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Simulations of structure formation and feedback at high redshift

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Submitted for the degree of Doctor of Philosophy

University of Sussex

6th December 2022

Declaration

I hereby declare that this thesis has not been and will not be submitted in whole or in part to another University for the award of any other degree.

Parts of this thesis have been undertaken in collaboration with others:

- Chapter 2: Ilian T. Iliev, Anastasia Fialkov, Keri L. Dixon and David Sullivan
- Chapter 3: Ilian T. Iliev, Sergey Pilipenko and Noam I. Libeskind
- Chapter 4: Ilian T. Iliev, Sergey Pilipenko, Gustavo Yepes, Julia Stadler and Celine Boehm
- Chapter 5: the Cosmic Dawn collaboration

Where this is the case, we acknowledge their work at the beginning of the relevant chapter.

Chapter 2 has been submitted for publication in MNRAS [[astro-ph/2207.11614](#)] and Chapter 3 has been submitted to the John von Neumann Institute for Computing (NIC) Symposium 2022. Both texts have been modified to better fit the thesis.

Signature:

Luke Conaboy

UNIVERSITY OF SUSSEX

LUKE CONABOY

SIMULATIONS OF STRUCTURE FORMATION AND FEEDBACK AT HIGH REDSHIFTSUMMARY

Understanding how structure formation progressed in the time between the emission of the cosmic microwave background and the formation of the first galaxies is essential to our models of the reionisation of the universe. Processes which can impact the formation and abundance of small-scale structures are of particular interest, since it is these structures which are thought to, initially, be the primary drivers of reionisation. In this thesis, we present a range of works using numerical simulations to model structure formation, and associated feedback processes, in the high-redshift universe.

To this end, we present our methodology for studying the impact of supersonic relative baryon-dark matter velocities on small-scale structure formation and demonstrate its effect on the halo baryon fraction and early star formation. We find a suppression in the baryon fraction of haloes and a delay in the onset of star formation, in qualitative agreement with previous works. This is the first simulation, to our knowledge, to self-consistently sample the relative velocity from a large box, making it useful for future works exploring the effect of the spatial fluctuations of the relative velocity.

Extending previous works, we begin to model the impact of reionisation on the Local Group of galaxies, using extremely high-resolution radiation-hydrodynamics simulations. We ran an extremely high-resolution constrained dark matter-only simulation (containing 16384^3 effective particles in the zoom region—the highest-resolution simulation in the HESTIA suite to date) of the Local Group down to $z = 0$, demonstrating excellent agreement with previous HESTIA runs. Further, we presented preliminary work on calibrating the star formation and supernova feedback to produce a realistic ionisation history.

Through the analysis of high-resolution N -body simulations, we assess the impact of initial small-scale suppression (due to interactions between radiation and dark matter in the very early universe) in the matter power spectrum on high-redshift halo formation and evolution. We find that the initial small-scale suppression is washed out to some extent, as

power cascades from larger (less suppressed) scales down to small scales. We also find that the abundance of low-mass ($M \lesssim 10^{10} h^{-1} \text{ M}_\odot$) haloes is reduced, and that the haloes in the interacting dark matter case accrete more of their mass later than in the standard cold dark matter case.

Finally, we present analysis of structure formation in the latest in a series of state-of-the-art fully-coupled radiation-hydrodynamics simulations of reionisation, containing 8192^3 dark matter particles and cells. We present a comparison to a companion dark matter-only simulation, finding good agreement at low redshifts and high masses. We also identify cases of overlinking in the halo analysis, whereby two unbound structures have been spuriously linked.

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Chapter 1

Introduction

1.1 This thesis

The main theme of this thesis is the use of numerical simulations to explore structure formation in the (mostly) high-redshift universe, with a particular focus on small scales. In this introductory chapter we will outline concepts required later in the thesis, starting with the cosmological background, moving to structure formation and reionisation, before finishing with discussions of numerical methods for simulations and their analysis.

In § 1.2.2 we detail the fluid equations that model the evolution of perturbations in the matter density and velocity, which are used in Chapter 2 to incorporate the effect of relative baryon-dark matter velocities into simulation initial conditions (a more detailed exposition, including the effect of baryon temperature perturbations, is given in § 2.2). A general discussion of simulation methods is given in § 1.4, with a focus on N -body methods (similar to those used in Chapter 4) in § 1.4.1 and the **RAMSES** simulation code (used in Chapters 2, 3 and 5) in § 1.4.8.

In addition to discussing the simulation methods, we also outline the generation of initial conditions for these simulations in § 1.4.4. In § 1.4.6, we outline a technique that allows for a compromise between high-resolution and large-volume simulations, called ‘zoom’ simulations, which are applied in Chapters 2 and 3. In § 1.4.7, we also discuss a method that attempts to reproduce the observed local matter distribution (e.g. the Virgo cluster), known as ‘constrained’ simulations. This type of simulation is used in Chapter 3, which relies on initial conditions generated by the **HESTIA** collaboration.

Finally, in § 1.5 we outline some of the techniques used throughout this thesis to analyse simulations. We discuss the computation of power spectra (§ 1.5.1), identification of haloes (§ 1.5.2) and the modelling of their growth and evolution (§ 1.5.3).

1.2 Cosmology

We are in an era of precision cosmology, with experiments like the Planck mission ([Planck Collaboration et al., 2020](#)) supporting the standard cosmological model of our universe, termed ‘ Λ CDM’. In such a model, most of the matter is in the form of cold dark matter (CDM), with baryons occupying a relatively small fraction of the matter budget ($\sim 15\%$). The nascent universe underwent a period of rapid exponential expansion (inflation) and has been expanding (at a much slower rate) ever since. In recent cosmic history, the rate of expansion has been increasing due to the influence of a cosmological constant (Λ), which dominates the energy density budget of the universe.

1.2.1 Modern cosmology

Our best model of the universe predicts that it has always been expanding. [Hubble \(1929\)](#) showed that the radial velocities of ‘extragalactic nebulae’ increase with increasing distance from us. In an expanding universe, the proper distance $\mathbf{r}$ to an object is given by

$$\mathbf{r} = \mathbf{x}a(t) \quad (1.2.1)$$

where $\mathbf{x}$ is the distance comoving with the expansion and $a(t)$ is a measure of the expansion, called the scale factor, and is normalised such that today $a(t_0) = 1$. The velocity of a receding object then becomes

$$\mathbf{u} = \frac{d\mathbf{r}}{dt} = \frac{d\mathbf{x}}{dt}a + \mathbf{x}\frac{da}{dt} = \mathbf{v} + \mathbf{x}\frac{da}{dt}, \quad (1.2.2)$$

which reduces to $d\mathbf{r}/dt = \mathbf{x}da/dt$ if we ignore peculiar velocities $\mathbf{v}$ such that $d\mathbf{x}/dt = 0$. Defining the Hubble rate as

$$H(t) \equiv \frac{1}{a} \frac{da}{dt}, \quad (1.2.3)$$

we get the recession velocity of an object (at least over relatively small distances from us) as

$$\mathbf{v} = H_0 \mathbf{r} \quad (1.2.4)$$

where H_0 is the value of the Hubble rate measured today, called the Hubble constant. We can observe the effect of this recession velocity through cosmological redshift z ,

$$\frac{\lambda_o}{\lambda_e} = 1 + z = \frac{1}{a(t_e)}. \quad (1.2.5)$$

which is where the wavelength of light emitted by a receding galaxy λ_e is extended (i.e. shifted to redder wavelengths) when observed today λ_o , due to the expansion of the universe

In the Friedmann-Lemaître-Robertson-Walker (FLRW) model of the universe, we make some assumptions about our universe on large scales—namely that it is homogeneous and isotropic. This is known as the cosmological principle and means that the universe is the same everywhere (homogeneous) and from every direction (isotropic), and it allows us to write the metric giving the distance between two points in this universe (in spherical polar coordinates)

$$ds^2 = -c^2 dt^2 + a^2(t) \left[\frac{dr^2}{1 - kr^2} + r^2 (d\theta^2 + \sin^2 \theta d\phi^2) \right], \quad (1.2.6)$$

where c is the speed of light and k is a constant describing the curvature, and consequent type, of the universe, with $k = 0$ describing flat, $k > 0$ closed and $k < 0$ open universes. The expansion of an FLRW universe including a cosmological constant Λ is described by the Friedmann equation

$$H^2 = \frac{8\pi G}{3} \rho + \frac{\Lambda c^2}{3} - \frac{kc^2}{a^2}, \quad (1.2.7)$$

where G is Newton's gravitational constant, and ρ is the mass density of the universe comprised of the matter ρ_m and radiation ρ_r densities

$$\rho = \rho_m + \rho_r, \quad (1.2.8)$$

where the matter density can be split into $\rho_m = \rho_b + \rho_c$, with 'b' denoting baryons, and 'c' cold dark matter. Describing the cosmological constant as a fluid with density

$$\rho_\Lambda \equiv \frac{\Lambda c^2}{8\pi G} \quad (1.2.9)$$

allows us to rewrite Equation (1.2.7) as

$$H^2 = \frac{8\pi G}{3} \rho - \frac{kc^2}{a^2}, \quad (1.2.10)$$

where we redefine $\rho = \rho_m + \rho_r + \rho_\Lambda$. Using Equation (1.2.10), we find a critical density for which the universe is flat ($k = 0$)

$$\rho_{\text{cr}} = \frac{3H^2}{8\pi G}, \quad (1.2.11)$$

which has a value of $2.78 \times 10^{11} h^2 \text{ M}_\odot \text{ Mpc}^{-3}$ today, where we have factored out the dependence on the current value of the Hubble parameter as $h \equiv H_0 / (100 \text{ km s}^{-1} \text{ Mpc}^{-1})$.

