boosted. The population of black holes where the Bondi radius is unresolved/resolved is seen in Figure 2.2. The use of the boost factor was first described in [232], however instead of using a constant value for  $\alpha$ , we let it

depend on parameters relating to the environment around the MBH.

In this case we adopt the prescription from [233], where they use the surrounding number density of gas to calculate the boost factor, more precisely,

$$\alpha = \begin{cases} \left( \frac{n_{\text{H}}}{n_{\text{H}^*}} \right)^\beta & \text{for } n_{\text{H}} > n_{\text{H}^*} \\ 1 & \text{otherwise} \end{cases} \quad (2.11)$$

where the parameter  $\beta = 2$ . While [233] use a critical density of  $n_{\text{H}^*} = 0.1 \text{ cm}^{-3}$ , we adopt the more appropriate value of  $n_{\text{H}^*} = 10^4 \text{ cm}^{-3}$ , for our case where the chemistry is somewhat different and the gas is able to cool to much lower values and hence the density increases. At this density, the  $\text{H}_2$  starts to rapidly increase with density, the chemistry starts to change and gas starts to cool rapidly - a phase change which *Renaissance* largely misses.

We adopt the boost factor implementation only for the  $\text{DM}_{\text{proxy}}$  method for our calculations. The  $\rho_{\text{max}}$  method is already an optimistic case for the accretion onto the black holes and we believe that adding a boost for this model will only make this case even less physically meaningful.

### 2.2.6 Tracking Mergers of Massive Black Holes

To track the MBHs as they merge and grow with time, we need to track the progress of the host dark matter halos. To do this *Rockstar* [196] is used to build a halo catalog which contains information on the growth and merging of halos with decreasing redshift. Consistent-trees was used to make a merger catalog from the Rockstar data [195]. We then analyse the consistent-trees outputs using *ytree* [234]. As a halo merges with another halo we employ two different methods to calculate the merger timescale in the

case where the two haloes contain MBHs. On the one hand we assume instantaneous MBH mergers (which gives the most optimistic merger times) and in the other we assign delays to the MBHs. We now discuss the implementation of delay times in our model.

## 2.2.7 MBH Merger Delay Times

The four stages of black hole mergers are: dynamical friction [79], stellar loss cone [235, 236, 237], circumbinary discs [238, 239] and energy loss due to gravitational wave emission [240]. We can therefore add in a delay time due to an analytical prescription for dynamical friction. We do not calculate the time delays for the final three stages. To do so we would need information on the stellar populations and eccentricity of the black hole binaries. Neither of these quantities are available to us. Since we only calculate the delay due to dynamical friction the time delays we impose should be taken as lower limits.

Despite the clumpy nature of the high redshift galaxies, the dynamical friction from the MBHs passage through the interstellar matter of the host halo can be approximated as an isothermal sphere where the time delay due to the dynamical friction is given by [80, 241]

$$t_{\text{df}} = 0.67 \left( \frac{a}{4 \text{ kpc}} \right)^2 \left( \frac{\sigma}{100 \text{ km s}^{-1}} \right) \left( \frac{10^8 \text{ M}_{\odot}}{M_{\text{BH},2}} \right) \frac{1}{\Lambda} \text{ Gyr} \quad (2.12)$$

where  $a$  represents the initial distance between the two black holes. The stellar velocity dispersion,  $\sigma$ , is given by

$$\sigma = \left( 0.25 \frac{GM_*}{R_{\text{eff}}} \right)^{1/2} \quad (2.13)$$

where  $M_*$  is the stellar mass of the post merger galaxy and  $R_{\text{eff}} = 0.1R_{\text{vir}}$ . Finally, the Coulomb logarithm is defined as

$$\Lambda = \ln\left(1 + \frac{M_*}{M_{\text{BH},2}}\right) \quad (2.14)$$

We also assume that the stellar mass of the halo remains constant as the black holes move through it. In reality and depending on the time scale of the MBH binary merger this may not be the case. Nonetheless, the approximation gives us a sense of the time scale for the binary merger and particularly whether or not we would expect the binary to merge prior to  $z = 0$ .

## 2.3 Results

The premise of this work is to postprocess the data from the *Renaissance* datasets in order to first of all identify heavy seed haloes and then within those haloes to examine the growth of heavy seeds via accretion and mergers. We therefore begin by identifying sites for heavy seed formation.

### 2.3.1 MBH Host Halo Identification

Using the metadata from the Normal and RP regions from *Renaissance*, we are able to search for halos which satisfy the metallicity conditions, inflow rate conditions and compactness conditions. In Figure 2.3 we show the number of halos that satisfy each and all of these conditions. The solid lines in Figure 2.3 are for the RP region, the dashed lines for the Normal region. The strictest condition for the identifying haloes is the mass inflow criteria. This is the criteria which dominates the seeding identification. In

each case only haloes with masses in excess of the atomic cooling limit are considered (condition 1, see §2.2.2). Following this, the metallicity condition ( $Z < 10^{-3} Z_{\odot}$ ) is the easiest condition to satisfy (green line). The next “easiest” condition to satisfy is the compactness condition followed by the inflow rate condition. The black line in each panel gives the total number of haloes satisfying our conditions for heavy seed production at each timestep.

Once a halo is seeded with a black hole, it cannot be seeded again. From Figure 2.3 it is clear that for overdense regions such as the RP region the number of heavy seeds forming is greater overall and that the haloes are also seeded much earlier at  $z \sim 22$ , in contrast to the Normal region which starts seeding at  $z \sim 16$ . Because of the criteria of the halo to reach atomic cooling limit ( $\sim 10^6 M_{\odot}$ ), and the capabilities of **Renaissance** to resolve halos of this mass, we can be assured that **Renaissance** is able to capture the possible halos that are seeding black holes at high redshifts. Out of all the halos identified in the RP region using Rockstar, 371 ( $\sim 4\%$  of atomic cooling halos) are seeded with central MBHs (by  $z = 15$ ). For the Normal region, 53 ( $\sim 1\%$ ) are seeded with central MBHs (by  $z = 11.6$ ). We note that the conditions required for seeding show no signs of slowing down after the cessation of each region, leaving the possibility of additional black holes being formed in these high redshift regimes.

It is clear from Figure 2.3 that the level of isolation that permits black holes from seeding in **Renaissance** plays an important role. We see that an overdense region, such as RP, is able to produce black holes earlier and at an order of magnitude higher at its simulation end time compared to that of the Normal region. In contrast, the Void region, which exists at a higher level of isolation fails to produce any halos capable of seeding heavy seed black holes.

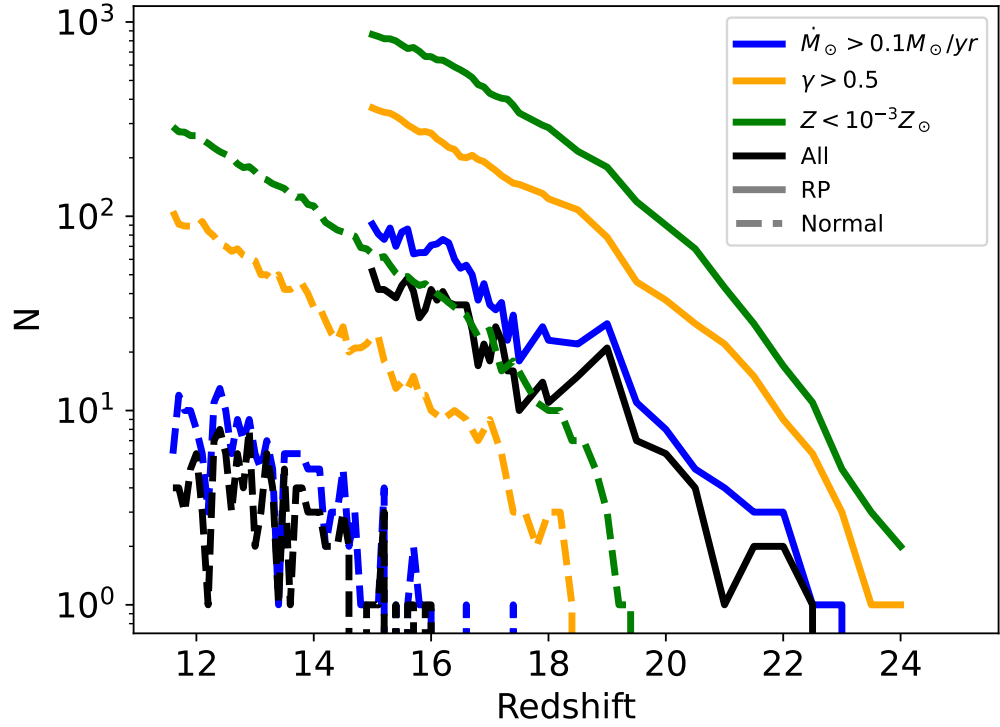


Figure 2.3: The number of halos that satisfy each and all of the conditions for a heavy black hole seed host halo. solid line represents the RP region, while the dashed line represents the Normal region. Once a halo meets all the seeding conditions, the halo is seeded if the corresponding MBH mass is greater than  $10^2 M_{\odot}$ . As we can see from the figure the mass inflow rate criteria is the strictest with the other criteria (metallicity and compactness) only having second order effects.

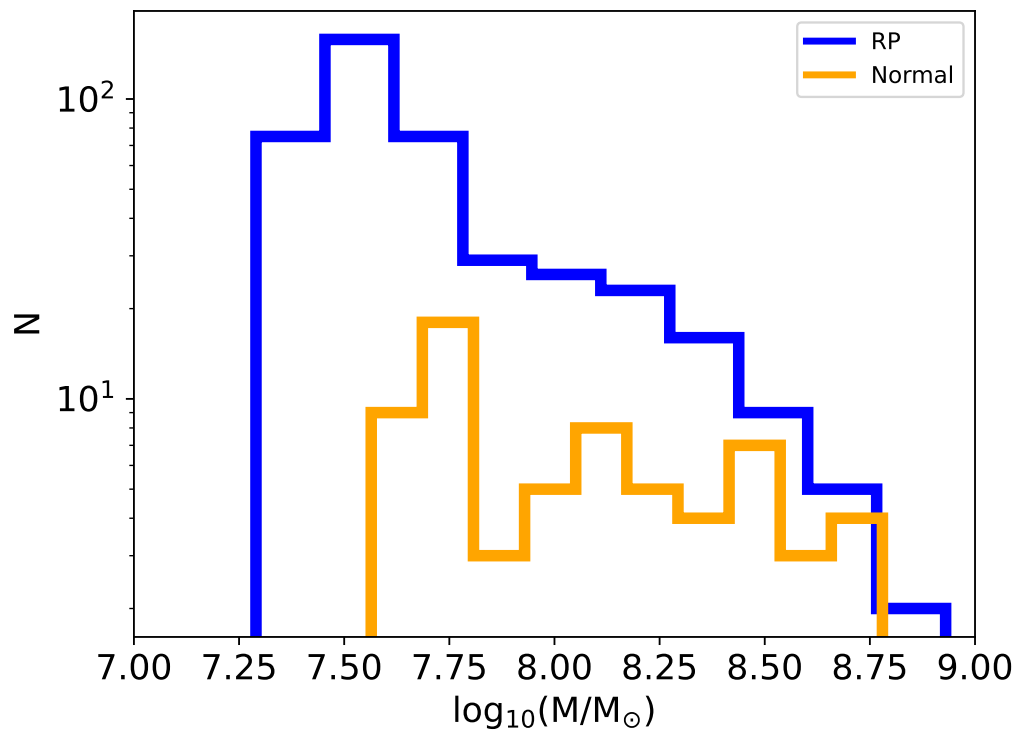


Figure 2.4: Histogram showing the distribution of virial masses of the host halos at the time of their respective black hole seeding.

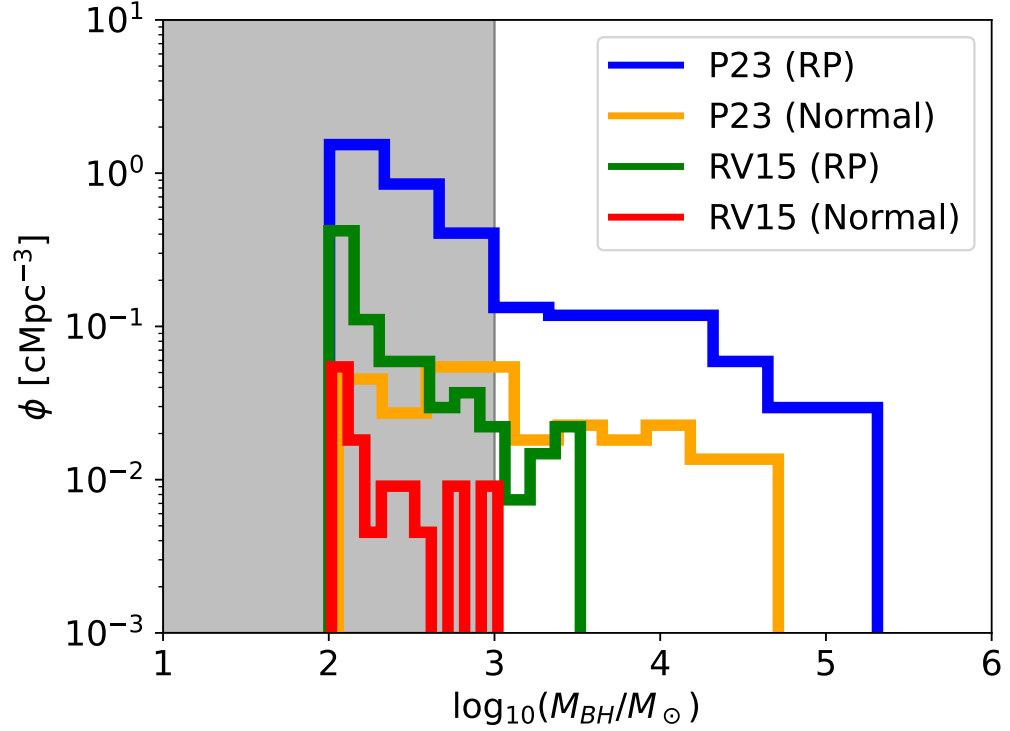


Figure 2.5: Initial Mass Function (IMF) of the MBHs that we seed in post-processing of the *Renaissance* Simulations once all the conditions for seeding in the halo have been met. We show here the IMF for both the Rarepeak region and the Normal region for both  $M_{\text{BH}} - M_*$  scaling relations that we employ, from [223] and [123]. The grey shaded region denote BH masses  $< 10^3 M_\odot$ , ie. light seeds. Everything above  $10^3 M_\odot$  we consider as a heavy seed.