Equation (1.2.11) allows us to define the density parameter of a species as

$$\Omega_i = \frac{\rho_i}{\rho_{\text{cr}}}, \quad (1.2.12)$$

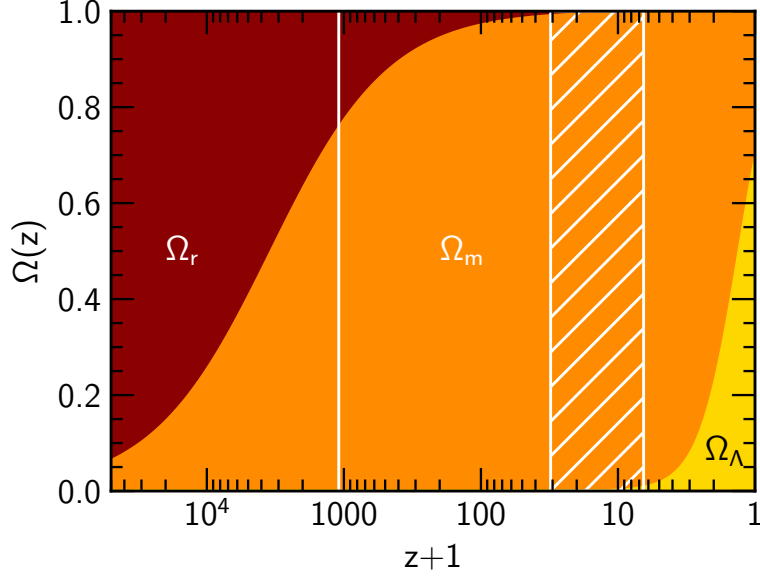


Figure 1.1: Density parameter of radiation (Ω_r , red), matter (Ω_m , orange) and the cosmological constant (Ω_Λ , yellow) as a function of redshift, the coloured fraction indicates the value of Ω . The vertical white line indicates the redshift of recombination $z \approx 1090$ and the hatched region indicates the EoR, from the formation of the first stars at $z \sim 30$ to the end of reionisation $z \approx 5.5$.

which, along with a rearrangement of the Friedmann equation, gives us the dependence of the Hubble parameter on density (ignoring contributions from massive neutrinos)

$$H^2(a) = H_0^2 \left[\frac{\Omega_{m,0}}{a^3} + \frac{\Omega_{r,0}}{a^4} + \Omega_\Lambda + \frac{\Omega - 1}{a^2} \right]. \quad (1.2.13)$$

In Figure 1.1 we show the contribution of each species to the total density as a function of z for a flat universe ($\Omega = 1$). At high redshift ($z \gtrsim 3400$), radiation is the dominant component in the density budget. Radiation density scales as $(1+z)^4$ whereas matter density goes as $(1+z)^3$, so as z decreases matter will become dominant over radiation. Indeed, at $z_{\text{eq}} \approx 3400$ the density of the two components becomes equal and below this z we enter the period of matter domination. Matter domination persists until $z \approx 0.3$ whereupon the cosmological constant begins to dominate, driving the accelerated expansion of the universe. Two particularly relevant periods are highlighted on Figure 1.1—recombination (solid white line) and the Epoch of Reionisation (EoR) (white hatched region). Recombination ($z \approx 1090$) is the point where the universe has expanded to the extent that atoms can form without being instantly ionised. The supersonic relative baryon-dark matter velocities discussed in Chapter 2 arise after recombination, when the baryons decouple from the photons. We mark the EoR as the period from the formation of the first stars ($z \sim 30$) to the end of reionisation $z \approx 5.5$.

1.2.2 Structure formation

On very large scales, the density of the universe is close to being homogeneous. However, on small scales this is not the case. Tiny overdensities collapse under gravity, eventually forming the galaxies and clusters of galaxies that we see today. To characterise these overdensities, we define the density contrast at a position $\mathbf{x}$ (as defined by Equation (1.2.1)) as

$$\delta(\mathbf{x}, t) = \frac{\rho(\mathbf{x}, t) - \rho_m(t)}{\rho_m(t)} \quad (1.2.14)$$

where ρ_m is the average density of the universe, $\delta(\mathbf{x}) > 0$ corresponds to an overdensity and $\delta(\mathbf{x}) < 0$ to an underdensity. To follow this growth of structure we can model the non-relativistic matter in the universe as an ideal fluid and derive equations governing its motion. We do not reproduce the entire derivation here, instead just presenting the results below, but for detailed expositions see e.g. Peebles (1980), Padmanabhan (1993), Peacock (1999) or Mo et al. (2010). The conservation equations appears simplest when described in the Lagrangian formalism,

$$\text{continuity: } \frac{1}{\rho} \frac{D\rho}{Dt} + \nabla \cdot \mathbf{u} = 0 \quad (1.2.15)$$

$$\text{Euler: } \frac{D}{Dt}(\rho \mathbf{u}) + \nabla p = -\rho \nabla \phi \quad (1.2.16)$$

where ρ is the mass density, $\mathbf{u}$ is the fluid velocity, p is the pressure, and ϕ is the potential. The Lagrangian derivative D/Dt is the derivative *following* the motion of the flow and we can translate it to the Eulerian derivative at a point by (Binney & Tremaine, 1987)

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla. \quad (1.2.17)$$

Now, we can use Equation (1.2.14) to write $\rho = \rho_m(\delta + 1)$ and, using Equation (1.2.17), we have the Eulerian conservation equations

$$\text{continuity: } \frac{\partial \delta}{\partial t} + \frac{1}{a} \nabla \cdot (1 + \delta) \mathbf{v} = 0 \quad (1.2.18)$$

$$\text{Euler: } \frac{\partial \mathbf{v}}{\partial t} + \frac{\dot{a}}{a} \mathbf{v} + \frac{1}{a} (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{\nabla p}{a \rho_m (1 + \delta)} - \frac{\nabla \phi}{a} \quad (1.2.19)$$

$$\text{Poisson: } \nabla^2 \phi = 4\pi G a^2 \rho_m \delta. \quad (1.2.20)$$

Considering an ideal fluid with an equation of state $p(\rho)$, where the pressure depends only on the density, we can rewrite the first term on the right-hand side (RHS) of the Euler equation (Equation (1.2.19)) as

$$\frac{\nabla p}{\rho_m} = \frac{\nabla \rho}{\rho_m} \frac{\partial p}{\partial \rho} \quad (1.2.21)$$

$$= c_s^2 \nabla \delta \quad (1.2.22)$$

where $c_s^2 = (\partial p / \partial \rho)$ is the fluid sound speed. Now looking at the linear regime, where $|\delta| \ll 1$, Equations (1.2.18) and (1.2.19) reduce to

$$\frac{\partial \delta}{\partial t} + \frac{1}{a} \nabla \cdot \mathbf{v} = 0 \quad (1.2.23)$$

$$\frac{\partial \mathbf{v}}{\partial t} + \frac{\dot{a}}{a} \mathbf{v} = -\frac{c_s^2 \nabla \delta}{a} - \frac{\nabla \phi}{a}, \quad (1.2.24)$$

where we have also used Equation (1.2.22). Combining Equations (1.2.23) and (1.2.24) yields

$$\frac{\partial^2 \delta}{\partial t^2} + 2 \frac{\dot{a}}{a} \frac{\partial \delta}{\partial t} = \left(4\pi G \rho_m + \frac{c_s^2}{a^2} \nabla^2 \right) \delta \quad (1.2.25)$$

where the $\nabla^2 \phi$ term has been replaced using Equation (1.2.20). Taking the Fourier transform of Equation (1.2.25), and using the relation $\nabla f(\mathbf{x}) \rightarrow i\mathbf{k}f(\mathbf{k})$ gives

$$\frac{\partial^2 \delta}{\partial t^2} + 2 \frac{\dot{a}}{a} \frac{\partial \delta}{\partial t} = \left(4\pi G \rho_m - \frac{c_s^2 k^2}{a^2} \right) \delta \quad (1.2.26)$$

and we can immediately see that there is some point at which the two terms on the rhs are equal, meaning that collapse due to gravitational instability is balanced by pressure support. This leads to a characteristic comoving wavenumber

$$k_J = \frac{2a}{c_s} \sqrt{\pi G \rho_m} \quad (1.2.27)$$

which can be translated into a proper length scale using the relation

$$\lambda_J = \frac{2\pi a}{k_J} = c_s \sqrt{\frac{\pi}{G \rho_m}} \quad (1.2.28)$$

and a corresponding mass scale as

$$M_J = \frac{4\pi \rho_m}{3} \left(\frac{\lambda_J}{2} \right)^3. \quad (1.2.29)$$

This length and mass scale are called the *Jeans length* and *Jeans mass* and dictate the size of perturbations whose pressure support stops them collapsing under gravity. The Jeans mass then gives the smallest mass object which can form at a given redshift at mean density. Throughout this section we made the simplifying assumption of a spatially uniform sound speed $c_s(t)$, whose pressure was a function of density only $p(\rho)$, however [Naoz & Barkana \(2005\)](#) made the argument that a more accurate treatment requires a spatially varying sound speed determined by tracking fluctuations in the baryon temperature. In § 2.2) we derive the sound speed including the effects of temperature perturbations, which are important at high redshift.

1.2.3 Haloes

As δ becomes close to 1, the description of § 1.2.2 breaks down and we say that structure formation has gone nonlinear. In this case, it is still possible to make some analytic predictions for nonlinear collapse, given some simplifying assumptions. As before, we will only briefly outline the details here—for the gory details see the references in § 1.2.2.

Consider a spherically-symmetric overdense region in an Einstein-de Sitter universe (i.e. $\Omega = \Omega_m = 1$ and $\Lambda = 0$, which is an excellent approximation to matter domination, the period in which the majority of this thesis is set). The acceleration felt by a test particle on a spherical shell some distance r from the centre of the overdensity is

$$\frac{d^2r}{dt^2} = \frac{-GM}{r^2}, \quad (1.2.30)$$

where $M = M(< r)$, since the particle will only experience a gravitation force due to the mass contained within the shell. Equation (1.2.30) can be integrated once to give

$$\frac{1}{2} \left(\frac{dr}{dt} \right)^2 - \frac{GM}{r} = C, \quad (1.2.31)$$

and is now in the form $T + U = E$, where T is the kinetic energy

$$T = \frac{1}{2} \left(\frac{dr}{dt} \right)^2, \quad (1.2.32)$$

U the potential energy

$$U = \frac{-GM}{r}, \quad (1.2.33)$$

and the constant of integration E the total energy. Equation (1.2.31) has the parametric solution

$$r(\theta) = \frac{r_{\text{ta}}}{2} (1 - \cos \theta) \quad (1.2.34)$$

$$t(\theta) = \frac{t_{\text{ta}}}{\pi} (\theta - \sin \theta), \quad (1.2.35)$$

where r_{ta} and t_{ta} are the radius and time at ‘turnaround’, where the perturbation begins to collapse, which occurs at $\theta = \pi$. The evolution of the overdensity goes like this: i) initially the overdensity expands with the universe at large, growing in r ; ii) the overdensity reaches a maximum radius $r = r_{\text{ta}}$ at $\theta = \pi$, for which

$$\left. \frac{dr}{dt} \right|_{r=r_{\text{ta}}} = 0 \quad (1.2.36)$$

$$U(r_{\text{ta}}) = E, \quad (1.2.37)$$

and begins to collapse; iii) the overdensity fully collapses at $\theta = 2\pi$, where $r = 0$. We can calculate the linear theory prediction the critical density contrast for collapse as $\delta_c = 1.686$. In reality, collapse does not proceed all the way to $\theta = 2\pi$, as a virialised structure forms before then since the shells of particles pass each other and interact gravitationally. If we define the condition for virialisation as

$$U = -2K, \quad (1.2.38)$$

and use Equation (1.2.37) and that $U \propto r^{-1}$, then we can show that $r_{\text{vir}} = r_{\text{ta}}/2$, corresponding to $\theta = 3\pi/2$. The overdensity $\Delta = \rho/\rho_m$ at which virialisation occurs is $\Delta = 18\pi^2 \approx 178$. In the real universe, overdensities are not spherically symmetric, and nonlinear collapse is usually treated using numerical simulations (see § 1.4). These virialised objects, called haloes, are the building blocks of structure in the universe. Structure formation proceeds in a hierarchical fashion with low-mass haloes forming earliest and merging to form larger haloes, since the small scales of the density distribution are first to go nonlinear.

Since haloes form at density peaks (e.g. [Bardeen et al., 1986](#)), studying the abundance of haloes can provide insights into the underlying matter distribution. Predictions for the abundance of haloes are couched in terms of the halo mass function dn/dM , i.e. how many haloes with mass in the range $(M, M + dM)$ exist in a given volume. In some cases, it is possible to use analytic arguments to derive the halo mass function, such as the model of [Press & Schechter \(1974\)](#) (PS), which uses the ‘peak formalism’ and assumes spherical collapse, or the improved model of [Sheth et al. \(2001\)](#), which extends the PS formalism to ellipsoidal collapse. More recent functional forms for the mass function have been derived by fitting to numerical simulations (e.g. [Warren et al., 2006](#); [Reed et al., 2007](#); [Tinker et al., 2008](#); [Bhattacharya et al., 2011](#)) and throughout this thesis we will use one such fitting formula, due to [Watson et al. \(2013\)](#). The [Watson et al. \(2013\)](#) mass function is based on a suite of CUBEP3M simulations of varying box size, resolution and redshift and functions are provided for FoF, SO and high-redshift catalogues. For a discussion on calculating the halo mass function in numerical simulations, see § 1.5.2.

1.2.4 Galaxies

Dark matter haloes provide a good starting point for discussing galaxy formation, but in order to accurately model the objects we observe it is imperative to consider the baryonic physics involved. Here we outline the physical processes around early galaxy formation (for more details see [Bromm & Yoshida, 2011](#); [Bromm, 2013](#)).

The gas accreted by the very first galaxies would have been metal-free, composed of hydrogen and helium. It is thought that the first stars would form in $\sim 10^6 M_\odot$ ‘minihaloes’, which form around $z \sim 20 - 30$. The virial temperature of gas collapsing into these minihaloes is approximately (Bromm, 2013)

$$T_{\text{vir}} \approx 2 \times 10^3 \text{ K} \left(\frac{M}{10^6 M_\odot} \right)^{\frac{2}{3}} \left(\frac{1+z}{20} \right), \quad (1.2.39)$$

and so we can see that these minihaloes will have a virial temperature $T_{\text{vir}} < 10^4 \text{ K}$. This is a key point, because below 10^4 K atomic cooling is ineffective and the dominant source of cooling is molecular hydrogen (Saslaw & Zipoy, 1967).

The very first generation of stars formed from metal-free primordial gas. After the first generation of Population (Pop) III metal-free stars go supernova, they pollute their surroundings with metals, vastly enhancing the range of cooling channels available and marking the transition to Pop II (metal-poor) star formation (e.g. Maio et al., 2007).

Beyond the first stars and galaxies, supernova feedback is an important regulator of star formation as it prevents gas collapsing too efficiently. Radiative feedback also has an impact, photoheating the gas—this is particularly important for low-mass galaxies, and the effect of reionisation can be to radiatively suppress low-mass galaxies (e.g. Dawoodbhoy et al., 2018).

1.3 Reionisation

From the recombination of hydrogen gas at $z \sim 1090$ to the formation of the first structures at $z \sim 30$ the universe was in a period known as the ‘dark ages’. At $z \sim 30$ the emission of UV photons from the first luminous sources began the reionisation of the largely neutral post-recombination intergalactic medium (IGM). This period, $z \sim 30 - 5.5$, is known as the EoR. The progress of reionisation depends on the growth of structure in a complex way, and as such is best studied theoretically through the use of numerical simulations (see § 1.4.5).

1.3.1 Observations

Most models predict that reionisation is complete by $z \sim 6 - 5.5$. One method of determining when reionisation finished is by looking for the Gunn-Peterson trough (Gunn & Peterson, 1965) in observations of high-redshift quasars. This feature is due to neutral hydrogen between us and the distant quasar absorbing the Lyman continuum (LyC) photons. The idea is that if a significant amount of neutral hydrogen is present along

the line of sight (i.e. reionisation is not complete) then this absorption feature will be seen. [Becker et al. \(2001\)](#) found a drop to near zero flux in this wavelength range for a quasar at $z = 6.28$ compared with the non-zero flux found by [Fan et al. \(2000\)](#) for a quasar at $z = 5.80$, supporting the theory that redshift finishes at $z \sim 6$. More recently, [Mortlock et al. \(2011\)](#) observed a similar feature in the spectrum of a quasar at $z = 7.085$. The spectra of the final sample of 52 high-redshift quasars found by SDSS is shown in [Figure 1.2](#) and the appearance of the Gunn-Peterson trough is clearly visible as redshift increases. Indeed recent results looking at the mean free path of ionising radiation found that there is significant evolution in the mean free path between $5 < z < 6$, meaning that reionisation could quite plausibly have finished at $z \leq 6$ ([Becker et al., 2021](#)).

Another reionisation observable is the integrated optical depth to reionisation, defined along the line of sight from $z = 0$ to some redshift z as

$$\tau(z) = c\sigma_T \int_z^0 d\tilde{z} n_e(\tilde{z}) \frac{dt}{d\tilde{z}}, \quad (1.3.1)$$

where c is the speed of light, σ_T is the Thompson scattering cross-section and $n_e(z)$ is the number density of free electrons at redshift z . Free electrons produced during reionisation can scatter photons from the cosmic microwave background (CMB) produced during recombination and affect the anisotropies seen in the CMB. The Planck satellite could detect this effect and measure an optical depth to reionisation. Using this optical depth [Planck Collaboration et al. \(2020\)](#) derived the redshift for the midpoint of reionisation to be $z_{\text{re}} = 7.67 \pm 0.73$.