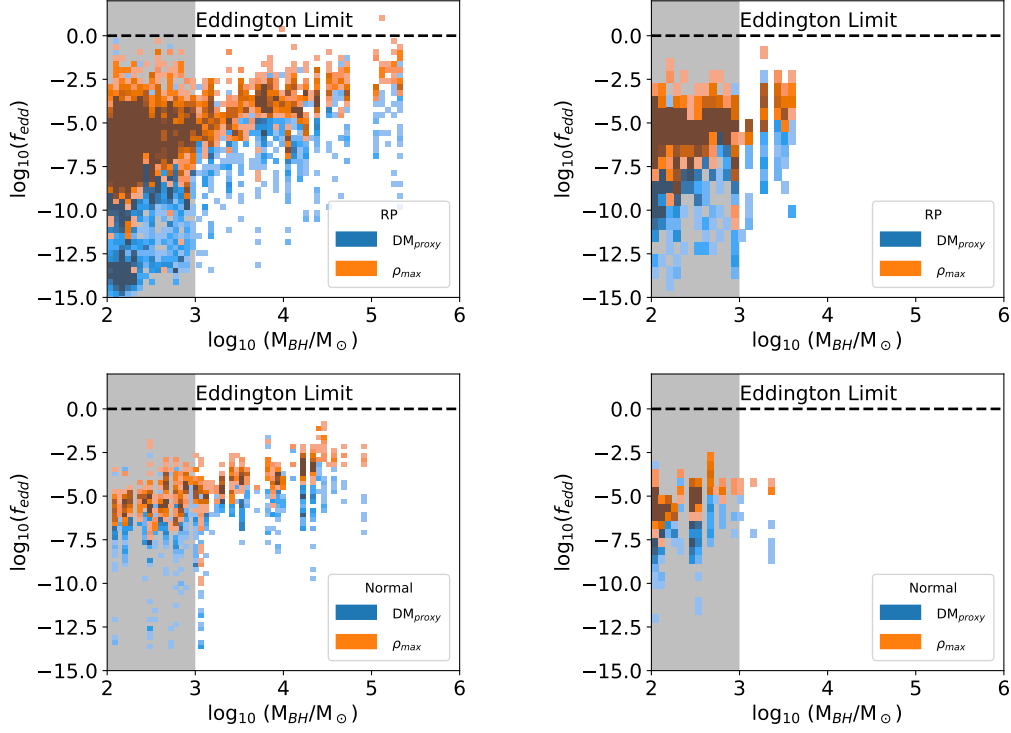


Figure 2.6: 2-D histograms of the Eddington fraction, for the massive black holes that exist in all the redshift snapshots from each region in **Renaissance**, in terms of Eddington fractions of the massive black holes from the Rarepeak region (top) and the Normal region (bottom). The orange represents the accretion values calculated via the  $\rho_{\max}$  method, while the blue represents the accretion via the  $\text{DM}_{\text{proxy}}$  method. The left column represents the black holes that are seeded from the P23 scaling relation, while the right is for the black holes seeded with the RV15 relation. A dashed black line showing the Eddington limit is displayed at the top of each of the figures for reference. The grey shaded regions denote BH masses  $< 10^3 M_{\odot}$ .

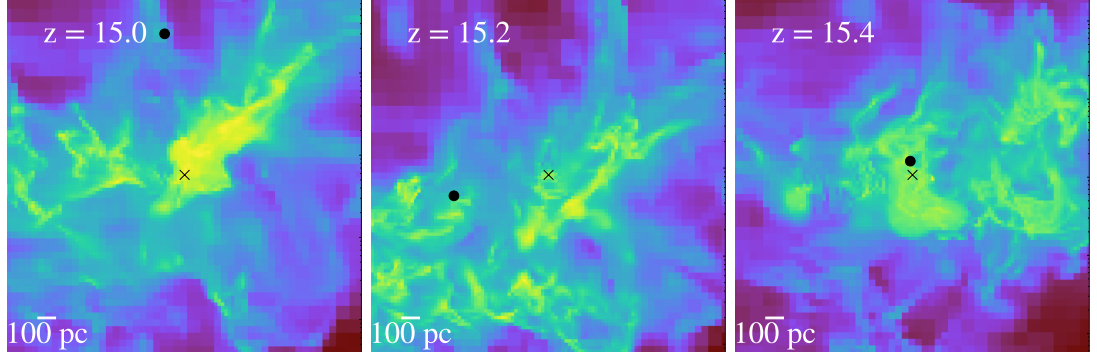


Figure 2.7: A series of examples showing the wandering nature of the  $\text{DM}_{\text{proxy}}$  BH particle. The dot represents the proxy particle while the cross represents the region of highest density in the host halo. This example was taken from the Rarepeak region with the host halo reaching an order of  $2 \times 10^9 M_{\odot}$ .

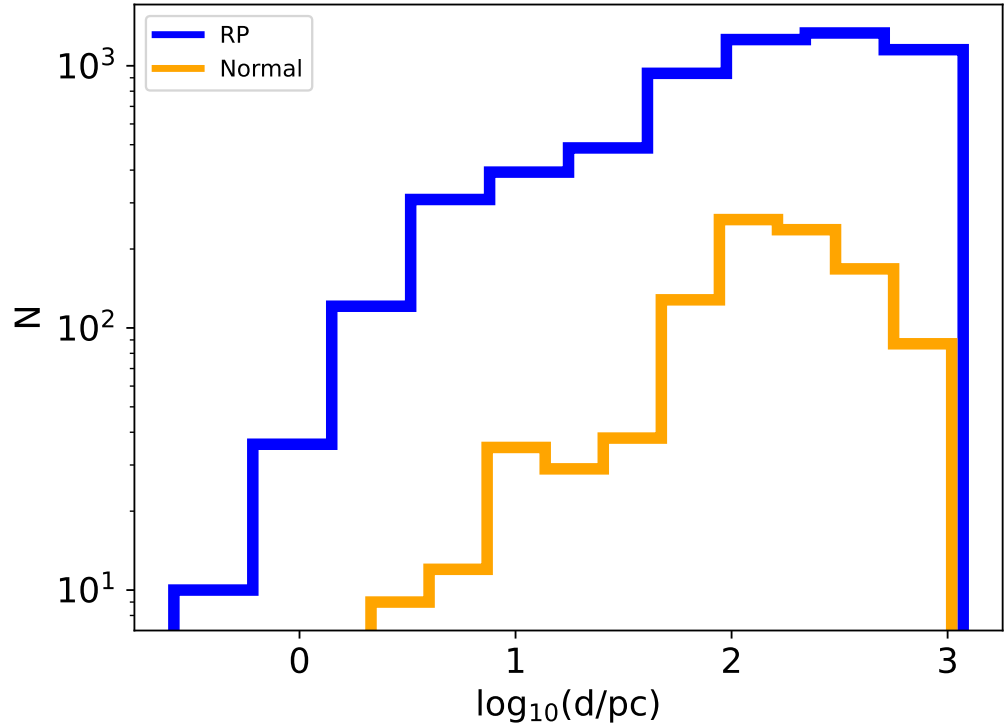


Figure 2.8: Histogram showing the all the distances between the  $\text{DM}_{\text{proxy}}$  particle with its respective  $\rho_{\text{max}}$  position, at all redshifts outputs, for both the RP and Normal region.

### 2.3.2 The MBH Mass Spectrum from Renaissance Galaxies

Once the halos that satisfy the heavy seeding conditions have been identified, the scaling relations, that were discussed in section 2.2.3, are used to assign seed masses to black holes. As discussed, we employ two separate scaling relations, one derived from the high- $z$  “over-massive” black hole population observed primarily by JWST [123] and the other derived from the local MBH-Galaxy Mass relationship [223]. As a result we end up with two (slightly) different black hole populations that we analyse independently. In Figure 2.5 we show the spectrum of initial MBH masses that emerge from employing our scaling relations. After seeding and assigning masses to black holes in halos that meet the heavy seed conditions, we allow them to grow within their environment. The accretion onto each MBH is then calculated using the Bondi-Hoyle formula as described in §2.2.4.

### 2.3.3 The Growth of Heavy Seed MBHs in renaissance

Accretion onto the MBHs is calculated using the analytical Bondi-Hoyle formula (§2.2.4) for two different values for the density,  $\rho$ : one value representing the highest density point of the halo ( $\rho_{max}$ ), and the other value extracted from the position of the dark matter proxy particle ( $DM_{proxy}$ ).

We examine the accretion onto the MBHs by computing the Eddington fraction,  $f_{edd} = \dot{m}/\dot{m}_{edd}$ , for both regions’ (i.e. Rarepeak & Normal) populations. In Figure 2.6 we show 2-D histograms of accretion (as a fraction of the Eddington rate) as a function of black hole mass. The accretion rate shown is the maximum rate across the entire redshift range and hence does not truly reflect the mass growth but instead gives a flavour for the maximum instantaneous growth rates. The top panel shows

the maximum accretion rate from the RP region while the bottom panels show the maximum instantaneous accretion rate from the Normal region. The left column uses MBHs with initial masses assigned from the P23 relationship, the right hand panel shows initial MBH masses assigned from the RV15 relationship. In orange we show the result when the black holes are positioned consistently at the highest density point while in blue we show the results for when the MBHs follow the dynamics due to the initially nearest DM particle.

In all cases the MBH growth increases as a function of MBH mass as expected (since the Bondi-Hoyle accretion prescription depend on  $M_{\text{BH}}^2$ ). Since the P23 relationship gives larger black hole masses as a function of stellar mass we immediately see a greater spread to higher masses in the left hand column. Additionally, allowing the MBHs to consistently sit at the highest density point allows for the most optimistic growth. As a result the most optimistic result is found by looking at the top left panel and focusing on the orange pixels.

This can be contrasted with the bottom right panel and focusing on the blue pixels. In this case the spread of masses is much reduced as we employ the RV15 scaling relationship and hence the masses of our seeds are significantly reduced. The bottom right panel also examines the Normal region where the number of host haloes is also significantly suppressed compared to the Rarepeak region. Finally, the blue pixels also use the  $\text{DM}_{\text{proxy}}$  method and therefore account for the dynamics (via a proxy DM particle). This additionally suppresses the accretion. In this (pessimistic) case seeds are effectively light (i.e.  $10^3 M_{\odot}$ ) and do not grow since the average accretion rates are at least five orders of magnitude below the Eddington rate. This is the case even when the accretion is boosted, due to unresolved gas, from Eqn.2.11

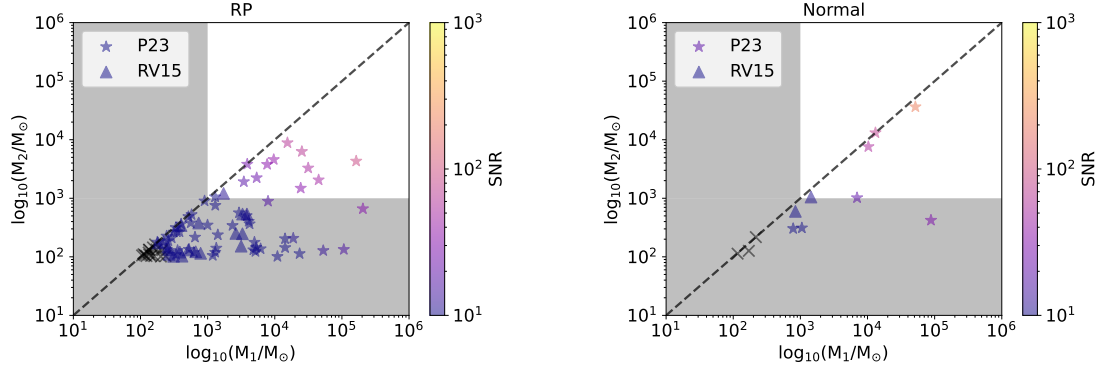


Figure 2.9: The SNR of the mergers, for the no-delay scenario, found in the **Renaissance** simulations, with the SNR of the mergers calculated from [242]. Due to the lack of growth for the black holes, the  $\rho_{max}$  methods and the  $DM_{proxy}$  methods are included in the same markers. The black crosses represent the mergers where the SNR could not be calculated and the black dashed line represents the case where the mass ratio between the two merging black holes is 1. The grey shaded regions denote BH masses  $< 10^3 M_{\odot}$ .

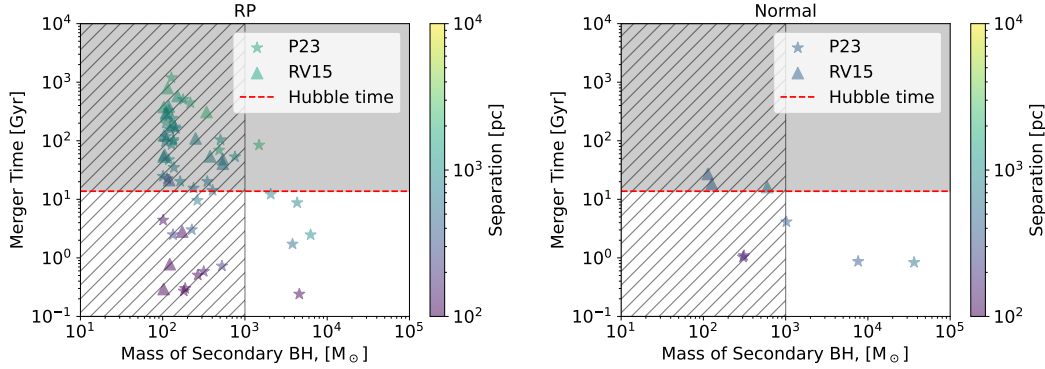


Figure 2.10: The merger times of the black holes from **Renaissance** with the effects of dynamical friction taken into account. The separation is the recorded distance between the two black holes in the snapshot before host galaxies have merged and is measured in proper units. As in Figure 2.9, due to the lack of growth for the MBHs, the  $\rho_{max}$  methods and the  $DM_{proxy}$  methods are included in the same markers. The grey shaded region denotes mergers that would not be detected due to the fact that they would not have occurred yet. The hatched regions denote BH masses  $< 10^3 M_{\odot}$ . The region of interest, or at least the region of detectability with LISA, is then the bottom right quadrant.

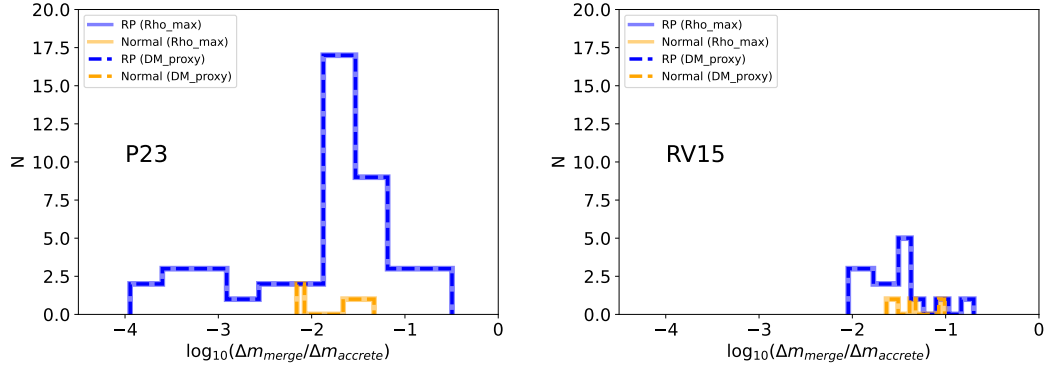


Figure 2.11: Fraction of MBH growth from mergers compared to growth from accretion for the two regions (RP and Normal). The ratio scale is displayed broadly here to emphasise the point that there is negligible difference between the two regions when it comes to the amount of matter accreted onto the black holes compared to the amount of matter gained from merging. It is noted that the lines for the  $\rho_{\max}$  and the  $DM_{\text{proxy}}$  method are indistinguishable here.

### 2.3.4 Growth Through Mergers

In order to examine the growth of MBH via mergers, we investigate two scenarios for Binary Black Hole (BBH) mergers. In the first case we have the naive situation of the MBH binaries merging immediately after the host halos merge, in the second, more realistic case, we account for delay times to the actual merger.

We begin by computing the Signal-to-Noise Ratio (SNR) of gravitational wave signals from BBHs which merge instantaneously. In this case the binaries are merged instantly once the host haloes merge. We compute the SNR expected by LISA using the prescription given in [242]. For the SNR calculation we use the masses of the primary and secondary MBHs as well as the redshift that they merge at (without delays). In our model the black holes are also spinless. Adding spin would change our results by a small but not significant amount, [242] state that the SNR would only change by at most a factor of 2 with spin. In Figure 2.9 we show the SNR for all of the merging black holes computed in our analysis. In the left panel we show the MBH mergers for

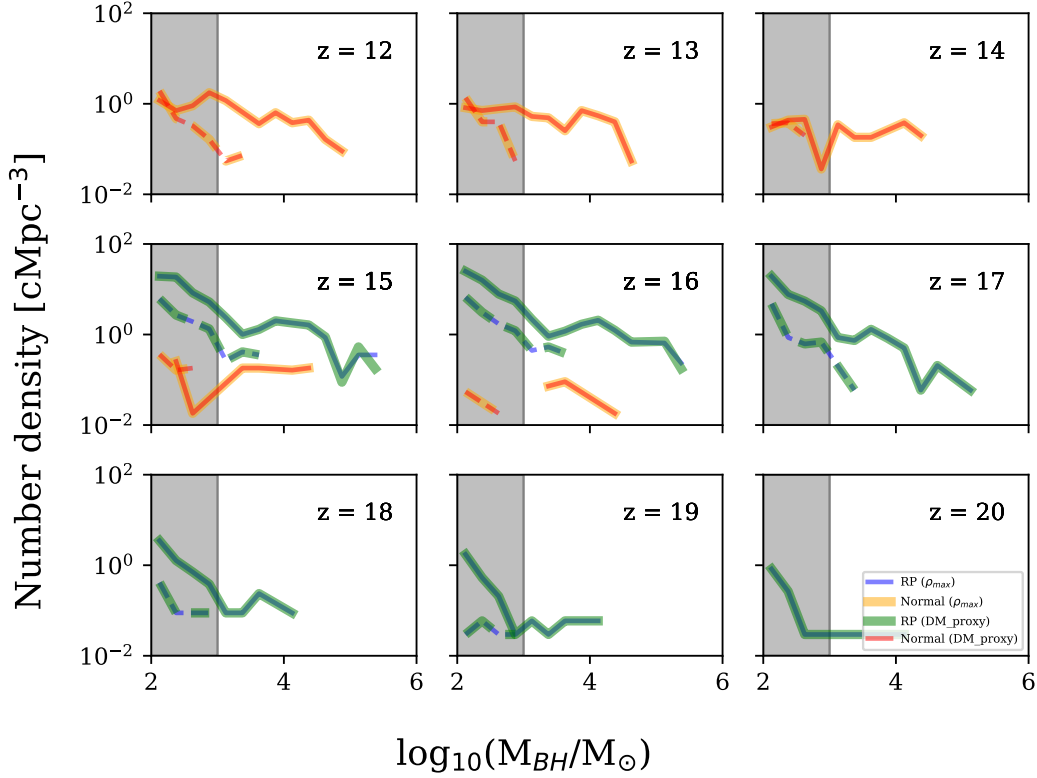


Figure 2.12: The MBH populations number densities as a function of mass for different redshifts. The solid lines represent the black holes that were seeded with masses derived from P23, and the dashed lines from RV15. The masses here are the result of the growth calculated from the accretion onto the black hole and through merger events with neighbouring halo. It is clear here that a black hole population becomes established earlier in the higher density Rarepeak region compared to the average density region represented by the Normal region. As the population grows the number density follows a power law with the mass dependence. The Rarepeak simulations finish at  $z = 15$  which is why there is an absence of black hole population at lower redshift. The grey shaded regions denote BH masses  $< 10^3 M_\odot$ . It is noted that the lines for both accretion methods, in each region, tend to overlap causing a change in the colour of the line compared to the legend.

the Rarepeak region while in the right panel we show the results for the Normal region. The Rarepeak being a more clustered region experiences many more halo mergers and hosts more, by number, MBHs. Hence the number of mergers in the Rarepeak regions vastly exceeds those in the Normal region as expected. On top of this the different prescriptions we employ for the MBH seed masses as well as their growth patterns enters.

We can see from Figure 2.9 that the low mass black holes, from  $10^2 - 10^4 M_{\odot}$ , produce the lowest SNR values as expected and will be extremely challenging to detect with LISA but may be detectable with the Einstein Telescope [128]. Black crosses in each panel represent SNR values too small to be reliably calculated. As the MBH masses prior to merger increase, the SNR values increase too. For mergers where both MBH masses are close to or above  $10^4 M_{\odot}$ , the signal becomes strong enough that it presents the opportunity for these black holes to be candidates for LISA to detect with SNR values reaching upwards of 100. However, even in the case where the SNR values are high ( $\text{SNR} > 100$ ) the errors on the luminosity distance will nonetheless present a significant challenge to host galaxy identification and ultimately a strong uncertainty on the masses [243, 244].

Having analysed the SNR from the instantaneous merger case we now move onto determining the merger timescales for a more realistic case i.e. where the MBHs take some additional time to merge following the host halo merger. Using the equations described in §2.2.7 we compute the delay times for the MBH mergers, for MBHs seeded with both scaling relations and both growth methods, and display them in Figure 2.10. As before the Rarepeak region is displayed in the left panel with the Normal region in the right panel, for all the growth models we calculated in this analysis. On the x-axis we show the mass of the secondary black hole and on the y-axis the merger time. Each merger candidate is coloured by the initial separation.

What we see from Figure 2.10 is that almost half of the mergers have delay times exceeding the Hubble time particularly for the lower mass end of the MBH mass spectrum. There is also a very clear function of separation in determining the merger timescales. The initial separation between the black holes is calculated by taking the minimum of the distance between the black holes in the snapshot before the host halos are considered merged and the radius of the merged halo. For the higher MBH masses which are involved in a merger (i.e. those with masses in excess of at least  $10^3 M_\odot$ ) we see that dynamical friction can drag these MBH to coalescence in less than a Hubble time and with delay times at low as 100 Myr. Our calculations also show a number of light seeds with masses less than  $10^3 M_\odot$  with delay times less than a Hubble time. These lighter seed mergers have short delay times because of the small separations that exist between them just after the galactic merger. It must be noted that the delay time here is based on the parameters and structure of the halo at the time of merger. As the halo evolves through cosmic time it will grow and change in structure, thus affecting the delay time for the mergers.

We end by stressing that BH growth is however primarily driven by accretion rather than mergers. In Figure 2.11 we show the fraction of growth coming from mergers relative to accretion. For both MBHs in the Rarepeak (blue) and Normal regions (yellow) the growth from accretion surpasses the growth from mergers by several orders of magnitude.

However, even though mergers account for approximately 1% of the MBH growth they crucially allow us to probe the MBH population demographics and potentially the seeding mechanisms [245, 246]. As such it is worth calculating both the number of MBH mergers as well as their potential detectability with LISA [247, 248]. Moreover, the growth via accretion prior to mergers allows for higher SNR values within the LISA

band.

We also note that as the host halos grow through mergers with smaller halos, there is an increase in the Star Formation Rate in the halo, as shown in [191]. Provided that the halo is massive enough to overcome the effects of stellar feedback, the amount of gas accretion onto the halo also increases. The replenishing of this gas reservoir provides an opportunity for the massive black hole that a halo could host, to gain a boost in the accretion from this gas.

### 2.3.5 The Number Density of Heavy Seed MBHs

Finally, having accounted for the initial masses of the heavy seeds, the growth of the black holes via both accretion and mergers we can now calculate the number density of heavy seed MBHs as a function of black hole mass and redshift. In Figure 2.12 we show the number densities of heavy seed MBH. In each panel solid lines represent MBH masses derived from the “over-massive” scaling relations from P23 while the dashed lines are derived using the scaling relations from RV15. The blue and green lines are from the Rarepeak region, while the red and yellow lines from the Normal region. Overall, there is little difference between the number densities of the  $\rho_{\text{max}}$  method and the  $\text{DM}_{\text{proxy}}$  method so there is considerable overlap between the respective lines. The solid lines (being the more optimistic values for the masses) extend to higher masses while the dashed lines (being the more pessimistic values for the masses) extend to less than  $\sim 10^4 M_{\odot}$  in most galaxies simply because our galaxy masses are small.

If we consider the  $z = 15$  panel (which is the final output from the Rarepeak region and there is also a substantial contribution in the Normal region) we see that even for MBH masses of approximately  $10^4 M_{\odot}$ , number densities are as high as  $1 \text{ cMpc}^{-3}$  for

the Rarepeak region and as high as  $10^{-1}\text{cMpc}^{-3}$  for the Normal region. These number densities while admittedly somewhat optimistic as they are derived from the “over-massive” relationship show that if heavy seeds can form at high- $z$  in haloes matching conditions similar to what we prescribe then they can easily explain the abundances of AGN currently being detected by JWST [249, 250, 251]. Moreover, even the most pessimistic case where early MBHs are not over-massive (see top left panel at  $z = 12$ , dashed line) we still have number densities greater than  $10^{-3}\text{cMpc}^{-3}$  for masses of approximately  $10^4 M_{\odot}$  (extrapolating the dashed line). Again, if we take this value as a lower limit then it would appear that a subset of haloes with conditions conducive to heavy seed formation can still explain the AGN candidates being put forward by JWST observations - albeit somewhat more marginally [251].

Taking our predictions at face value our calculations predict number densities for MBHs with masses of approximately  $10^4 M_{\odot}$  from  $10^{-2} \text{ cMpc}^{-3}$  up to  $1 \text{ cMpc}^{-3}$  at  $z = 15$ . Our ability to predict number densities at lower redshifts is hampered by our underlying simulation suite which does not provide statistics for us at significantly lower redshifts. However, if we take the outputs at  $z = 12$  from the Normal region and again assume an over-massive population then the number densities hold and we predict number densities for MBHs with masses of approximately  $10^4 M_{\odot}$  again up to  $1 \text{ cMpc}^{-3}$  at  $z = 12$ . The number densities for more massive objects (as is being detected as high- $z$  AGN by JWST) will be lower by a couple of orders of magnitude but this nonetheless fits well with current AGN candidate estimates [249, 250, 251].

### 2.3.6 Comparing our Number Density Rates to the Existing Literature

Calculating the number density of MBHs in the high- $z$  Universe is a hugely important goal in modern astrophysics. The number density itself is a key parameter in further calculating the active fraction of MBHs in galaxies [e.g. 252] and in calculations of merger rates of MBHs potentially detectable by the next generation of space based gravitational wave observatories [247].

Over the last two decades many studies have attempted to calculate the overall number density values as a function of redshift as we have done here. The initial calculations from the early part of the last decade came from [253] and [254]. Their calculation were primarily driven by assuming that MBHs form in haloes subject to a supercritical Lyman-Werner(LW) flux. Depending on the strength of the flux assumed the values calculated by both authors are between approximately  $10^{-10}$  to  $10^{-6}$   $\text{cMpc}^{-3}$  at  $z \sim 10$  and so many orders of magnitude more pessimistic than the values found here (see Figure 2.12).

Higher values for the expected number density of MBHs can be obtained by reducing the value of the super-critical flux required. The values quoted previously are for  $J_{\text{crit}} = 300 J_{21}^2$  but by lowering the threshold to  $J_{\text{crit}} = 30 J_{21}$  values aligning closer to the values obtained in this study. However, the majority of research in the literature suggests that the higher threshold of  $J_{\text{crit}} = 300 J_{21}$  (or even higher is required) [255, 256, 257, 258, 259, 260].

[261] similarly found that number densities of order  $10^{-6}$   $\text{cMpc}^{-3}$  at  $z \sim 10$  result from a threshold  $J_{\text{crit}} = 300$  when analysing output from several cosmological hydrodynamical simulations that cover a large range of box sizes and resolutions. Lessening the

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<sup>2</sup>where  $J_{21}$  is in units of  $10^{-21} \text{erg cm}^{-2} \text{ Hz}^{-1} \text{ s}^{-1} \text{ str}^{-1}$

metallicity constraint to incorporate metal-poor rather than metal-free haloes improves the number densities somewhat [262, 263, 264] bringing number density values up to approximately  $10^{-4} \text{ cMpc}^{-3}$  at  $z \sim 10$  [265, 183, 266, 267].

However, such models are always somewhat sensitive to the parameters used to analyse the data as no model can yet follow, in a cosmological context, the formation of MBH seeds self-consistently. Some models therefore predict somewhat higher number densities even for the LW pathway [e.g. 268] but the consensus of the bulk of the literature appears to suggest number densities of approximately  $10^{-6} \text{ cMpc}^{-3}$  to  $10^{-4} \text{ cMpc}^{-3}$  at  $z \sim 10$  for reasonable values of  $J_{\text{crit}}$  (i.e.  $J_{\text{crit}} > 300 J_{21}$ ).

The values we find, through appealing to the so-called ‘rapid assembly model’ [e.g. 218, 181], are at least two to three orders of magnitude higher than the more optimistic LW channel results (and in fact are closer to some semi-analytic models based on very efficient growth of light seeds [e.g. 266, 267]). As discussed in §XYZ our values are founded on the rapid growth of the host halo predominantly following on from the results of [181]. A comparable study by [183] used a semi-analytical treatment on top of n-body only calculations of a quasar progenitor environment to calculate number densities in a similar way. [183] found number density values of approximately  $0.1 \text{ cMpc}^{-3}$  at  $z \sim 10$  (after accounting for the impact of their overdense realisation). This value compares extremely well to our estimate (see again Figure 2.12).