A further tool for exploring reionisation is the 21-cm line, due to the hyperfine transition in neutral hydrogen ([Furlanetto et al., 2006](#)). This emission line is specially interesting because it *directly* probes the neutral gas, as opposed to the indirect measures described above. Even better, since it is a spectral line with a frequency $\nu_{21} = 1420$ MHz ([Santos et al., 2005](#)), it can be used to produce 3D tomographic maps ([Fan et al., 2006](#)) (the many challenges pertaining to sensitivity and foreground subtraction aside) with the observed frequency going as

$$\nu = \frac{\nu_{21}}{1+z}. \quad (1.3.2)$$

The 21-cm observable is the differential brightness temperature between the neutral hydrogen spin temperature T_S and the temperature of the CMB radiation T_{CMB} at a given

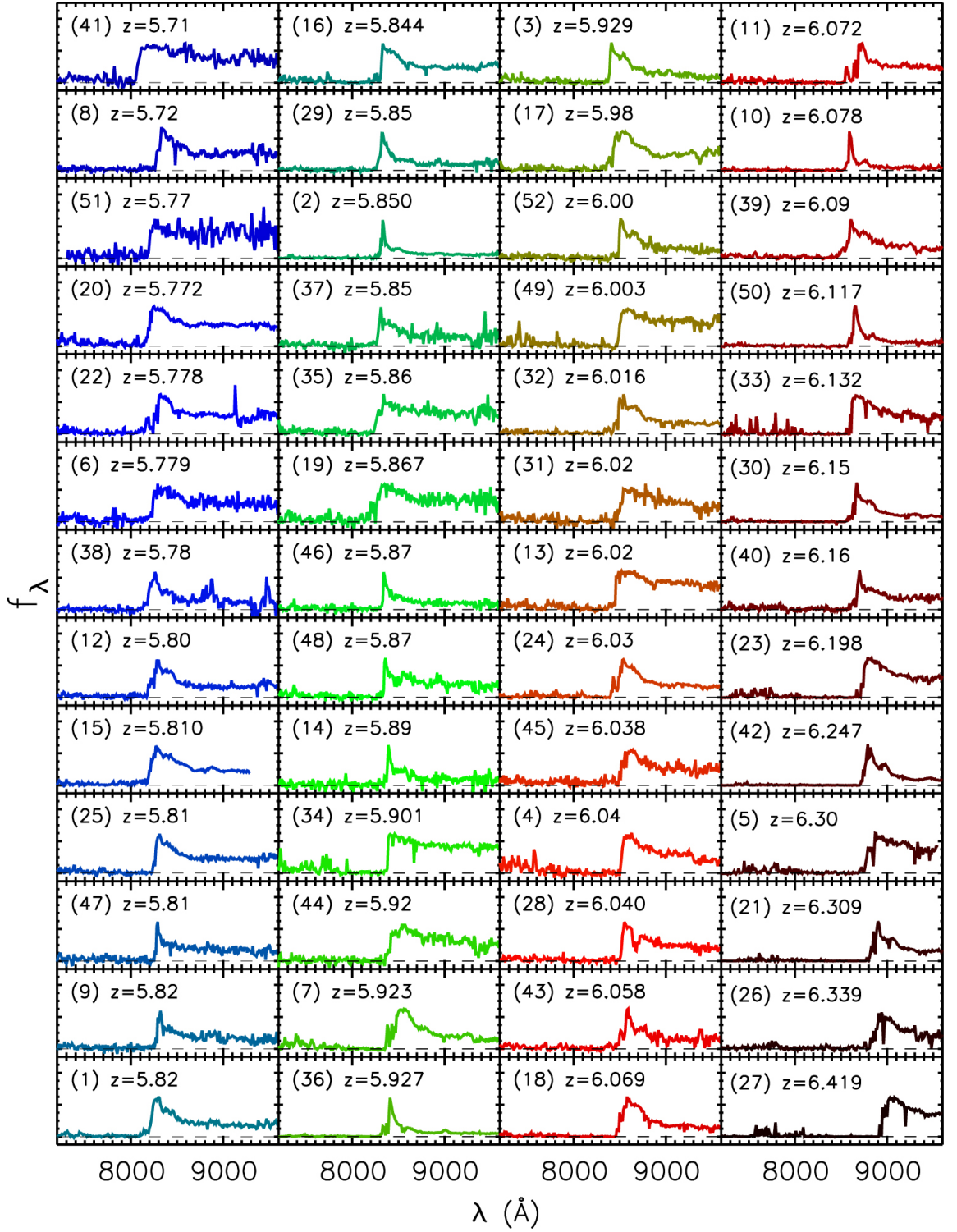


Figure 1.2: Absorption spectra of all 52 high-redshift quasars found in the SDSS sample. For $z \gtrsim 6$ the drop in flux in the LyC band (between $(1+z)(912-1216)$ Å) can be seen, indicating the presence of neutral hydrogen along the line of sight. Figure originally from [Jiang et al. \(2016\)](#).

redshift z

$$\delta T_b(z) = \frac{T_S - T_{\text{CMB}}}{1+z} (1 - e^{-\tau}) \quad (1.3.3)$$

$$= 28.5 \left(\frac{1+z}{10} \right)^{\frac{1}{2}} (1+\delta) x_{\text{HI}} \left(\frac{\Omega_b}{0.042} \right) \left(\frac{h}{0.73} \right) \left(\frac{0.24}{\Omega_m} \right)^{\frac{1}{2}} \text{ mK} \quad (1.3.4)$$

where τ is the 21-cm optical depth (assumed to be $\ll 1$ in Equation (1.3.4)), and $(1+\delta)x_{\text{HI}} = n_{\text{HI}}/\langle n_{\text{H}} \rangle$ is the mean number density of neutral hydrogen over the mean number density of hydrogen at that redshift (Iliev et al., 2014). One interesting feature in the 21-cm brightness temperature is an absorption feature caused by the formation of the first stars, as Lyman- α photons from the first stars couple T_S to the adiabatically cooled gas temperature, which is smaller than T_{CMB} (Chen & Miralda-Escudé, 2008; Pritchard & Loeb, 2012).

The redshifted signal falls into the radio part of the spectrum and will be detectable by the upcoming Square Kilometre Array (SKA) (Iliev et al., 2015). In fact, the EDGES experiment recently claimed to have detected an absorption profile due to radiation from the first stars in the sky-averaged 21-cm signal (Bowman et al., 2018), although the signal is much stronger than expected and requires extensions to known physics to explain it, such as interactions between baryons and dark matter (Barkana, 2018). A more recent experiment also looking at cosmic dawn has claimed to be unable to reproduce the EDGES signal (Singh et al., 2022).

1.4 Simulations

To aid the discussion of certain concepts in this and the following section (§ 1.4 and § 1.5), we use results from a test simulation produced with RAMSES (Teyssier, 2002). This simulation considered only dark matter particles and was performed in a $64 h^{-1}$ Mpc box, with the dark matter modelled using 128^3 particles. The initial conditions were set up using MUSIC (Hahn & Abel, 2011), with transfer functions from CAMB (Lewis et al., 2000) generated with the following cosmological parameters: $\Omega_m = 0.307$, $\Omega_\Lambda = 0.693$, $\Omega_b = 0.045$, $n_s = 0.961$, $\sigma_8 = 0.8288$ and $h = 0.6777$.

1.4.1 N -body

Since the large-scale structure in our universe is governed by the underlying distribution of dark matter, it follows that the simplest type of simulation would look only at the dynamics of dark matter. Modelling the dark matter as a collisionless system of N particles (i.e. an

N -body system), the equations to be solved are the Newtonian equations of motion

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p \quad (1.4.1)$$

$$\frac{d\mathbf{v}_p}{dt} = -\nabla\phi \quad (1.4.2)$$

where $\mathbf{x}_p$ are the particle positions, $\mathbf{v}_p$ are the particle velocities and $\nabla^2\phi$ can be found from

$$\nabla^2\phi = 4\pi G\rho. \quad (1.4.3)$$

There are many variants of N -body simulation, but three classic types are: the particle-particle (PP); particle-mesh (PM) and particle-particle-particle-mesh (P³M) models. A quite aged but classic introduction to computer simulation methods can be found in [Hockney & Eastwood \(1981\)](#).

Conceptually the simplest, the PP model directly computes the force between each particle and all its neighbours, using this to integrate the equations of motion and step forward in time. Whilst the PP method is simple, it is also expensive and scales as $\mathcal{O}(N_p^2)$ where N_p is the number of particles in the simulation, since $N_p - 1$ computations must be performed for each particle.

Next in terms of complexity comes the PM model. In this case, a mesh is applied to the simulation volume. The density ρ is computed by assigning particles to nearby points on the mesh, using some interpolation scheme. One such scheme is the nearest grid point (NGP) method whereby particles are assigned to the nearest part of the mesh, and another is the cloud-in-cell (CIC) scheme whereby the contribution by a particle to each mesh point is weighted by its distance to the grid point. With the density in hand, the potential ϕ is calculated on the mesh, using Equation (1.4.3), and this is used to compute the acceleration on particles from the mesh. Computing the potential can be drastically sped up by using Fourier methods to solve Equation (1.4.3), as the fast Fourier transform (FFT) scales as $\mathcal{O}(N_m \log N_m)$ where N_m is the number of mesh points and is usually a power of two. The main drawback of this method is that the resolution depends on how fine the mesh is, and a very fine mesh makes for a very expensive simulation. Poor resolution in PM codes can be improved by introducing adaptive resolution (i.e. decreasing the mesh size) in regions of high density, as is done in adaptive mesh refinement (AMR) codes such as [Enzo \(Bryan et al., 2014\)](#) and [RAMSES](#).