In general terms a heavy seed model relying solely on the influence of a LW background will struggle to meet the number density demands currently being set by JWST [e.g. 249, 251]. Our methodology, based primarily on rapid halo growth, achieves rates that match and exceed those required by current observations with number densities reaching well above  $10^{-2} \text{ cMpc}^{-3}$  at  $z \sim 10$  (for MBHs with masses of approximately  $10^4 M_{\odot}$ ).

### 2.3.7 LISA Event Rates from Mergers of Heavy Seed Massive Black Holes

Using the mergers that are predicted at high-redshift with *Renaissance*, we are able to make an estimation for the merger rate of these MBHs that will then be observed during LISA’s 4–10 year lifespan. We calculate the merger rate using the following formula:

$$\frac{dN}{dzdt_{\text{obs}}} = 4\pi cr_c^2 \frac{dN}{dzdV} \quad (2.15)$$

where  $r_c$  is the comoving distance to the merger events and  $dN/dz dV$  is the number density of mergers per redshift and per comoving volume [269, 270, 241]. We compute the merger rate for both the instant mergers (after the merging of the host galaxies) and the mergers that are time delayed due to the effects of dynamical friction. We show the merger rate calculation in Figure 2.13.

It must be noted that the merger rate appears to decrease for the time delayed case because the Normal region does not simulate past  $z = 11.6$ , and therefore the mergers of any MBHs after this time are not simulated. Using Figure 2.13, we can see that in the proposed 10 year lifetime, LISA should expect to see around  $\sim 80$  mergers, using the predictions from the Normal region. With the RP predictions we expect to see around  $10^2 - 10^3$  mergers in LISA’s lifetime. With the addition of dynamical friction into the merger model we can expect to see signals from binaries formed in the early Universe, merging at redshifts closer to the local Universe.

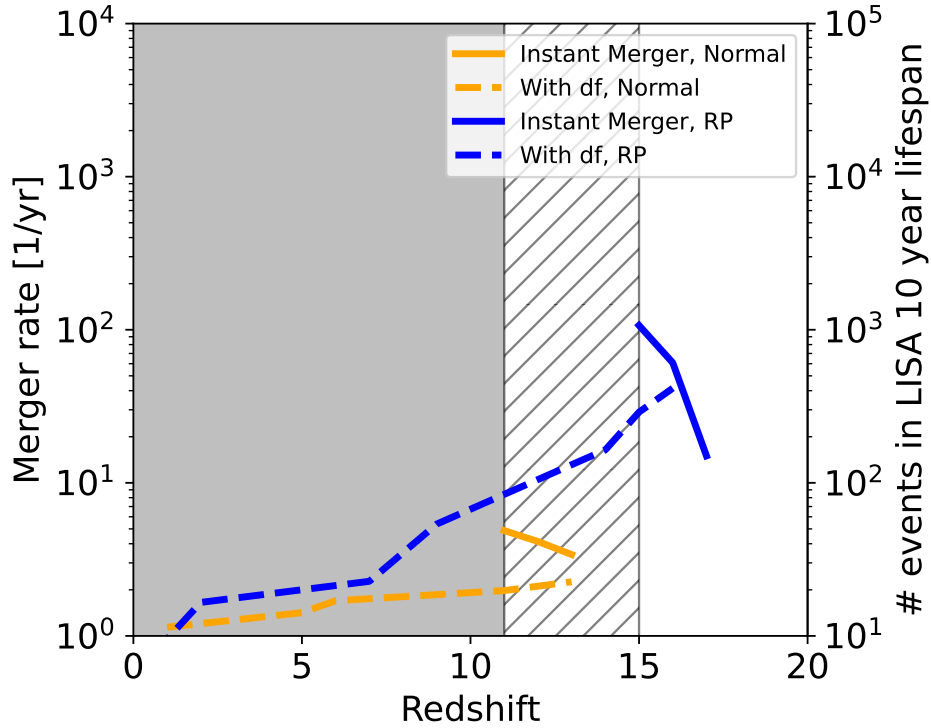


Figure 2.13: The merger rate of the massive black holes from *Renaissance*, for both the instant mergers and the mergers with time delay due to dynamical friction. The hatched dashed region denotes the redshift regime where the Rarepeak model not run, whilst the solid grey region denotes where both the RP and Normal region are unable to simulate. In the lifetime of LISA ( $\sim 10$  yrs) we should expect to see  $\sim 80$  mergers from MBH binaries using the results from the Normal region.

### 2.3.8 Detection of High-z Black Holes and Comparison with Other Semi-analytical Models

The high redshift nature of the black holes modelled in this analysis makes them difficult to detect using current observation techniques. While JWST is continuing to make measurements of high- $z$  AGN, the extreme nature of these active black holes are potentially causing a bias in the predicted mass spectrum of MBHs in the early Universe [271]. The low accretion values of our black holes will lead to low bolometric luminosity and thus the need for other detection techniques becomes greater. With the future gravitational wave detector LISA due to be launched in the 2030's, it will present us with the opportunity to detect gravitational wave signatures from merging black holes like the ones modelled here. The ESA led space-based gravitational wave detector is designed to detect mergers from black holes in the intermediate mass range, up to and at very high redshifts ( $z > 15$ ). LISA will not be alone in the search for higher mass black hole binaries, the Chinese led missions Taiji [272] and Tianqin [273] will operate with the same principles as LISA, while the ground based Einstein telescope [274] and Cosmic Explorer [275] will join the search for black hole mergers up to the cosmic dark ages.

Other semi-analytical and simulation models have explored the extent to which GW observatories will explore the the high- $z$  population of massive black holes [e.g. 276, 277, 278, 279]. The general consensus is that if we are able to constrain the parameters from black hole mergers and analyse a merger rate (whose predicted values range from  $10^1 - 10^3 \text{yr}^{-1}$  with LISA) using the synergy of various gravitational wave detectors, we should be able to constrain the massive black hole formation models which dominate the early Universe.

## 2.4 Summary & Conclusions

In this chapter, we set out to study the halo environments potentially conducive to heavy seeds formation in the early Universe via post-processed modelling in the **Renaissance** simulations. In order for a halo to host a heavy seed, it would need to satisfy four criteria: (i) reaching a mass needed for atomic cooling, (ii) a high inflow rate ( $\dot{M} > 0.1 M_{\odot} \text{ yr}^{-1}$ ), (iii) low metallicity ( $Z < 10^{-3} Z_{\odot}$ ) and (iv) compactness. In effect we find that the high mass inflow rate is the strictest criteria with the other criteria more easily attained. Because the final redshifts of each region are quite high, they don't fully capture the end of massive black hole formation, as can be seen in fig.2.3, therefore we are underestimating the mergers that will happen after the end times of **Renaissance**. Nonetheless it is important to include these mergers in our black hole formation models as they will contribute to the signal that LISA will detect.

Once the host haloes are identified, we assign masses to the black holes in one of two ways. On the one hand we assign MBH masses from a local relationship between galaxy masses and black holes masses from RV15 and on the other hand we utilise a more recent relationship specific to high- $z$  MBH obtained from JWST data (P23). The latter relationship predicts that high- $z$  black holes are “over-massive” with respect to their host galaxy. Following seeding, the black holes were then allowed to grow, both via accretion and mergers with each other. We based the accretion formalism on the Bondi-Hoyle-Lyttleton model and calculate the actual accretion rate using parameters obtained from the underlying **Renaissance** simulations. For the accretion we investigated two models, one where the MBHs are effectively pinned to the highest density point,  $\rho_{max}$ , and secondly where the MBH moves within the gravitational potential of the host galaxy. Because the accretion methods are applied to snapshots in

*Renaissance*, they are instantaneous values and may not accurately track the growth of black holes over the simulation time. Therefore, we may be over or under-predicting the final simulated masses of the MBH population. However, the predicted observed luminosity will not be affected by these calculations.

Finally, MBH mergers are also included in our analysis both from the point of view of growth but also from the point of view of observability with future gravitational wave observatories. For analysing MBH mergers we again consider two scenarios. In the naive case we assume that the BBHs merge instantly as part of the host halo merger and secondly we consider the case where the black holes must coalesce via dynamical friction. The latter case can, in some instances, result in significant delay times between the host galaxy merger and the BBH merger. Our main conclusions are:

1. Using a heavy seed model for populating dark matter haloes we find that the number density of MBHs from this channel can be as high as  $1 \text{ cMpc}^{-3}$  at  $z \sim 10 - 15$  in the most optimistic case. In a more pessimistic scenario this value can drop by three orders of magnitude, for masses in the range of  $10^2 - 10^4 M_{\odot}$ . However, even at this lower level of  $10^{-2} \text{ cMpc}^{-3}$  at  $z \sim 10 - 15$  a heavy seed model can still explain the number of AGN candidates currently being detected by JWST. Moreover, what this tells us is that host galaxy environments with high inflow rates, low metallicity and high compactness exist in sufficient numbers to explain the JWST candidate AGN.
2. MBH growth following seeding is in general sub-Eddington. Only the most massive MBHs ( $M_{\text{MBH}} \sim 10^{4-5} M_{\odot}$ ) can grow at values approaching the Eddington rate. This also only occurs for those MBHs which are pinned to the highest density regions. MBHs which undergo (random) motions around the galactic nucleus

show strongly suppressed growth.

3. MBH growth comes primarily, by several orders of magnitude, from gas accretion rather than MBH mergers.
4. MBH mergers are in principle observable with LISA for primary black hole masses in excess of  $10^4 M_\odot$  and secondary black hole masses in excess of  $10^3 M_\odot$ . In these cases SNR values in excess of 100 are viable with delay times (assuming they are shorter than the age of the Universe) increasing the SNR values and potentially also easing difficulties with host galaxy detection by overcoming the gravitational wave background noise that may exist at corresponding frequencies.
5. We calculate LISA event rates of both the Normal and Rarepeak regions and find that the high redshift regime will provide numerous candidates for LISA detection in its proposed 10 year lifespan, with  $\sim 80$  mergers expected to be observed using the merger predictions from the Normal region (with  $\sim 10^3$  mergers predicted from the RP region). If LISA is able to detect the signals from these mergers, we will be able to further constrain the formation processes of the black hole populations at this epoch.

# Chapter 3

## Using Renaissance to validate the existence of High- $z$ galaxies

### 3.1 Introduction

With the launch, and now the first observations with JWST, the high-redshift Universe is being unveiled with unprecedented detail for the first time. As exquisitely detailed measurements of distant early galaxies are now within the range of observations, it allows for the opportunity to compare the results of these observations against high resolution simulations of early galaxy formation which was previously intractable.

The JWST Advanced Deep Extragalactic Survey (JADES) [280] has provided measurements on five galaxies with spectroscopically confirmed redshifts at  $z > 10$ . Three of these galaxies are the most distant yet detected. [108], [109] and [281] have constrained physical properties of these five galaxies, finding that the galaxies lie at (mean) spectroscopic redshifts of  $z = 10.38$  (GS-z10-0),  $z = 11.58$  (GS-z11-0),  $z = 12.63$  (GS-z12-0),  $z = 13.20$  (GS-z13-0) and  $z = 10.60$  (GN-z11). Additionally the CEERS project [282]

has also provided measurements for Maisie’s galaxy which has a redshift of 11.44 [283]. In total there are six spectroscopically confirmed galaxies against which we can directly compare.

The JADES survey, performed using the NIRCam instrument on JWST, targets a region, previously studied by the Hubble Space Telescope [284], in nine different wavelength bands. JADES was conducted with the aim of detecting faint galaxies using the dropout-technique [280]. The dropout technique involves observing an object in different wavelength filters. Hydrogen surrounding the galaxy will absorb any light at a threshold wavelength, which is subject to cosmological redshift. Any wavelengths shorter than the threshold wavelength won’t appear in the filtered image, thus allowing for fast identification of high redshift galaxy candidates. However, the photometry alone is not enough to confirm the candidates’ redshift and a follow-up spectrum, using an instrument like NIRSpec, is needed to confidently quantify the redshift of the candidates as noted above.

Similar to JADES, CEERS aims to study the first 500 Myr of galaxy evolution again by using a combination of the NIRCam instrument for fast identification followed by a longer duration follow-up using NIRSpec. Initial photometric measurements of Maisie’s galaxy and of CEERS-93316 placed them at photometric redshifts of  $z_{\text{phot}} = 11.08$  [285] and  $z_{\text{phot}} = 16.45$  [286], respectively. Spectroscopic follow-up measurements of these galaxies confirmed their redshifts to be  $z_{\text{spec}} = 11.44$  and  $z_{\text{spec}} = 4.912$  [283], respectively. Due to the decrease in redshift of CEERS-93316 to a much lower redshift, we do not include it in the analysis in this paper and instead only include the high redshift Maisie’s galaxy.

The spectra of the galaxies found in JADES and CEERS were analysed using **Beagle** [112], to estimate the stellar mass and star formation rate of each galaxy which we com-

pare directly against our simulations. More details on the modelling procedure used to reduce the observational data can be found in the detection papers [e.g. 281, 283].

In a recent study [120, hereafter K23] tested the capabilities of a variety of cosmological simulations by investigating whether these simulations were able to reproduce galaxies with properties similar to the galaxies observed in the JADES and CEERS surveys. To do this, K23 utilised the EAGLE [89], Illustris [90], TNG100 [91], RomulusC [92], OBELISK [93] and Simba [94] simulations.

K23 concluded that the cosmological simulations they examined were able to reproduce galaxies with a similar stellar mass and star formation rate (SFR) compared to the galaxies observed in the JADES simulations and that the observed galaxies are consistent with a flat  $\Lambda$ CDM model. In this chapter, we build-on the work of K23 by comparing the JADES and CEERS results against high resolution simulations that were designed to specifically examine a high-redshift environment and to model the early assembly history of the first galaxies. By considering simulation data from both the higher halo mass regime of K23 and the lower halo mass data from this paper, we strengthen the argument that there exists no tension between the measurements of JWST and the  $\Lambda$ CDM model of the Universe.

This study accomplishes this using the *Renaissance* simulation suite [287, 191, 192]. The *Renaissance* simulations model early galaxy formation in three regions which differ from each other by their level of overdensity [see 192, for details]. Using a similar methodology to K23, we compare the results from these simulations to the JADES and CEERS galaxy property estimates, observationally validating our simulation results and also determining the likelihood of such massive galaxies forming early in a  $\Lambda$ CDM cosmology.

There have been significant concerns that the early measurements by JWST are in

conflict with the  $\Lambda$ CDM model of the Universe. In particular, there are claims that the stellar masses of the galaxies observed by JWST are simply too high to be explained in the context of a  $\Lambda$ CDM cosmology [e.g. 288] and that the masses of the JWST galaxies, as measured at redshifts between 7 and 10 by [289] in particular, are testing the upper limits on the available baryonic mass available according to  $\Lambda$ CDM [290]. See also [115], [114], [116], [117], [118], and [119] for more discussion and analysis on the proposed tension between the JWST measurements and  $\Lambda$ CDM.

This chapter addresses these concerns by showing that simulations (based on a  $\Lambda$ CDM cosmology) are able to reproduce galaxies consistent with the early findings of JWST at least at the very highest redshifts explored by it. If the [289] result holds under spectroscopic scrutiny and the galaxies are found to lie in typical regions of a  $\Lambda$ CDM Universe, then, as pointed out by [290], this represents a major challenge to standard cosmology. However, see also [291] which offers an alternative explanation to the large stellar masses found by [289].

The chapter is laid out as follows: §3.2 describes the high-resolution **Renaissance** simulations as well as the methodology and code used to run the suite, §3.3 discusses the results of the analysis performed and in §3.4 we discuss the implications of the results and the case for further analysis of the high redshift Universe using cosmological simulations.

## 3.2 Methodology

### 3.2.1 The Renaissance Simulations

The **Renaissance** simulations [287, 191, 192, 224, 181] were run using the massively parallel adaptive mesh refinement **Enzo** code [95, 96]. We briefly describe the methods

used here, but refer the interested reader to the previous papers listed before for a more complete discussion. The *Renaissance* simulation suite is composed of three zoom-in regions (see Figure 1.7) extracted from a parent comoving volume of 40 Mpc on a side. The three separate zoom-in regions were named the Rarepeak (RP) region, the Normal region and the Void region. The zoom-in volumes ranged from 200 to 430 comoving Mpc<sup>3</sup>.

The RP region is centred on a  $3 \times 10^{10} M_{\odot}$  halo at  $z = 6$  with an enclosing comoving volume of  $(3.8 \times 5.4 \times 6.6) \text{ Mpc}^3$ . The Normal and Void volumes have comoving volumes of  $(6.0 \times 6.0 \times 6.125) \text{ Mpc}^3$ . All three regions have projected areas comparable to the NIRCам field of view with the RP, Normal, and Void regions respectively subtending  $(1.2' \times 1.8' \times 2.2')$  at  $z = 15$ ,  $(2.1' \times 2.1' \times 2.1')$  at  $z = 11.6$ ,  $(2.2' \times 2.2' \times 2.3')$  at  $z = 8$ . The *Renaissance* suite uses the cosmological parameters from the 7-year WMAP  $\Lambda\text{CDM}+\text{SZ}+\text{LENS}$  best fit [292] with  $\Omega_{\text{M}} = 0.266$ ,  $\Omega_{\Lambda} = 0.734$ ,  $\Omega_{\text{b}} = 0.0449$ ,  $h = 0.71$ ,  $\sigma_8 = 0.81$  and  $n = 0.963$ . The (dark matter) particle mass resolution of the *Renaissance* suite is  $2.9 \times 10^4 M_{\odot}$  and the maximum spatial resolution afforded by the adaptive mesh is 19 comoving pc. This allows the *Renaissance* suite to resolve most of the minihaloes in which the first stars are expected to form [e.g. 293, 294, 268].

In particular, *Renaissance* employs a model for metal-free (Population III) and metal-poor (Population II) star formation [295, 296] allowing for the stochastic sampling of the formation of the first stars and galaxies, inspired by star formation simulations and observations rather than their galactic counterparts because they resolve individual star-forming clouds. Under the assumption that metal-enriched star formation is insensitive to redshift, [296] used an efficiency of 7 per cent of the cold gas within a dense cloud being converted into Population II star particles, similar to what

was found in present-day star formation simulations [297], which were themselves consistent with observations [298] at the time of the method’s formulation. The stellar feedback is modelled via adaptive ray tracing of  $\text{H}_2$  ionising radiation,  $\text{H}_2$  dissociating Lyman Werner radiation and feedback from supernova which enriches the surrounding environment with metals. There is no AGN feedback modelled in **Renaissance**. They calibrated the feedback models against local dwarf galaxy properties, in particular the metallicity distribution function, ensuring that they avoided the “overcooling problem” that overestimates the stellar mass and thus metallicities. The resulting metal enrichment driven from the collapse of the first stars results in the emergence of the second generation of stars which ultimately lead to the birth of the first massive galaxies - the galaxies which JWST is now observing.

The computational complexity of the **Renaissance** suite means that evolving these simulations to the present day is completely intractable. As such the RP simulation was evolved to  $z = 15$ , the Normal simulation evolved to  $z = 11.6$  and the Void region to  $z = 8$ . As some of the JADES and CEERS results are at somewhat lower redshifts (compared to the RP and Normal runs) we extrapolate our results to the JADES and CEERS spectroscopic redshifts in some cases.

As discussed in the Introduction, the comparison study undertaken by K23 uses the simulation datasets from the EAGLE, Illustris, TNG100, RomulusC, OBELISK and Simba simulations. In Table 3.1 we compare the simulation datasets used in K23 versus the one used here (i.e. against **Renaissance**). The simulations used in K23 do not have sufficient resolution to probe the formation of the first stars and can resolve, at best, the formation of the first atomic cooling haloes. The **Renaissance** suite allows us to probe the assembly processes involved in forming the haloes that appear in the simulations used in K23 as well as the building blocks of the galaxies now being observed

Table 3.1: Simulation domain sizes and resolution

| Simulation  | Box size [cMpc] | $M_{\text{DM}}$ [ $M_{\odot}$ ] | $\Delta x_{\text{DM},*}$ [pc] |
|-------------|-----------------|---------------------------------|-------------------------------|
| Simba       | 147.7           | $9.7 \times 10^7$               | 500                           |
| EAGLE       | 100             | $9.7 \times 10^6$               | 2660                          |
| TNG100      | 110.7           | $7.5 \times 10^6$               | 740                           |
| Illustris   | 106.5           | $6.3 \times 10^6$               | 710                           |
| OBELISK     | 142.0           | $1.2 \times 10^6$               | 540                           |
| RomulusC    | 50              | $3.4 \times 10^5$               | 250                           |
| Renaissance | 40              | $2.4 \times 10^4$               | 19                            |

**Notes:** The first column gives the simulation suite name, the second column the comoving box size length of each simulation used in K23, the third column gives the dark matter particle resolution,  $M_{\text{DM}}$ , and finally the fourth column gives the spatial resolution. The spatial resolution was based on the gravitational softening lengths for the SPH simulations and for the AMR simulations it is based on the cell length. For the *Renaissance* suite we give the parent box size (40 cMpc) but note that the results we show here are for the zoom in regions which have box lengths of approximately 6 cMpc.

with JWST.

### 3.2.2 Extrapolating the Stellar Mass of the Simulated Galaxies based on the Star Formation History

To properly compare the simulated galaxy conditions against observations, we need to have simulated values at the same redshift as the JADES and CEERS measurements. However, as discussed above, both the Normal and RP regions of the *Renaissance* simulations only reach a redshift of  $z = 11.6$  and  $z = 15$  respectively. Therefore, the Normal region does not reach sufficiently low redshifts so as to be directly comparable against two of the JADES and CEERS galaxies, while the RP region cannot be directly compared, in terms of redshift, against any of the JADES and CEERS galaxies. To rectify this, we extrapolate the stellar masses of the most massive galaxy in both the Normal and RP region based on their respective specific Star Formation Rates (sSFR)

forward in time to connect with the observational redshifts.

The definition of the sSFR is

$$\Psi_{\text{S}} \equiv \frac{\Psi}{M_*} \quad (3.1)$$

where  $\Psi$  is the SFR and  $M_*$  is the stellar mass. We use three values for  $\Psi_{\text{S}}$  in our extrapolation method: A maximum value of  $10^{-7} \text{ yr}^{-1}$ , a nominal value of  $10^{-8} \text{ yr}^{-1}$ , and a minimum value of  $10^{-9} \text{ yr}^{-1}$ . These values were chosen from the range of sSFR values found in *Renaissance* (see also Figure 3.3). The extrapolated mass is dictated by the differential equation

$$\Psi \equiv \frac{dM_*}{dt} = \Psi_{\text{S}} M_*, \quad (3.2)$$

where the solution of this equation is

$$M_*(t) = M_0 e^{\Psi_{\text{S}}(t-t_0)}. \quad (3.3)$$

Here,  $M_0$  is the final simulated stellar mass of the halo and  $t_0$  is the final simulated time. Using Equation (3.3) we can then predict the stellar mass of the galaxy past the final simulation time. We justify using an exponential method to estimate the future stellar masses as we expect these galaxies to be clumpy and exhibit periods of starbursts, as opposed to the constant star formation rate that you would expect in the disc component of a local Milky-Way type galaxy [299, 300, 301, 302]. We will discuss the impact of this extrapolation method in more detail next.

### 3.3 Results

We begin here by comparing the most massive galaxy in each of the RP, Normal and Void regions against the JADES and CEERS results. We then follow this by comparing

the global galaxy assembly history of all of the galaxies in the *Renaissance* suite against the JADES and CEERS results.

### 3.3.1 Comparing the Most Massive Galaxies in Renaissance with the JADES and CEERS measurements

In Figure 3.1 we plot the stellar masses of the most massive galaxy in each region in *Renaissance* against the stellar masses of each of the JADES and CEERS survey galaxies. As discussed in §3.2.2, we extrapolate the stellar masses to the observed redshifts for the comparison.

From Figure 3.1 we can immediately see that the most massive galaxy in the Normal region (blue line), which evolves to  $z = 11.6$ , has a stellar mass greater than GS-z10-0 and is consistent with or within a factor of a few compared to the stellar mass of the remaining five galaxies. The RP region, which does not overlap in redshift with any of the JADES and CEERS galaxies, is consistent in terms of stellar mass with each of the observed galaxies once extrapolation (using the sSFR) is considered. The upper bounds of both shaded regions is based on a constant sSFR value of  $10^{-7} \text{ yr}^{-1}$ , the lower bounds being  $10^{-9} \text{ yr}^{-1}$ , and the dashed lines show the extrapolated stellar masses based on an nominal sSFR value of  $10^{-8} \text{ yr}^{-1}$ . The dashed line belonging to the RP region is overall consistent with each of the observed galaxies, with GS-z11-0 and GN-z11 lying within the bounds of the extrapolations. The Void region shows systematically lower stellar masses and does not achieve the same stellar masses as those found in JADES and CEERS.

Large-scale overdensities are directly related to the overabundances of galaxies through the halo mass function and the halo mass – stellar mass relation, shown by

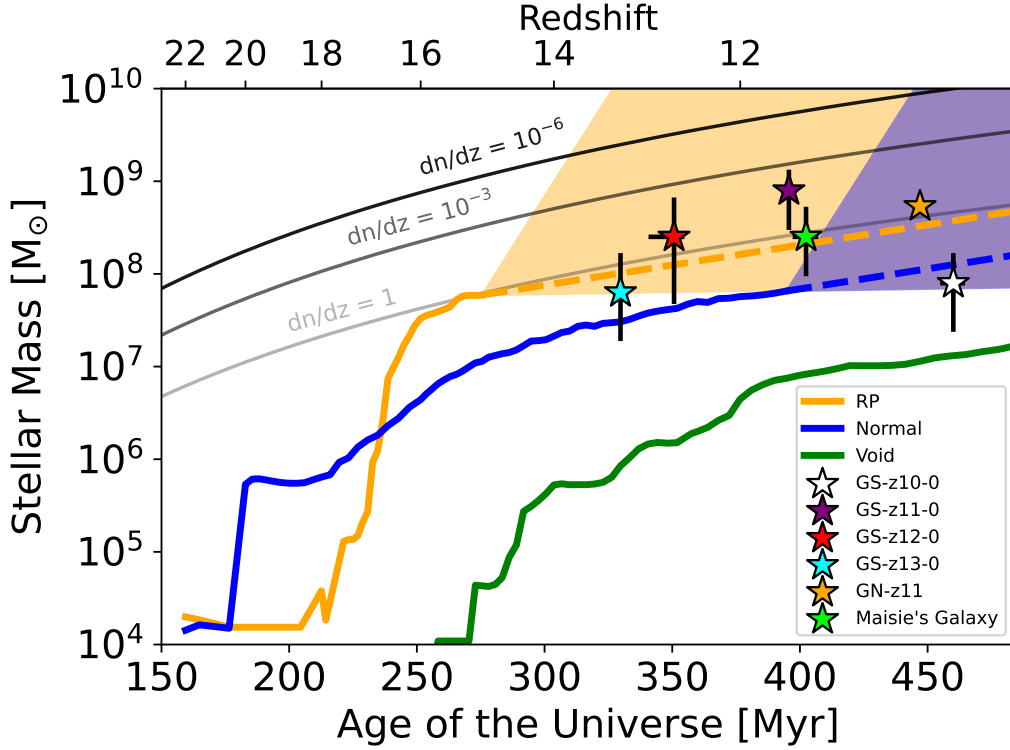


Figure 3.1: The most massive galaxy in each of the Rarepeak (RP, orange), Normal (blue) and Void (green) regions are shown. The six star shaped symbols identify the JADES and CEERS galaxies giving both their stellar masses and the redshift at which they were spectroscopically identified. The most massive galaxies in both the RP and the Normal regions are in excellent agreement with the JADES and CEERS observations. The shaded region denotes the extrapolation of the stellar masses based on the SFR history of the respective galaxy where the region is bounded from above by a specific star formation rate of  $10^{-7} \text{ yr}^{-1}$  and from below by a sSFR of  $10^{-9} \text{ yr}^{-1}$ . The dashed line represents an extrapolated mass based on a sSFR of  $10^{-8} \text{ yr}^{-1}$ . Finally, we plot lines labelled by  $dn/dz$  the expectation value for finding a galaxy of a given stellar mass at a given redshift in a field of view comparable to NIRCcam. For this we assume a gas mass corresponding to the baryon fraction and a star formation efficiency (SFE) of 0.1 using the Sheth-Tormen [303] halo mass function as the underlying framework. All of the JADES, CEERS and *Renaissance* haloes are consistent with  $\Lambda$ CDM predictions of finding at least one halo with these stellar masses in this volume. See text for further details on the consistency with respect to  $\Lambda$ CDM predictions, including commentary on the effects of cosmic variance and variance of the halo mass function at high- $z$ .

[98] for the *Renaissance* suite in particular. The observed stellar mass estimates suggest that the CEERS and JADES fields are not likely underdense regions. However, additional work would be needed to statistically conclude that the JADES and CEERS were observed in overdense regions.

To provide additional context and to quantify the rarity of haloes at these masses and redshifts, we plot lines in Figure 3.1 to represent the number of haloes of a certain (stellar) mass we expect JWST to see at a specific redshift. These lines are based on the baryon fraction obtained from WMAP7 and a star formation efficiency (SFE) of  $f_* \equiv M_* / [(\Omega_b / \Omega_M) M_{\text{halo}}] = 0.1$ , with the baryonic fraction being  $\Omega_b / \Omega_M \sim 0.17$ . While this value for the SFE may seem high [see e.g. 304] for this redshift regime, *Renaissance* shows an increasing SFE value dependent on the halo mass (see Figure 3.4), for this reason a value of 0.1 seems appropriate for the extrapolation. The value of  $dn(M_*, z)/dz$  represents the number of galaxies of stellar mass  $M_*$  or greater we expect to see at redshift  $z$  in the NIRCcam field of view. For example  $dn/dz = 10^{-3}$  tells us that we expect to see one galaxy with stellar mass  $M_*$  or greater at redshift  $z$  in every one thousand frames with the angular size of NIRCcam ( $9.7 \text{ arcmin}^2$ ).