A compromise between the two methods described above is the P³M model, where long-range forces on a particle are calculated via the PM method and supplemented with PP forces calculated for nearby particles. This method can suffer from performance issues

if particles begin to cluster and the PP calculations start to dominate, although on the whole is a good compromise between the efficiency of PM and the accuracy of PP.

Further advancements can be made on the methods listed above to improve speed or reduce memory usage. One such example is ‘tree’ algorithms (e.g. **GADGET**, [Springel et al., 2001](#); [Springel, 2005](#)) where each cubical cell is recursively sub-divided until each cell contains only one particle ([Aarseth, 2003](#)). Another method is the use of adaptive algorithms, where high-density regions are split into finer regions in order to minimise the cost imposed by expensive short-range interactions. For example, the adaptive P³M code **Hydra** overcomes the performance issues due to clustering in standard P³M by subdividing high-density regions, thereby replacing the short-range PP calculations with PM and PP calculations over a finer mesh ([Couchman et al., 1995](#)).

1.4.2 Hydrodynamics

While N -body simulations are useful for capturing large-scale structure, to resolve processes such as galaxy formation we have to include the baryonic physics, in the form of numerical hydrodynamics, which solve the fluid equations presented in § 1.2.2. Numerical hydrodynamic codes can be broadly grouped into two categories: Lagrangian and Eulerian. Lagrangian codes move, as best as possible, with the flow while Eulerian codes follow the flux through cells.

A typical example of a Lagrangian implementation would be smoothed-particle hydrodynamics (SPH) where tracer particles follow the geometry of the flow and fluid quantities are obtained by interpolation using some smoothing kernel. Perhaps the most widely used SPH code today is **GADGET** ([Springel et al., 2001](#); [Springel, 2005](#); [Springel et al., 2022](#)), which is publicly on its fourth release. Another SPH code is **SWIFT**, which uses clever load balancing to improve performance ([Schaller et al., 2016](#)).

There are plenty of Eulerian codes out there, but the one we use throughout this thesis is **RAMSES**, which is discussed in detail in § 1.4.8. It is an adaptive mesh refinement (AMR) code, where the local resolution of the simulation is dependent upon the local density, and can be refined on-the-fly to better resolve high-density regions.

1.4.3 Radiative transfer

Many problems in astrophysics and cosmology now require an understanding of how photons propagate and interact in different environments, which in turn necessitates the use of radiative transfer (RT) recipes. There are many RT codes available, often spe-

cifically designed for use with other hydrodynamical codes, and for a comparison of their various strengths and weaknesses see Parts I and II of the Cosmological Radiative Transfer Comparison Project (Iliev et al., 2006b, 2009). Below I will briefly outline the radiative transfer equation and two of the main methods for solving it.

First we define $I_\nu(\mathbf{x}, \mathbf{n}, t)$ as the specific intensity for radiation, at a position $\mathbf{x}$, in a direction $\mathbf{n}$ and at time t . From this we find the energy of photons passing through an area dA , in time dt , through the solid angle $d\Omega$ and in the frequency range $\nu + d\nu$ is given by

$$dE = I_\nu dA dt d\Omega d\nu. \quad (1.4.4)$$

Incorporating the effects of emission and absorption, we arrive at the equation of radiative transfer (e.g. Rybicki & Lightman, 1979), which describes the change in I_ν along a ray

$$\frac{1}{c} \frac{\partial I_\nu}{\partial t} + \mathbf{n} \cdot \nabla I_\nu = -\alpha_\nu I_\nu + j_\nu \quad (1.4.5)$$

where α_ν is the absorption coefficient and j_ν is the emission coefficient.

One method of solving Equation (1.4.5) is to assume that the contribution to the radiation field is dominated by a few sources, and cast ‘rays’ from each source radially outward, casting enough that every cell is crossed by at least one ray on average. The specific intensity I_ν is then determined as a function of the optical depth τ from the source (Abel et al., 1999). More advanced codes get rid of the redundancy of having lots of rays passing through cells close to the source, but few in cells far away, by adaptively subdividing rays in cells (Abel & Wandelt, 2002). However, ray-based codes still scale linearly with the number of sources and don’t lend themselves to multiprocessor parallelisation.

The other main method for solving Equation (1.4.5) is by switching to a fluid description of the radiation field, taking the angular moments of the equation (Rosdahl & Teyssier, 2015). Hence, the two angular dimensions are removed, simplifying the problem, and the fluid nature means the radiation can be more easily coupled to hydrodynamical codes (this is the method used in RAMSES-RT, see § 1.4.8). RT codes that use this methodology scale independently of the number of sources. Despite bringing a huge improvement in efficiency, averaging over the angular dimensions means that the radiation loses its directionality, and so moment-based codes do not produce sharp shadows. A further problem is that the speed of light requires (prohibitively) small time steps to ensure that the Courant-Friedrichs-Lewy condition, which dictates that the radiation should cross less than a whole cell in a single timestep, is satisfied. A solution to alleviate the problem of small time steps is to employ the reduced speed of light approximation (RSLA)

(Gnedin & Abel, 2001) where we define a new speed of light

$$\hat{c} = f_c c \quad (1.4.6)$$

with f_c typically in the range $0.01 - 0.1$. The idea behind the RSLA in the context of reionisation simulations is that ionisation fronts in dense regions do not propagate anywhere near the speed of light. However, Ocvirk et al. (2018) found that the use of the RSLA can lead to an overestimation of the neutral hydrogen fraction after reionisation, which is important to remember when analysing the results of simulations using the RSLA.

1.4.4 Initial conditions

For any cosmological simulation, we first need to create the initial conditions (ICs), which dictate the starting state of the simulation. To do this, we first generate linear transfer functions at the start time of the simulation $T(k, z_{\text{ini}})$ which map primordial density perturbations to their late-time counterparts. The choice of z_{ini} is somewhat free and comes from a tradeoff between numerical noise overriding the early density fluctuations and missing out on the late-time growth of structure. Typically, $z_{\text{ini}} \sim 100 - 200$ but this is heavily dependent upon resolution (Oñorbe et al., 2014). These $T(k, z_{\text{ini}})$ can be computed from fitting formulae (e.g. Eisenstein & Hu, 1998) or, more accurately, using a Boltzmann solver such as CAMB (Lewis et al., 2000) or CLASS (Blas et al., 2011). One advantage of using a Boltzmann solver over fitting formulae is that a Boltzmann solver will return distinct amplitudes for the dark matter and baryon perturbations, whereas a fitting formula assumes that the baryons trace the dark matter exactly.

These transfer functions are then related to the power spectrum by

$$P(k, z_{\text{ini}}) = A k^{n_s} T^2(k, z_{\text{ini}}) \quad (1.4.7)$$

where A is a normalisation constant and n_s is the spectral index after inflation. At the simplest level, ICs are generated through a convolution of this power spectrum with a Gaussian random field, which imposes the amplitudes dictated by $P(k)$ onto the modes of the white noise field. IC generators used in practice make many improvements on this, such as the use of anti-aliasing filters (Bertschinger, 2001) or the use of real-space (as opposed to Fourier-space) transfer functions (Hahn & Abel, 2011). Figure 1.3 shows a slice through a test set of ICs generated with MUSIC (Hahn & Abel, 2011). In the top panel, we show the white noise field used to set the ICs and in the bottom panel we show the same white noise field after convolution with the matter power spectrum produced by CAMB.