All of the galaxies are consistent with the  $dn/dz = 1$  line except the GS-z11-0 galaxy whose error bars are marginally above the  $dn/dz = 1$  line. This means that we should expect to observe at least one galaxy of that stellar mass in the field of view of NIRCcam. The lines at  $dn/dz = 10^{-3}$  and  $10^{-6}$  represent a mass scale that would be increasingly unlikely to observe at that redshift. The calculations used in the creation of these values is described in §3.5.

We can observe that the Normal region does not contain a galaxy that exceeds the  $dn/dz = 1$  line. This can, however, be explained through cosmic variance [305, 306] which would provide an uncertainty in the expectation values of the stellar mass of

$\sim \pm 100\%$  [e.g. 307]. It may also be explained by a variance in the halo mass function used at high redshifts [308], which would provide an additional uncertainty up to an order of magnitude in the abundances of halos at fixed stellar mass. Combining these two uncertainties can easily move the  $dn/dz = 1$  lines up (or down) by a factor of a few.

In summary, the JWST observed galaxies are overall consistent with both the Normal and RP regions once the extrapolation methods and cosmic variance are taken into account. Both GN-z11 and GS-z11-0 are unusual galaxies and detailed hydrodynamic simulations are clearly struggling to match their luminosities and stellar masses perfectly. It may be that these galaxies contain star formation processes not currently correctly modelled by our subgrid recipes - by this we mean that these JWST galaxies may contain stars born from an extremely top heavy IMF including a population of extremely massive stars [e.g. 309, 310] or unusually strong bursts of star formation [e.g. 311]. In addition to this, GN-z11 shows signatures of AGN activity [312, 313] which is not currently modelled by **Renaissance** for example and the processes responsible for seeding this massive black hole may well be a factor in explaining its large luminosity. Finally, we make no attempt here to analyse absolute cosmic abundances of high mass galaxies. The galaxies found thus far by JWST at these redshifts are at the absolute limit of the **Renaissance** simulations and we are not in a position to quantify such abundances. This is due to the small volume of the **Renaissance** simulations and thus the limitation in quantifying the statistics of high mass haloes in this epoch of the Universe.

Figure 3.2 shows the SFR history of the most massive galaxy in the RP, Normal and Void regions - the same as Figure 3.1. Here and thereafter we consider the average SFR over the previous 20 Myr, i.e. the stellar mass of star particles younger than 20

Myr divided by 20 Myr. Comparing the observed (coloured symbols) and simulated galaxies (solid coloured lines), it is clear that *Renaissance* is able to reproduce galaxies with star formation rates generally consistent with the galaxies observed in JADES and CEERS. This is achieved due to the excellent mass and spatial resolution afforded by *Renaissance* which gives *Renaissance* the unique capability to follow the formation of the galaxy stellar population(s) from approximately  $10^4 M_{\odot}$  up to the final simulated stellar masses of a few times  $10^7 M_{\odot}$ . What we see is that the star formation rates start several orders of magnitude below that observed but in very inefficient, star forming, haloes. As the star formation efficiency increases (see also Figure 3.3) the simulated values quickly level off to the observed values ultimately reaching values of approximately  $1 M_{\odot} \text{ yr}^{-1}$ .

It is the higher mass resolution of *Renaissance*, afforded through the use of adaptive grids in a zoom-in setup, that allows us to follow the build up of the galaxy from initially very small stellar masses ( $\sim 10^4 M_{\odot}$ ) up to a final stellar mass of more than  $> 10^7 M_{\odot}$ . Additionally, the spatial resolution of 19 comoving pc allows for the internal structure and dynamics of these early galaxies to be well resolved.

We observe an initial burst of star formation in the *Renaissance* galaxies plotted in Figure 3.2 with a leveling off in the SFR as the halo continues to evolve. This can be explained via the following mechanisms. In the initial stages of star formation in the haloes, the mass resolution of *Renaissance* is sufficient to capture the early assembly history. Once the halo mass exceeds the atomic cooling threshold and gas can cool via atomic line emission, the gas begins to collapse and form Population II stars more readily and the star formation efficiency increases rapidly. The feedback from the Population II star formation heats up the surrounding environment thus regulating further star formation. This results in an equilibrium in the SFR of the halo and is represented

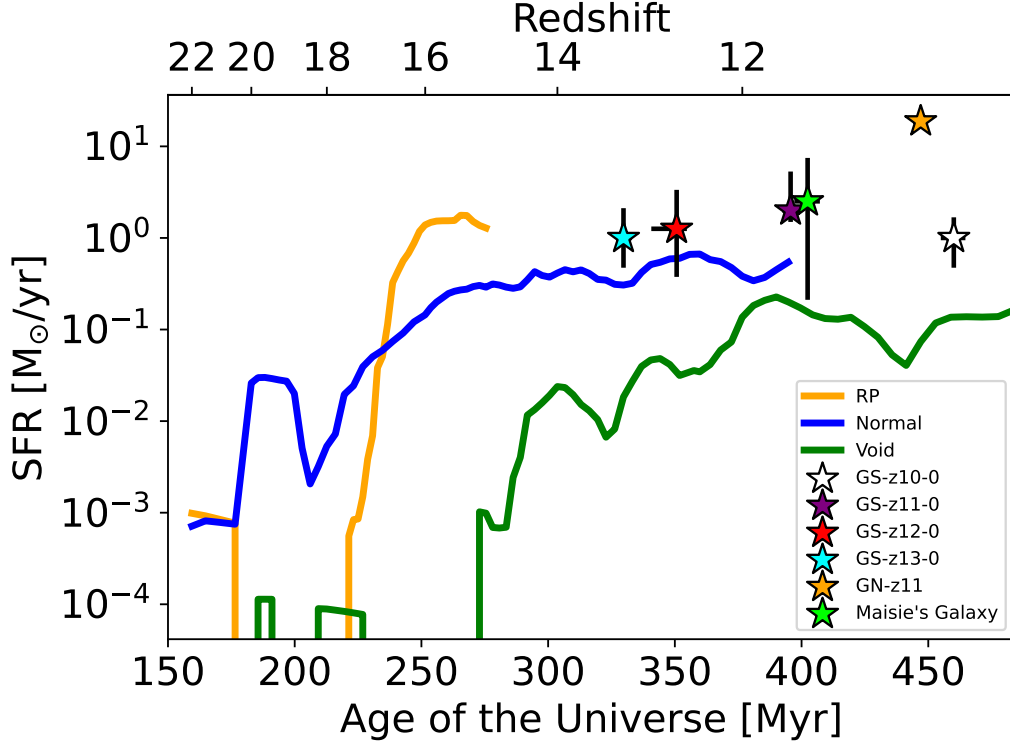


Figure 3.2: The star formation rates (SFRs) of the most massive galaxy in each of the RP (orange), Normal (blue) and Void (green) regions. The SFR of the JADES and CEERS galaxies are also plotted as star symbols with associated error bars [108, 283, 281]. All of the modelled galaxies show an initial burst of star formation at the early stages of evolution with a leveling off as each halo continues to evolve. In the cases where the observed galaxies overlap with the modelled galaxies, the SFRs found are consistent with each other within an order of magnitude. Both the Normal and RP regions show SFRs, for their highest mass galaxies of between 0.5 and 1  $M_{\odot} \text{ yr}^{-1}$ . The most massive galaxy in the Void region shows a lower SFR as expected [e.g. 98].

by the leveling off seen in Figure 3.2.

### 3.3.2 Comparing all Galaxies in Renaissance with JADES Measurements and Simulation Results

We now expand our analysis to a larger set of high-redshift simulated galaxies to determine how the observed galaxies compare. Figure 3.3 shows the SFR of each galaxy

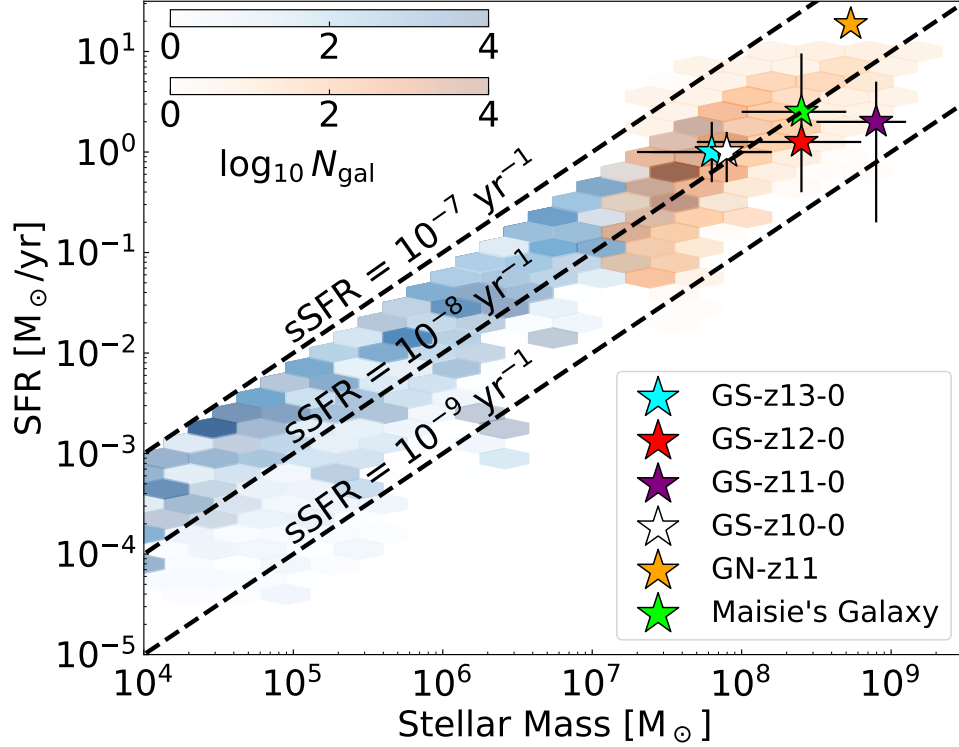


Figure 3.3: The star formation rates of the galaxies in the *Renaissance* simulations, which occupy lower masses in the plot and shown in blue hexbins, and the galaxies in the K23 simulations, which exist at higher masses and shown in orange hexbins, as a function of stellar mass. The bin saturation depicts the number of galaxies on a log-scale. The galaxies from the *Renaissance* simulations (blue hexbins) exist at redshifts greater than 15, 11.6, and 8 for the RP, Normal, and Void region, respectively. The K23 simulations are in the range of  $z = 10-14$  for four full-box and two zoom-in simulations. We consider all outputs from the simulations as a stack over all snapshots. Lines of constant sSFR are plotted that are representative of the majority of the galaxies in the simulations. We plot the JADES and CEERS observations as stars, consistent with the simulation data.

as a function of the stellar mass of each galaxy in *Renaissance* along with the galaxies from the simulations included in K23. By including the data from our simulations and the K23 simulations, we see how both lower and higher mass galaxies compare to the JADES and CEERS data that is plotted on Figure 3.3 as coloured stars. The data

on GS-z13-0, GS-z12-0, GS-z11-0 and GS-z10-0 are taken from [108], GN-z11 is taken from [281] while the data on Maisie’s Galaxy is taken from [283]. In this comparison, we consider all galaxies in the RP, Normal, and Void regions of the **Renaissance** simulations that extend to very low stellar masses, shown starting from  $10^4 M_\odot$  (blue hexbins), while the K23 simulations (orange hexbins) provide insight into the higher galaxy mass regime. As shown by Figure 3.3, the trends found in the **Renaissance** simulations compliment the K23 simulations at higher masses that overlap with the JADES and CEERS observations, showing the cohesion between the simulations and the observed data.

We show lines of constant sSFRs that are representative of the majority of the data in Figure 3.3. The figure shows that most galaxies at high-redshift quickly assemble, with the sSFR lying in the range  $10^{-7} - 10^{-9} \text{ yr}^{-1}$  corresponding to  $e$ -folding times of 10 Myr to 1 Gyr. While it is difficult to see any definite trends in the heatmap because of the differing simulations and zoom-in regions, this figure demonstrates that early galaxy formation progresses at a fairly rapid rate with the lower mass galaxies having higher sSFR values. The plot shows that the **Renaissance** simulation follows closely with the trend shown in the K23 simulations. For both sets of data, we can see that the distribution of the SFRs increases as stellar mass increases with a constant slope. The **Renaissance** data connects smoothly to the K23 and JADES data, showing how the galaxies in the **Renaissance** simulations could evolve over 200 Myr to become the JADES and CEERS galaxies. The consistent progression of SFR in Figure 3.3 from the low-mass regime (blue hexbins) to higher masses (orange hexbins) indicates that these  $z > 10$  galaxies detected by JADES and CEERS are the most massive examples within a much larger and still undetected population of young and low-mass galaxies.

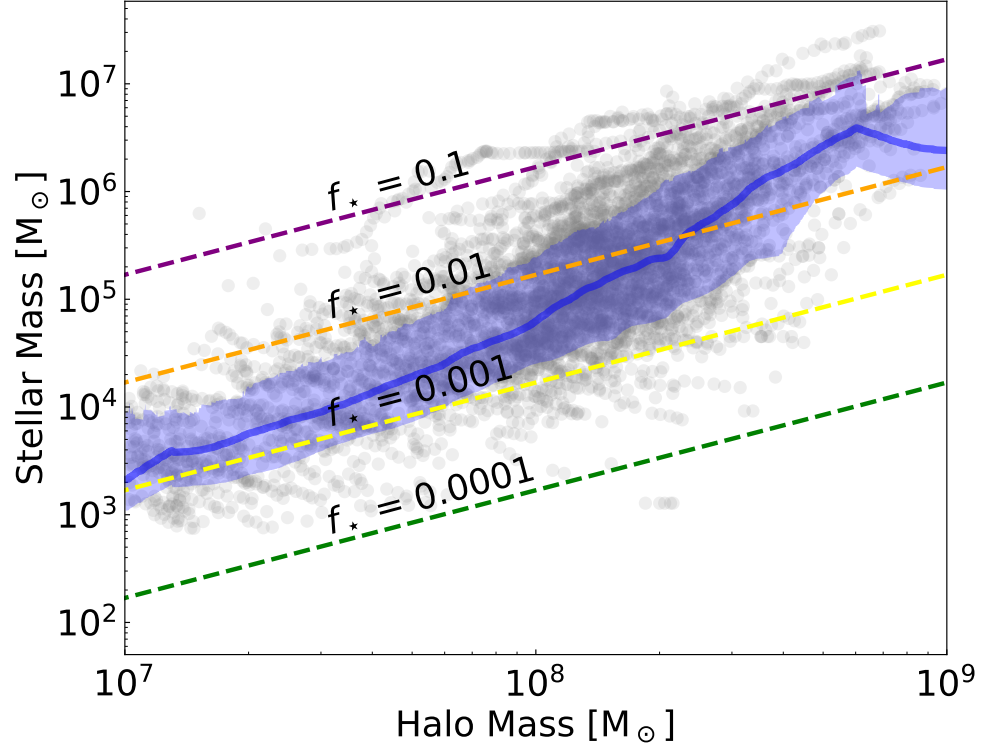


Figure 3.4: The stellar mass of each galaxy from the *Renaissance* simulation plotted against the dark matter halo mass of each galaxy over time. The green, yellow, orange, and purple dashed lines show the stellar mass given a constant SFE of 0.01, 0.1, 1, and 10 per cent, respectively. The blue solid line shows the median stellar mass while the shaded blue region shows one standard deviation, each of them as a function of the halo mass.

### 3.3.3 Simulated Stellar Mass – Halo Mass Relation

The growth of low-mass galaxies is ultimately controlled by the host dark matter halo growth, thus we turn our attention to the stellar mass - halo mass relationship of the galaxies in the *Renaissance* Simulations to shed light on the origins of the galaxies observed in CEERS and JADES. Figure 3.4 shows the stellar mass of each galaxy in the *Renaissance* simulation against its host dark matter halo mass from all zoom-in regions which shows the linear relationship between the halo mass and the stellar mass

in the **Renaissance** galaxies until reaching the atomic cooling limit. We plot data from all outputs in the simulation suite. We can combine these datasets because galaxy scaling relations do not vary greatly, though with a large galaxy-to-galaxy scatter, with redshift at these early times [see Figure 15 and Table 2 in 98]. Here we focus on the trends between stellar mass and halo mass in this low-mass regime. From the raw data alone, there is a large scatter at all halo masses, culminating from highly variable SFRs that arise from periodic gas expulsions from stellar feedback.

To better show any trends, we show the median value (solid blue line) as a function of the halo mass for all galaxies. We depict the  $1\text{-}\sigma$  standard deviation as the shaded blue region, which remains fairly constant in log-space throughout this mass range. We also show lines of constant star formation efficiency (SFE) for convenience. As demonstrated in Figure 3.2, galaxy growth does not proceed at a constant SFR and thus SFE, especially at these low masses when star formation can be bursty. Each galaxy makes its unique path through this parameter space. When a population of bursty galaxies are considered, these variable tracks transform into a relationship shown in the figure. Throughout most of the plot, the slope of the median line is steeper than the slopes of the constant SFE lines, meaning that the galaxies are, on average, forming stars more efficiently as they grow.

This trend clearly shows as an increase in the  $M_* - M_{\text{halo}}$  slope around the atomic cooling limit at  $\sim 10^8 M_\odot$ . Gas cooling and thus star formation within these nascent galaxies are inefficient below this limit with a median SFE of  $f_* \sim 2 \times 10^{-3}$ . Once the gas can cool through atomic processes, star formation becomes more efficient, depicted by the increase in the slope and associated SFE. By the time haloes reach  $10^9 M_\odot$ , the median SFEs are a few per cent, similar to the more massive galaxies probed by the simulations highlighted in K23. With this information, we are able to justify our use

for the SFE value of  $\text{SFE} = 0.1$  that we use for the mass extrapolation discussed in §3.2.2.

We note that the turnover to a negative slope is an artefact of limited galaxy sample at these highest halo masses in the *Renaissance* simulations. In principle, the stellar mass should continue to grow as the halo grows. These most massive haloes have lower stellar masses than some of slightly less massive haloes. This is not unexpected because of the large scatter in the stellar mass - halo mass relation, caused by the stochastic nature of early galaxy formation.

### 3.4 Discussion and Conclusions

The goal of this chapter was to investigate whether or not the initial findings of JWST, via the JADES and CEERS surveys, are consistent with state-of-the-art high resolution simulations. Additionally, the high (mass) resolution simulations allow us to study in detail the assembly history of these galaxies and allow us to connect the modelled galaxies with those observed in JADES and CEERS. We find that, using the high spatial and mass resolution *Renaissance* simulations, that excellent agreement exists between observations and simulations. There is a limitation in the fact that we are unable to compare the simulations and measurements at similar redshifts. To address this, an extrapolation method was applied to the end masses of the most massive haloes in the RP and Normal regions. We justify this caveat, by extracting directly the range of sSFR values found across all halo mass ranges in *Renaissance* (see Figure 3.3). These sSFR values were then used to put lower and upper bounds on the mass of the most massive galaxies in both the Normal and RP regions.

We also address the fact that both the GN-z11 and GS-z11-0 galaxies are above the

(extrapolated) mass of the most massive galaxy in the RP region (when a sSFR of  $10^{-8} \text{ yr}^{-1}$  is used). GN-z11 was recently found to have an anomalously high abundance of N/O [314] and likely hosts an active AGN [140, 313], a characteristic that will be missed by **Renaissance**. These outliers may also be explained by an uncertainty associated with cosmic variance, as discussed in §3.3.1 or an uncertainty associated with the higher ends of the redshift ranges [308].

Our results are consistent with a similar study by [120] who compared a range of somewhat larger scale simulations against the initial JADES and CEERS results. The combination of the larger scale study by K23 with the higher resolution simulations here, which can accurately track the initial assembly history of the galaxies subsequently found in the K23 simulations, provides compelling evidence for an excellent agreement between the JADES and CEERS results and the  $\Lambda$ CDM model. It is the combination of the two regimes that is crucial in this regard. Our overall findings can be broken down as:

- The most massive haloes in **Renaissance** have comparable stellar masses to the JADES and CEERS galaxies after extrapolating the masses. The **Renaissance** simulation suite does not evolve in time to the same epoch as all of the observations and so we must extrapolate the (specific) star formation rate forward in time for some galaxies - but nonetheless the agreement is overall remarkable. Comparing with the theoretical expectation of galaxies within a field of view identical to NIRCam, we find that the  $z > 10$  galaxies detected in JADES and CEERS are consistent with that expected from a  $\Lambda$ CDM cosmology.
- The star formation rates for the most massive galaxies in **Renaissance** are overall consistent with the JADES and CEERS measurements. The star formation his-

tories show specific star formation rates, as a function of stellar mass, generally consistent with these latest  $z > 10$  JWST observations. Finally, it is also possible that the observed stellar masses may be affected by bursts of star formation close to the epoch of observation which may effect the derived results [315].

- The mass resolution of *Renaissance* allows us to capture the rapid assembly of galaxies in the early Universe. After inefficiently forming stars below the atomic cooling threshold at a median SFE of  $2 \times 10^{-3}$ , star formation becomes more rigorous yet feedback-regulated after the halo reaches a virial temperature of  $2 \times 10^4$  K (as can be seen in [316]), reaching levels of a few per cent at galaxy masses similar to the JADES and CEERS measurements.
- We conclude that both lower and higher resolution simulations agree that the JADES and CEERS measurements are not in tension with current galaxy formation models.

JWST has for the first time enabled a detailed view of the early Universe. Initial findings of massive early galaxies has surprised many with some discussion in the literature that the JWST results may be in conflict with  $\Lambda$ CDM [288, 290]. However, what we find is that in the context of a  $\Lambda$ CDM Universe there is no tension between theory and observation at the very highest redshifts that we can currently probe.

As more measurements are made with JWST and future record breaking observatories, it comes with more opportunity to utilise high-resolution simulations like *Renaissance* and further stress test the  $\Lambda$ CDM model.

### 3.5 Appendix A: Calculating the number of haloes expected to be seen by JWST

In Figure 3.1 we present predictions for the number of haloes of a certain stellar mass,  $M_*$  we expect to see in JWST’s FoV,  $\Omega$ , at a certain redshift,  $z$ . To do this we use the `hmf` module [317] to supply a halo mass function which we then use in our calculation. The halo mass function provides the number of haloes with a mass between  $M$  and  $M + dm$  at  $z$  per comoving volume. The number of haloes we expect to see per comoving Mpc in JWST’s field of view, with a mass greater than  $M_0$ , is calculated as follows:

$$\frac{dn}{dr_c} = A(z) \int_{M_0}^{\infty} \frac{dn}{dm}(M, z) dm \quad (3.4)$$

$A(z)$ , measured in  $\text{Mpc}^2$ , is the comoving area at redshift  $z$  and is calculated from

$$A(z) = \Omega r_c^2(z) \quad (3.5)$$

where  $r_c(z)$  is the comoving distance as a function of redshift. We can then convert it to the amount of haloes NIRCam should observe per redshift with

$$\frac{dn}{dz} = \frac{dn}{dr_c} \frac{dr_c}{dz} \quad (3.6)$$

It is noted that effects due to dust extinction and the angular resolution of JWST’s cameras are ignored for this calculation. For the field of view calculation, we use the FoV of the NIRCam instrument ( $9.7 \text{ arcmin}^2$ ).

# Chapter 4

## Beyond No Tension

### 4.1 Introduction

At the time of the publishing of the paper that this chapter consists of, it had been three years since JWST started providing fresh information on previously hidden parts of the Universe. From exoplanets to the extragalactic population, we have gained unprecedented access into astrophysics that previously remained theoretical. In this chapter specifically, we are focused on understanding the formation of the very first galaxies and how accurate well established cosmological models are at predicting the number densities and formation rates that these galaxies would exhibit. Not long after the commissioning of JWST that probes the high redshift Universe, questions started to arise into what observations were beginning to tell us about early galaxy formation. Surveys like JADES [318, 319, 320] and CEERS [321, 282, 322] unveiled a population of galaxies that appeared to even violate accepted formation models. They displayed high stellar masses and high star formation rates for this epoch of the Universe, reaching the order of  $10^8 - 10^9 M_{\odot}$  in stellar mass only a few hundred million years after the Big

Bang [108, 323]. These galaxies presented a problem as theoretical models predict that if these galaxies do in fact exist, they would have to possess star formation efficiencies close to 100%, given the accepted baryonic matter made available by  $\Lambda$ CDM – our most accepted cosmological model at the time of writing this chapter [113].

Resolutions to this tension include the possibility that the stellar masses from early galaxies are being overestimated, due to possible contribution of light from massive black holes in these high- $z$  galaxies [e.g. 324]. Other research lines find that for high mass dark matter halos, that star formation becomes more efficient with redshift, allowing for the existence of high stellar masses in these halos without violating  $\Lambda$ CDM [e.g. 325].

One way to see what kind of galaxy population  $\Lambda$ CDM would present us with is the use of cosmological simulations. With simulations we are able to construct a Universe using a priori assumptions based on the most basic physics with initial conditions provided by measurement of the Cosmic Microwave Background and also sophisticated state-of-the-art modelling of physical mechanisms. Due to current computational power, simulations are often limited in terms of the redshift regimes that are being examined along with the mass and spatial resolutions. To quantify this aspect of numerical work [326] utilised a number of cosmological simulations to try and see if they could reconstruct the high- $z$  galaxies that were being observed with JWST. While these simulations were able to produce galaxies on the same mass scale as the observations, they were not designed to focus on the high- $z$  galaxies, and so the build up of these galaxies is not accurately captured by the large-scale cosmological simulations such as EAGLE [327, 328], Illustris [329], TNG100 [330], RomulusC [331], Obelisk [332] and Simba [333]. In [121] (hereafter M23), we used the **Renaissance** simulations [12, 13, 14], a suite of high- $z$ , zoom-in simulations that were specifically designed for modelling early

Universe galaxy formation. With **Renaissance**, we were not only able to reproduce the high masses and star formation rates of the JADES/CEERS galaxies, but we were also able to show the build up of these galaxies from small mass scales due to the superior mass and spatial resolutions of **Renaissance**. In M23 we concluded that the existence of these high- $z$  observations were not in tension with  $\Lambda$ CDM and that more evidence would be needed to provide a strong argument that theoretical models needed revisions.

Fast forward to 2025 and JWST has continued to break the record of spectroscopically confirmed high- $z$  galaxies. Most recently, the Miracle-or-Mirage (MoM) survey has discovered a galaxy, MoM-z14, in the COSMOS Legacy field which has a spectroscopically confirmed redshift of  $z \sim 14.44$  and a measured stellar mass of  $10^{8.1} M_{\odot}$  [110]. The galaxy also exhibits a luminous UV signature suggesting high levels of star formation for this epoch of its lifetime. Along with MoM-z14, the JADES survey has unveiled a galaxy at  $z \sim 14.3$ , GS-z14, which has a mean spectroscopically derived stellar mass of  $10^{8.6} M_{\odot}$  [111], even higher than its high redshift counterpart MoM-z14. These extremely high- $z$  and rapidly forming galaxies force us to revisit the work of M23 and deduce whether or not these galaxies are in direct tension with our cosmological simulations, and if so, do we need to revisit models of star formation/feedback or do we need to adjust how we apply our models to observations of high- $z$  environments.

In this chapter, we are updating the results of M23 and comparing the galaxies from **Renaissance** to the highest redshift observations from JWST, along with other  $z > 10$  galaxies to provide context on the steadily forming census of early galaxies. We also examine the measured UV luminosity functions from these  $z \sim 14$  galaxies and see how they compare to the derived luminosity functions from the **Renaissance** simulations.

## 4.2 Methodology

We will now briefly outline the methods we applied to compare the JWST observations with the results from the **Renaissance** simulations. First we will describe the main attributes of the **Renaissance** simulations which are relevant to this work, more information on **Renaissance** can be found in [334], [12], [13], and [14]. **Renaissance** is a suite of N-body hydrodynamic simulations created using the adaptive mesh-refinement code Enzo [95, 96]. **Renaissance** consists of three zoom-in regions, defined by their level of overdensity: the Rarepeak (RP), Normal, and Void region. The RP region consists of a box of  $3.8 \times 5.4 \times 6.6 \text{ cMpc}^3$  run to  $z = 15$ , while the Normal and Void regions consists of boxes of dimensions  $6.0 \times 6.0 \times 6.125 \text{ cMpc}^3$ , respectively run to  $z = 11.6$  and  $z = 8$ . The advantages of **Renaissance** include its high mass resolution of dark matter particles, reaching down to  $2.4 \times 10^4 M_\odot$  and spatial resolution reaching down to 19 cpc. **Renaissance** also contains prescriptions for PopIII and PopII star formation and feedback, allowing for accurate galaxy formation modelling at high redshifts. Star formation in **Renaissance** relies on the stochastic sampling of the first generation of stars, based on individual star forming clouds which can be resolved in the simulations. A star formation efficiency of 7% is used to convert cold gas within the simulations into PopII stars, which is based on simulations of local star formations simulations by [335], who calibrated feedback models against local dwarf galaxies. This was to ensure that the simulations avoided the “over-cooling problem” which led to overestimation of stellar mass and metallicity.