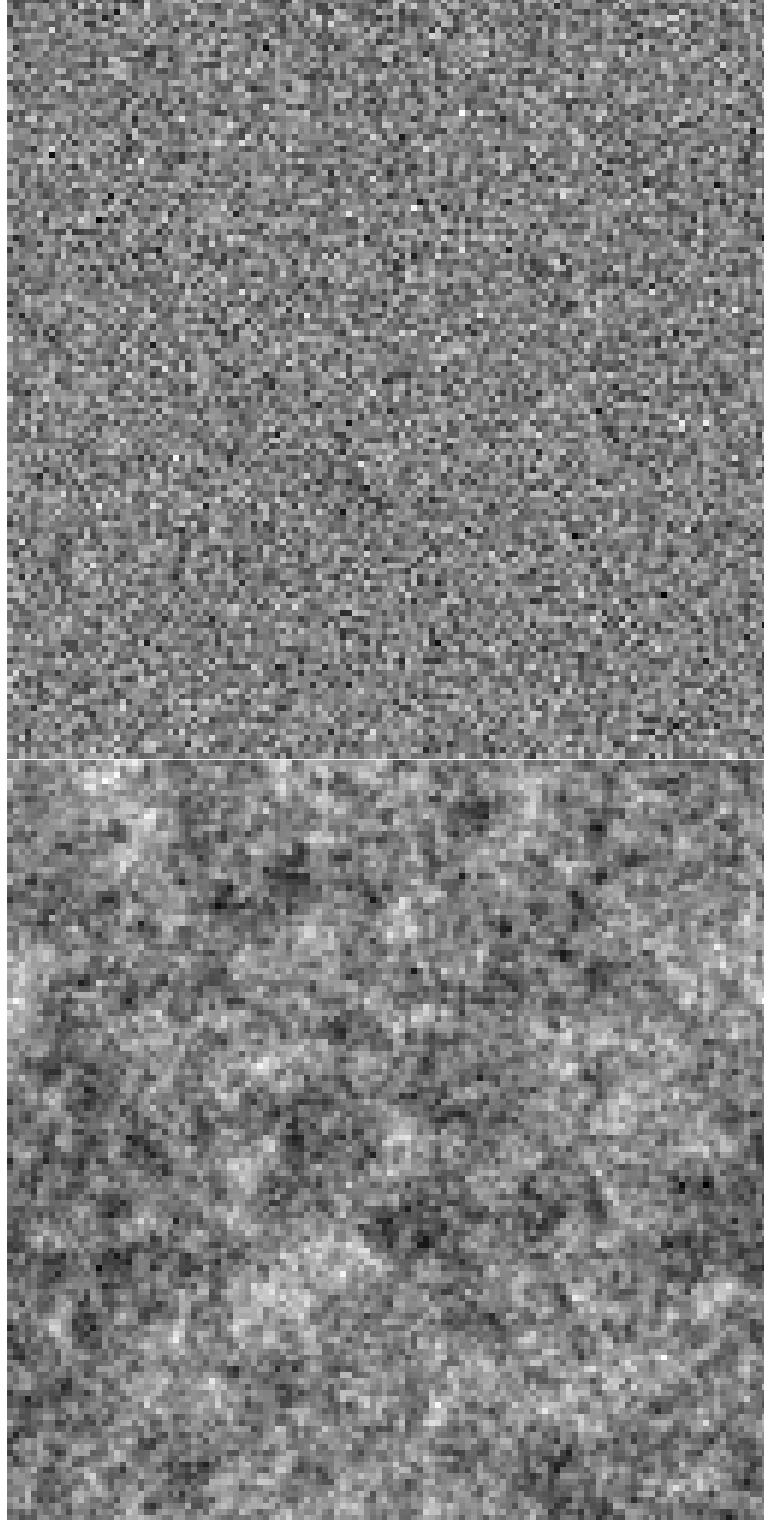


Figure 1.3: A slice, $64 h^{-1}$ Mpc wide and $0.5 h^{-1}$ Mpc thick, through the test set of 128^3 ICs produced with MUSIC. Top: the white noise field used to set the ICs. Bottom: the density contrast field δ , where black is $\delta < 0$ (i.e. underdense) and white is $\delta > 0$ (i.e. overdense). The bottom panel is produced through a convolution of the matter power spectrum produced by CAMB with the white noise field.

1.4.5 Reionisation simulations

[Iliev et al. \(2006a\)](#) undertook the first large-scale simulations of reionisation, using a $100 h^{-1}$ Mpc box to capture a representative sample of the universe. This was done by modelling structure formation using an N -body code (PMFAST, [Merz et al., 2005](#)) and then post-processing the radiative transfer with a ray tracing code (C²-RAY, [Mellema et al., 2006](#)). Among other things, they showed that the geometry of reionisation was ‘inside-out’, where high-density regions are ionised first, with low-density voids ionised last. This is in contrast with other studies, which predicted an ‘outside-in’ progression, where the voids are ionised first and densest regions last. A later study by [Iliev et al. \(2014\)](#) using box sizes up to $425 h^{-1}$ Mpc found that box sizes of at least $100 h^{-1}$ Mpc are required for convergent reionisation histories, while box sizes of $50 h^{-1}$ Mpc or less are not well converged.

Due to computational limitations, most large-scale simulations of reionisation are performed using the prescription described above (post-processing radiative transfer on to simulations of structure formation). However, these simulations miss the feedback effects that occur when radiation and gas dynamics are fully-coupled, such as the photoheating of gas by radiation. [Rosdahl et al. \(2018\)](#) self-consistently modelled the effects of using binary stellar population models, compared with using traditional single stellar population models, and found that the escape fraction of ionising photons was about three times larger for the binary stars. This can lead to a much earlier end to reionisation.

Due to the high computational cost of running reionisation simulations, the use of convolutional neural networks (CNN) in relation is starting to be explored. [Gillet et al. \(2019\)](#) proposed the idea of using CNNs recover astrophysical parameters from 21-cm images, while [Chardin et al. \(2019\)](#) suggest that a CNN could be used instead of full radiative transfer simulations.

1.4.6 Zoom simulations

In numerical simulations, it is desirable to be able to model the large-scale density environment (e.g. to include the effect of tidal fields due to large-scale structure), while at the same time having high spatial and mass resolution, in order to accurately sample the smaller scales on which individual galaxies form. Doing this in an ordinary simulation box would require an unfeasibly large dynamic range, from many megaparsecs down to a few kiloparsecs. ‘Zoom’ simulations offer a neat solution, by sampling the large-scale fields with low resolution, while embedding a small, high resolution region in an area of interest

(e.g. [Katz et al., 1994](#); [Bertschinger, 2001](#)). Throughout most of this work we use MUSIC ([Hahn & Abel, 2011](#)), which produces accurate high-resolution zoom initial conditions, such as those shown in Figure 1.4. It is important that zoom simulations are checked carefully after running, to ensure that no low resolution (i.e. high mass) particles end up in the final haloes being studied. Such contamination can artificially modify the matter the distribution inside galaxies, rendering them unusable ([Oñorbe et al., 2014](#)).

1.4.7 Constrained simulations

Multiple parts of this thesis (Chapter 3, Chapter 4 and Chapter 5) use results based on constrained simulations, run as part of the CLUES¹ project. These simulations are designed to produce galaxies that resemble the Local Group (LG) of galaxies (e.g. the Milky Way, M31, M33—see § 3.1 for a more detailed discussion) while also accurately modelling the larger-scale structure surrounding the LG. Here we detail some of the background to producing these constrained simulations (for a nice discussion of these topics, see [Doumler, 2012](#)).

Reversed Zel’dovich approximation

The reversed Zel’dovich approximation (RZA) ([Doumler et al., 2013](#); [Sorce et al., 2014](#)) is used to reproduce the initial positions of haloes.

Given a density field, discretised using particles, the Zel’dovich approximation connects the initial positions of these particles $\mathbf{q}$ at z_0 to their comoving positions $\mathbf{x}(\mathbf{q}, z)$ (here we use comoving coordinates as defined in Equation (1.2.1)) at some later z through

$$\mathbf{x}(\mathbf{q}, z) = \mathbf{q} + \boldsymbol{\psi}(\mathbf{q}, z) \quad (1.4.8)$$

where $\boldsymbol{\psi}(\mathbf{q}, z)$ is the displacement field

$$\boldsymbol{\psi}(\mathbf{q}, z) = D(z)\boldsymbol{\psi}(\mathbf{q}, z_0) \quad (1.4.9)$$

with $D(z)$ the linear growing mode and $\boldsymbol{\psi}(\mathbf{q}, z_0)$ the linear displacement field at the initial redshift z_0 . From now on, we drop the explicit dependencies for clarity. Taking the time derivative of Equation (1.4.8) and using the definition of peculiar velocity Equation (1.2.31)