We will use the results from the simulations to compare with the JWST measurements of MoM-z14 and GS-z14 and a number of other  $z > 10$  galaxies taken from [323, 281, 336, 337, 338, 339]. Due to the high redshifts of these galaxies, we now have the

chance to almost directly compare observations of high- $z$  galaxies with like counterparts of galaxies found in the RP region of **Renaissance**, which ends at  $z = 15$ , only tens of millions of years of separation away from the observations. We will analyse the observations by studying them as individual cases, with the masses being compared to the most massive galaxies in **Renaissance**, but we will also try to compare these exceptional galaxies against the simulated global population of **Renaissance**, by connecting their calculated UV luminosity functions against the luminosity functions derived from the simulations, analysing the star formation models in the process.

## 4.3 Results

In Figure 4.1 we plot the new stellar mass observations (MoM-z14 and GS-z14) against the values discussed in [121]. On top of each solid line, which denotes the stellar mass of the most massive galaxy in each **Renaissance** realisation we include a region of error on the stellar mass that can be attributed to a cosmic variance of +100%, which we obtained from [341]. We only include +100% to provide an upper limit to the stellar mass of the galaxies, in order to show the upper limits that the most massive galaxy from each region can reach due to cosmic variance. The dotted lines following the RP and Normal solid lines extrapolate the stellar masses based on the star formation rates found for those galaxies at the ending redshifts.

MoM-z14 appears to follow the established trend of the previously discovered  $z > 10$  galaxies, with its stellar mass lying safely within the predicted mass that the most massive galaxy of the RP region. Only three of the discovered galaxies have mass ranges that intersect the most massive galaxy in the Normal region, despite these galaxies likely coming from a Normal-like environment, suggesting that some revisions in stellar

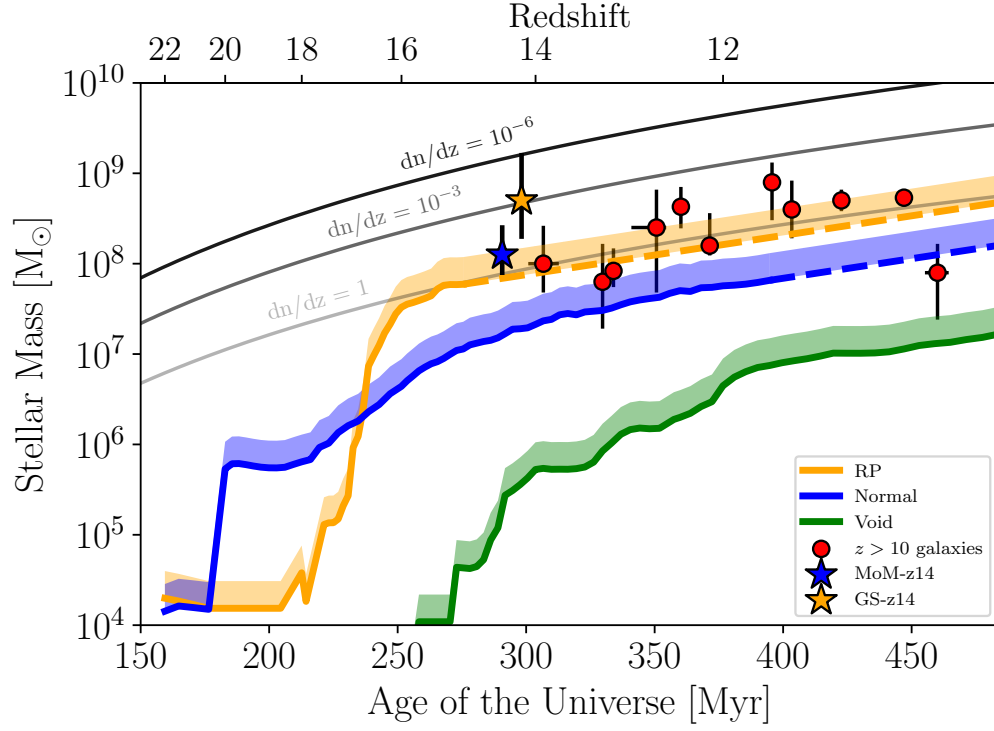


Figure 4.1: The growth evolution of the most massive galaxies from each region in *Renaissance* compared with observations from JWST. The dashed lines indicate where the stellar mass is extrapolated after the end time of each region in *Renaissance*, using a specific star formation rate of  $\text{sSFR} = 10^{-8} \text{ yr}^{-1}$ . The shaded regions denote the upper limit to these galaxies if we take into account an error from cosmic variance of +100%. The greyscale lines denoted by  $dn/dz$  indicate the probability of discovering a galaxy of a certain stellar mass and at a certain redshift in the FoV of the NIRCcam instrument on JWST. The calculation of these lines can be found in Section 3.5 of of the previous chapter.

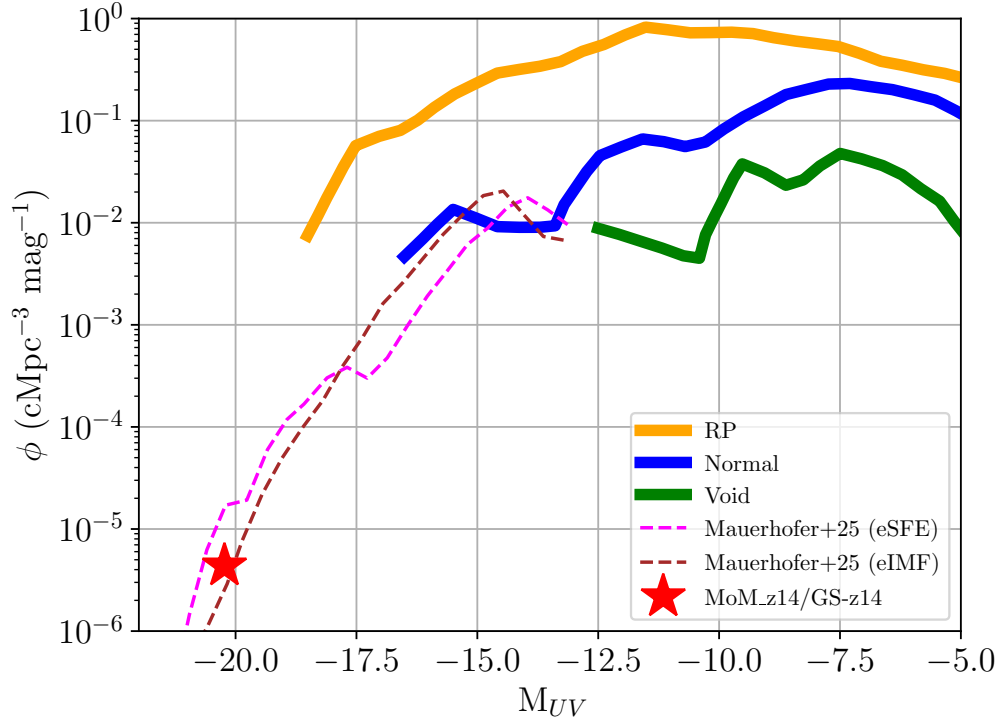


Figure 4.2: Luminosity function of the galaxies modelled in *Renaissance*, along with the luminosity function derived from the parameters constrained from GS-z14 and MoM-z14 [110]. We have also included estimates of the luminosity function derived from models which assume a top-heavy IMF in the early Universe (brown line) and a model which assumes that star formation efficiencies increase with increasing redshift [340]. It is noted that the luminosity function derived by [110] assumes that these galaxies are the only  $-21 < M_{UV} < -20$  galaxies to exist at  $z \sim 14 - 15$  in the UDS, GOODS-S and COSMOS fields, imaged by the PRIMER and JOF surveys.

formation modelling at this epoch is required. In contrast, GS-z14 appears to be testing the limits of **Renaissance**, with its stellar mass lying above the accepted range of simulated masses at that redshift even for the RP region. The anomalous nature of GS-z14 initially suggests that **Renaissance** is underestimating the star formation in select high mass environments at high-redshift, which may be resolved in future through higher mass and spatial resolutions and updates to star formation and feedback prescriptions in such environments.

We note however that this is one measurement that does not agree with simulations. This outlier, combined with the fact that JWST will only be detecting the most massive galaxies in this epoch, does not contradict simulations, but rather requires that adjustments be made to high- $z$  modelling of star formation. Overall, the masses from previous detection of  $z > 10$  galaxies and the new MoM-z14 and GS-z14 detections agree more with the predicted masses of the RP region rather than the Normal region, possibly highlighting the need to revise how we treat star formation in the most massive halos in the early Universe.

In Figure 4.2, we plot the UV luminosity functions of the simulated and measured galaxies. We use the UV luminosities calculated at  $z = 15$  using **Renaissance** from [12], which were derived from the stellar masses, star formation rates (SFRs and metallicities of galaxies from each region. There are concerns that there is an overabundance of luminous galaxies in the early Universe, suggesting high star formation efficiencies at this epoch [342, 343, 344]. Studying and comparing the UV luminosities from **Renaissance** with the values derived from observations and new theoretical models will be valuable in understanding where inaccuracies remain in the modelling of star formation at high- $z$ .

In Figure 4.2 we can see that the measured UV luminosity function from the com-

bination of GS-z14 and MoM-z14 lie at lower values than the simulations, with considerably brighter UV magnitudes, due to the large respective star formation rates of  $25_{-5}^{+6}$  and  $13_{-3.5}^{+3.7} \text{ M}_{\odot} \text{ yr}^{-1}$  for these galaxies. The luminosity function values that [110] calculate in their work comes from the assumptions that these are the only  $z \sim 14$  galaxies to exist in the FoV of the survey.

The UV luminosity functions from **Renaissance** fit well to the luminosity function calculations at  $z = 14$  from the adjustments made by [340], suggesting that **Renaissance**, for the most part, is agreeing with theoretical models that suggest adjustments need to be made in terms of the star formation of the first generation of stars. Where **Renaissance** is most likely breaking down is for the brightest galaxies (as found by JWST) where the rapid assembly and subsequent evolution driving these galaxies is not well captured by our physical models and/or resolution.

## 4.4 Conclusions

In conclusion, **Renaissance** is underestimating the stellar masses of the most massive high- $z$  galaxies with the majority of them fitting the RP line from Fig.4.1 but not the Normal region (as may be expected). The misalignment between the Normal region and the observed  $z > 10$  galaxies indicates that some adjustments need to be made to the star formation/feedback prescriptions and/or numerical resolution needed in future simulations to model these high- $z$ , extreme, galaxies.

It is unlikely, given the relatively small field of view of the JADES and MoM surveys that JWST by chance, happened to set its sights on a RP-like region in the early Universe. While the UV luminosities from the observations line up with the derived quantities from **Renaissance**, suggesting that the global star formation rate is accurately

modelled in the simulations, the high masses of these individual galaxies themselves may suggest that there needs to be some revisions on how we apply stellar formation prescriptions in select environments [e.g. [345](#), [346](#)]. These select environments may allow, for example, earlier star formation in rapidly accreting galaxies to account for this increase in galaxy size or even greater star formation efficiency for the most massive galaxies at high- $z$ . We conclude, however, that there is insufficient evidence to imply that our most accepted model of the Universe,  $\Lambda$ CDM, is in tension with the observations that JWST has been making for three years now. There is still not enough data relating to  $z > 10$  galaxies to arrive at the conclusion that we need to change the most fundamental foundations of our current framework of galaxy formation and cosmology.

## Chapter 5

# Conclusions & Outlook

In this thesis, we set out with the goal of understanding some of the mysteries that have been presenting themselves in the early Universe. Thanks to JWST, we are starting to answer some of these questions, while at the same time new questions arise, such as the population of early massive galaxies that are prevailing at high- $z$  and also the high mass black holes coexisting with these galaxies. This new window into the high- $z$  Universe allows us to test our theories and more specifically the simulations that were designed to probe this early epoch of the Universe. To do this, we used the **Renaissance** simulations, a suite of high- $z$  zoom-in simulations, built using the adaptive mesh-refinement code ENZO, designed to study early galaxy formation. In the second chapter of this thesis, we applied post-processing methods to investigate the formation and growth of heavy seed black holes in rapidly assembling halos. What we discovered was that were black holes to form in these high- $z$  redshift dynamical environments, the lower mass proportion of these black holes would have a hard time accreting matter, with their accretion values reaching a tiny fraction of the Eddington limit. We also find that mergers between black holes at this redshift are few and far between. However,

any mergers that should occur at this epoch should be easily detectable by the likes of future GW detectors like LISA.

In Chapter 3, which is based on the published [121], we investigated the existence of extremely high- $z$  galaxies that were discovered using the JWST-based JADES and CEERS surveys, using the **Renaissance** simulations. These galaxies have started to raise questions regarding the validity of the  $\Lambda$ CDM, with their masses seemingly approaching the limit of the amount of available baryonic matter dictated by  $\Lambda$ CDM that is able to convert to stellar material. We isolated the most massive galaxies in **Renaissance** and tracked their evolution from their foundational building blocks of high resolution dark matter particles up to galaxies ranging around  $10^{7-8} M_{\odot}$  in stellar masses at very high redshifts. In the case where **Renaissance** could not directly simulate at the redshifts these high- $z$  galaxies have been observed at, the specific SFRs from the population of galaxies in **Renaissance** were used to extrapolate the masses so we could make estimates that could be directly compared against observations. What we discovered was that the high- $z$  observations were not in direct tension with  $\Lambda$ CDM and that the existence of these galaxies could be easily explained using high resolution simulations akin to **Renaissance**.

In Chapter 4, we return to the matter of these high- $z$  galaxies. Since the publication of [121], more galaxies have been discovered by JWST which have broken the records of how far back in time these galaxies are observed to be at. In particular MoM-z14 and GS-z14 are two galaxies that are now even starting to test the results of the **Renaissance**. These galaxies are extremely high mass, at very high redshifts and thus exceeding the stellar mass of the most massive galaxy in the **Renaissance** Rarepeak region, even when accounting for cosmic variance. However, when examining the UV luminosity functions of these galaxies, the observed galaxies appear to have a

UV luminosity function value of  $\sim 10^{-5} \text{ cMpc}^{-3} \text{ mag}^{-1}$ , a number density that cannot be achieved by **Renaissance**, due to the volume restrictions of the simulations. We conclude that future simulations that are able to probe small areas of bursty star formation in these high- $z$  galaxies, should be able to account for the existence of these record breaking early Universe galaxies.

Throughout this thesis, we have utilised the **Renaissance** simulations to address open questions in the early Universe. We have found that these simulations are extremely valuable when it comes to studying the newly unveiled observations thanks to JWST and making predictions for what discoveries can be made in terms of black hole physics with future gravitational wave detectors. We anticipate that as computational advances continue to be made, more sophisticated simulations will be made to address the mysteries that are continuing to become more prevalent in the early Universe.



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