$$\mathbf{u} = a \frac{d\mathbf{x}}{dt} \quad (1.4.10)$$

and introducing the linear growth factor

$$f = \frac{d \ln D}{d \ln a} \quad (1.4.11)$$

¹Constrained Local Universe Simulations <https://www.clues-project.org/cms/>

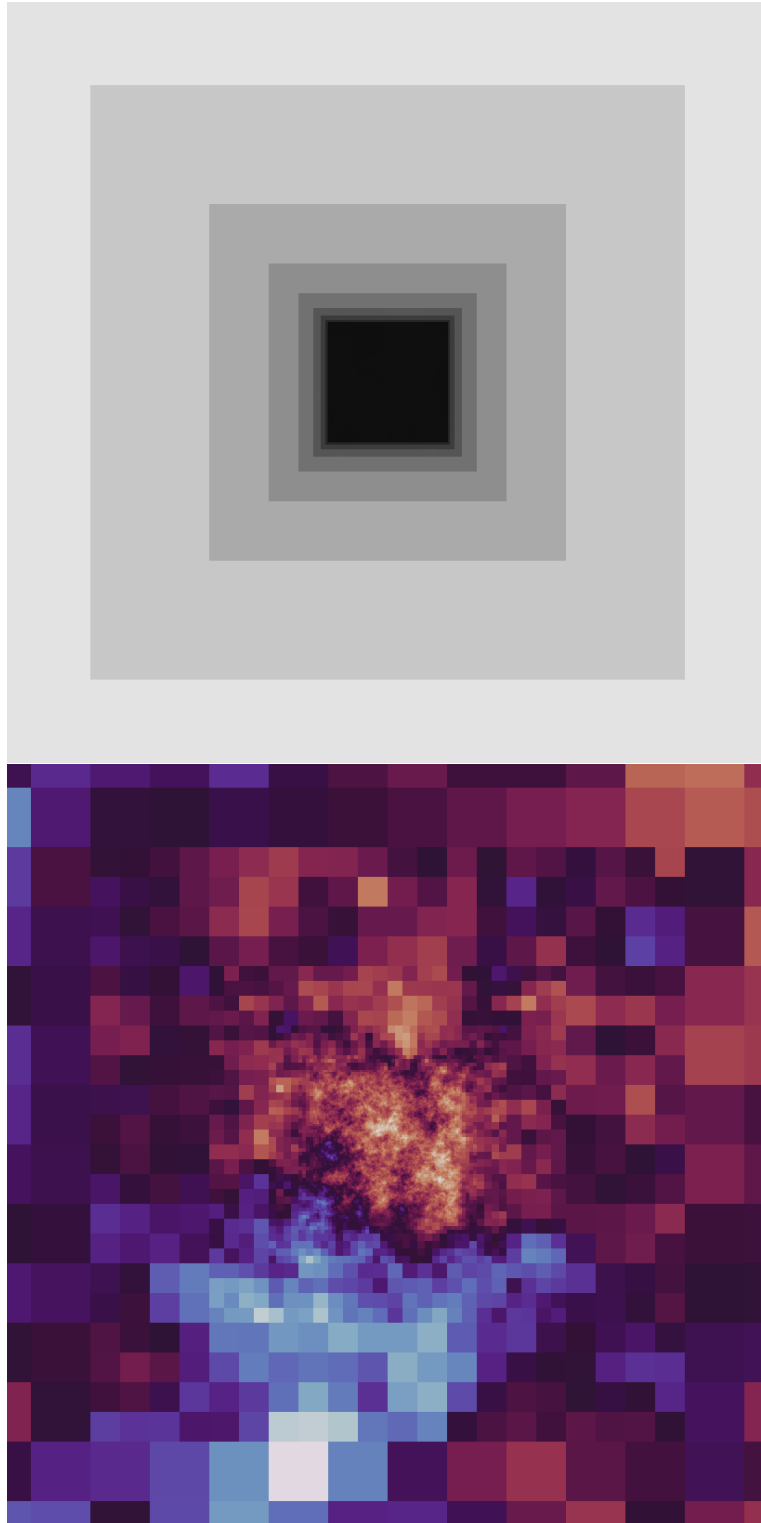


Figure 1.4: An example of high resolution zoom ICs produced by MUSIC. Top: the different levels of refinement, where each shade darker is twice better spatial resolution. Bottom: the corresponding density field, where the decrease in cell size can be clearly seen.

we can write the peculiar velocity in terms of the displacement field as

$$\mathbf{u} = \dot{a}f\boldsymbol{\psi}, \quad (1.4.12)$$

where $\dot{a} = da/dt$. At $z = 0$, $a = 1$ and so the comoving coordinates become equal to the physical coordinates, meaning

$$\mathbf{x} = \mathbf{r} = \mathbf{q} + \boldsymbol{\psi} \quad (1.4.13)$$

$$\mathbf{u} = \mathbf{v} = H_0 f \boldsymbol{\psi} \quad (1.4.14)$$

where H_0 is the Hubble constant today. This now yields a way to use observations of objects' positions today to map back to their initial locations $\mathbf{q}$, by reversing Equation (1.4.13)

$$\mathbf{q} = \mathbf{r} - \boldsymbol{\psi} \quad (1.4.15)$$

with

$$\boldsymbol{\psi} = \frac{\mathbf{v}}{H_0 f}. \quad (1.4.16)$$

The Zel'dovich approximation is only valid up to the first 'shell-crossing', where particles that were initially at different positions end up in the same position. Since Equation (1.4.8) does not account for interactions between particles, caustics form before promptly evaporating, as particles pass each other by without affecting each other. Hence, the RZA only works for structures whose dynamics have not deviated strongly from the linear theory prediction. If the dynamics of a structure have strongly deviated from the linear theory prediction, such as for orbiting substructure, then it is impossible to predict the dynamics at some time in the past from Equations (1.4.15) and (1.4.16) alone. This is one of the main limitations of the RZA.

Constrained initial conditions

Using observations of peculiar velocities in tandem with the RZA thus gives an estimate of the primordial positions of haloes. In order to translate these constraints into ICs, two further techniques are required: the Wiener filter (WF) (Zaroubi et al., 1995, 1999) and constrained realisations (CRs) (Bertschinger, 1987; Hoffman & Ribak, 1991). The WF is a method of reconstructing the three-dimensional density and velocity fields from observational data, such as galaxy peculiar velocities, including uncertainties. CRs enable simulators to generate cosmological ICs subject to a set of constraints. For further details

on the WF and CRs techniques, we direct the reader to the references in this section and to [Hoffman \(2009\)](#).

As pointed out earlier, the Zel’dovich approximation breaks down after shell-crossing, which means that the scales which determine the properties of the LG (such as the mass of MW and M31) are unconstrained by the RZA (as opposed to the scale on which, for example, Virgo forms). Thus, the extra small-scale information must be added in a trial-and-error fashion, by altering the random seeds for the large and small-scale fields, running the simulation and comparing to a set of cosmographic criteria.

1.4.8 RAMSES

For much of this thesis, we use the adaptive mesh refinement (AMR) N -body and hydrodynamical code called **RAMSES** ([Teyssier, 2002](#)). The N -body solver is similar to the one presented in [Kravtsov et al. \(1997\)](#). The N -body solver in **RAMSES** uses a multigrid method to solve Equation (1.4.3) on the AMR mesh, calculating the potential level-by-level starting from coarser levels and moving to finer levels ([Guillet & Teyssier, 2011](#)).

To use the fluid equations described in § 1.2.2, we need one final equation that describes the conservation of energy. In **RAMSES**, this is implemented as ([Teyssier, 2002](#))

$$\frac{\partial}{\partial t}(\rho e) + \nabla \cdot \left[\rho \mathbf{u} \left(e + \frac{p}{\rho} \right) \right] = -\rho \mathbf{u} \cdot \nabla \phi \quad (1.4.17)$$

where e is the specific total energy and the pressure p is given by

$$p = \rho(\gamma - 1) \left(e - \frac{1}{2} |\mathbf{u}|^2 \right), \quad (1.4.18)$$

where γ is a gas-dependent constant (for an ideal monatomic gas $\gamma = 5/3$). The solver that computes fluxes through cells is based on a second order Godunov method, while the gravitational source terms are solved with a fractional step approach (for details on these methods, see [Toro, 1999](#)). We use the atomic and metal cooling modules of **RAMSES**.

Originally, **RAMSES** only had N -body and hydrodynamical solvers but over the years different people have contributed extra features, making it a useful code for cosmological simulations. Current features include star formation ([Rasera & Teyssier, 2006](#)) and supernovae feedback ([Dubois & Teyssier, 2008](#)) (see § 1.4.9), magnetohydrodynamics ([Fromang et al., 2006](#)), and radiation hydrodynamics on both a fixed (**ATON**, [Aubert & Teyssier, 2008](#)) and adaptive grid (**RAMSES-RT**, [Rosdahl et al., 2013](#)).

1.4.9 Star formation and feedback

Even the highest-resolution **RAMSES** simulations presented in this thesis (Chapter 2 and Chapter 3) are too coarse to resolve the formation of individual stars. Instead, each stellar particle represents a population of stars, with masses of a few hundred to thousands of $M_\odot$. In these simulations, we use the traditional **RAMSES** density and temperature criteria to form stars (Rasera & Teyssier, 2006), allowing star formation where: i) the physical hydrogen number density n_H is greater than some threshold $n_\star$; ii) the local overdensity Δ is greater than $200\rho_{\text{cr}}$ and iii) wherever the temperature is below 2×10^4 K. The overdensity criterion is to stop spurious star formation at very high redshift, when all gas cells will exceed the threshold due simply to the small physical size of the universe. The temperature criterion is in place because gas with temperatures above $T > 2 \times 10^4$ K should be ionised and so hydrogen cooling becomes more inefficient, making it difficult to form stars. A temperature criterion such as this is often used in cosmological simulations (e.g. Stinson et al., 2006; Agertz et al., 2013; Ocvirk et al., 2016). Gas cells that satisfy these criteria are permitted to form star particles at a rate of

$$\frac{d\rho_\star}{dt} = \epsilon_\star \frac{\rho}{t_{\text{ff}}} \quad (1.4.19)$$

where $\epsilon_\star$ is the star formation efficiency (typically taken to be some small, global number e.g. $\epsilon_\star = 0.015$), ρ is the gas density and t_{ff} is the local free-fall time

$$t_{\text{ff}} = \left(\frac{32\pi}{3G\rho} \right)^{\frac{1}{2}}, \quad (1.4.20)$$

where G is Newton's gravitational constant. Star formation is a stochastic process, where N star particles form in a cell according to a Poisson process.

In simulations that employ star formation, we also include stellar feedback using the kinetic model of Dubois & Teyssier (2008), where part of the energy from a supernova is directly injected as kinetic energy into neighbouring cells and the rest is added as thermal energy. Supernovae also deposit metals into the surrounding cells.

1.5 Simulation analysis

1.5.1 Power spectra

One way of quantifying the growth of structure in the universe is through the power spectrum of density fluctuations. Taking the density contrast as defined in Equation (1.2.14)

at fixed cosmic time, we can transform into Fourier space using the convention

$$\delta(\mathbf{k}) = \int d^3\mathbf{x} \delta(\mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{x}} \quad (1.5.1)$$

from which the power spectrum $P(k)$ is defined as

$$\langle \delta(\mathbf{k}) \delta(\mathbf{k}') \rangle = (2\pi)^3 \delta_D(\mathbf{k} + \mathbf{k}') P(k) \quad (1.5.2)$$

δ_D is the Dirac delta function and $k = |\mathbf{k}|$ (e.g. [Bernardeau et al., 2002](#)). Matter in simulations is represented by discrete tracers, typically particles in the case of dark matter. Given that the number of particles in modern simulations can number many billions, tools like fast Fourier transforms (FFTs) are essential to rapidly compute the Fourier transforms required to compute $\delta(\mathbf{k})$. To estimate the density $\rho(\mathbf{x})$ in a form amenable to FFTs, the particle mass is first assigned to a regular grid, which is the same operation as computing the density for the PM method (see § 1.4.1). Each mass assignment method is imprinted on the power spectrum through the Fourier transform of the mass assignment function, which can be deconvolved from the power spectrum by dividing out the appropriate kernel ([Hockney & Eastwood, 1981](#); [Jing, 2005](#)).

In Figure 1.5 we show the power spectra in dimensionless form

$$\Delta^2(k) = \frac{k^3 P(k)}{2\pi^2} \quad (1.5.3)$$

from a test **RAMSES** N -body simulation, which contains 128^3 dark matter particles in a $64 h^{-1}$ Mpc box, for the ICs at $z = 99$ and evolved down to $z = 0$, calculated using **GenPK** ([Bird, 2017](#)). Also shown in Figure 1.5 is the input power spectrum at $z = 99$ calculated using **CAMB** (top) and linearly scaled down to $z = 0$ (bottom) using the linear growth factor as

$$P(k, z = 0) = \left[\frac{D(z = 0)}{D(z = 99)} \right]^2 P(k, z = 99) \quad (1.5.4)$$

where the growth factor is calculated as

$$D(z) = \frac{5E(z)\Omega_m}{2} \int_z^\infty d\tilde{z} \frac{1 + \tilde{z}}{E(\tilde{z})^3} \quad (1.5.5)$$

with

$$E(z) = \frac{H(z)}{H_0} \quad (1.5.6)$$

with $H(z)$ defined in Equation (1.2.13), with the appropriate change of variable $a = (1 + z)^{-1}$. From Figure 1.5 we can see that the ICs reproduce the input power spectrum

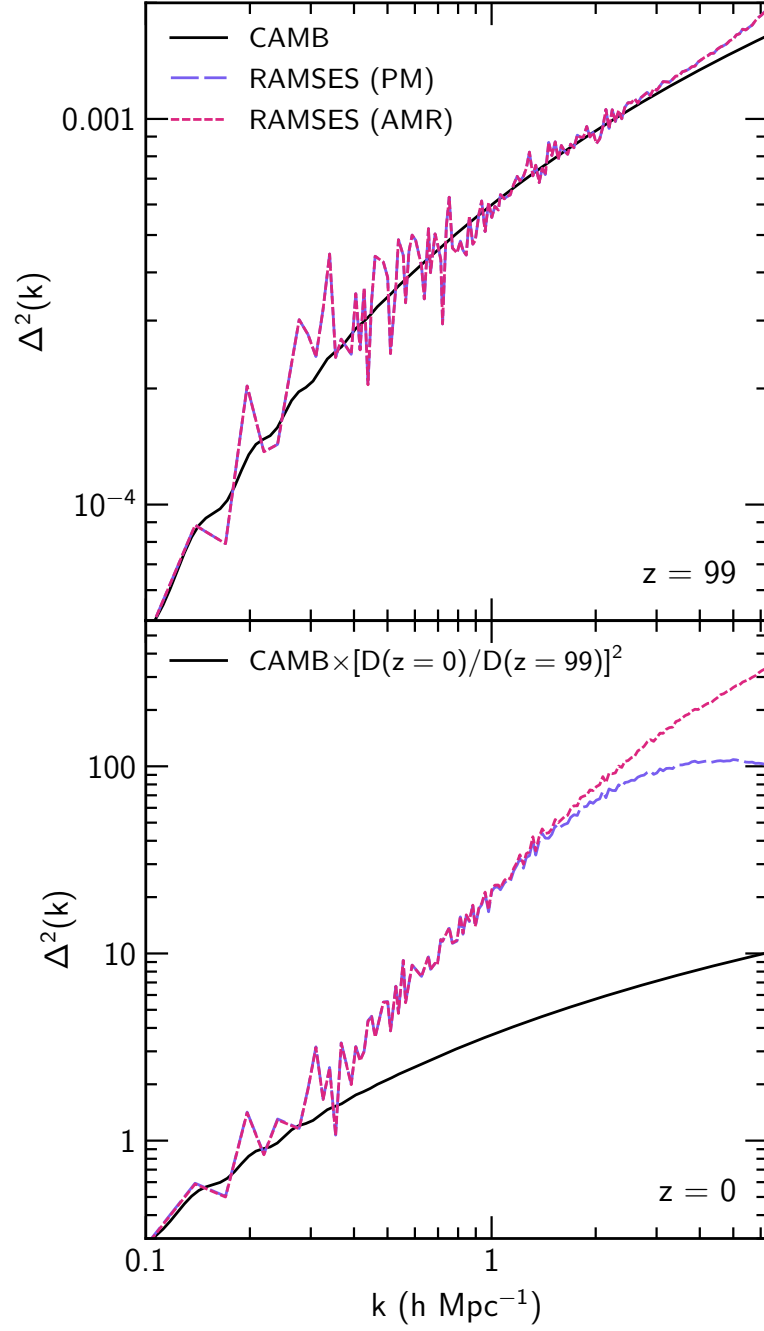


Figure 1.5: The measured matter power spectrum from a test N -body **RAMSES** simulation with 128^3 dark matter particles in a $64 h^{-1}$ Mpc box, for the simulation using only the particle-mesh solver (PM, blue long-dashed) and with four additional levels of refinement (AMR, pink short-dashed) along with the input power spectrum calculated by **CAMB**. We show the power spectrum in the ICs $z = 99$ (top) and at $z = 0$ (bottom) with the input power spectrum linearly scaled down to $z = 0$ using the linear growth factor $D(z)$.

closely, as expected. By $z = 0$ there is significant deviation from the linear theory prediction above $k \sim 0.3 \ h \text{ Mpc}^{-1}$ as nonlinear evolution takes over on small scales. The difference between the PM and AMR method becomes apparent too, as the extra refinement leads to a boost in small-scale power not present in the PM case.

1.5.2 Structure finding

Computing the power spectrum gives statistical information about the density field, but often we are interested in the properties of individual structures (see § 1.5.2). Extracting such structures from a cosmological simulation is a messy business and various tools exist for doing so. These tools can be broadly grouped into two main algorithms: friends-of-friends (FoF) (Davis et al., 1985) and spherical overdensity (SO) (Lacey & Cole, 1994). In the FoF method, all particles that are separated by less than some multiple b of the interparticle spacing $\bar{n}$ are grouped together, where typically $b = 0.2$. FoF algorithms have the advantage of not assuming any shape for the halo, instead allowing it to be dictated by the particle distribution, but have the disadvantage of potential ‘overlinking’ of nearby structures through a spurious particle connection. On the other hand, SO halo finders assume that haloes are spherical and work by growing shells out from some initial peak in the density field, until the average density inside these shells reaches some specified value. The threshold density is usually defined as some factor Δ times the mean or critical density in the universe, such that the mass M of a halo with radius R is given by

$$M = \frac{4\pi R^3}{3} \Delta \rho_\chi \quad (1.5.7)$$

with ρ_χ the choice of background density. Where SO haloes are used throughout this work, we take $\Delta = 200$ (close to $\Delta = 178$, cf. § 1.5.2) and $\rho_\chi = \rho_{\text{cr}}$. Halo masses computed using the SO method are sensitive to the choice of halo centre, as well as the method for identifying the initial peaks in the density field, and this constitutes the main differences between many SO implementations.

In this work we employ a variety of halo finders, including: **AHF** (Gill et al., 2004; Knollmann & Knebe, 2009) (Chapter 2, Chapter 3); **rockstar** (Behroozi et al., 2013a) (Chapter 4) and **pFoF** (Roy et al., 2014) (Chapter 5). Both **AHF** and **rockstar** are SO halo finders, though **rockstar** initially uses a spatial FoF search to identify groups for analysis, before searching in phase-space (i.e. using both position and velocity information) to identify subgroups which are eventually converted to haloes. **AHF** uses an adaptive grid to locate peaks in the density field and halo properties are calculated using particles determined to be gravitationally bound to this density peak. Removal of gravitationally

unbound particles is done by both **AHF** and **rockstar**. **pFoF** is a massively parallel version of a spatial FoF finder, designed to work with large **RAMSES** datasets. For a thorough comparison of halo finding methods, see [Knebe et al. \(2011\)](#).

With the halo catalogues in hand, we can construct halo mass functions. In the first instance, mass functions are computed by generating a histogram of the counts of haloes in each mass bin and dividing by the bin width and box volume, which yields an approximation to dn/dM . In this form, the halo mass function spans many orders of magnitude, so to clearly show deviations, we will plot a variant of the halo multiplicity function

$$g(M) = \frac{M^2}{\rho_m} \frac{dn}{dM} \quad (1.5.8)$$

which is related to the actual multiplicity function $f(\sigma)$ ([Jenkins et al., 2001](#)) by

$$f(\sigma) = g(M) \frac{d \ln M}{d \ln \sigma^{-1}} \quad (1.5.9)$$

where σ is the mass variance and is used here as a proxy for mass. Figure 1.6 shows the halo mass function for the test **RAMSES** N -body simulation highlighting, as with the power spectrum, the reduction in the low-mass halo abundance in the PM case compared to the AMR case.

1.5.3 Merger trees

The final piece of the puzzle in analysing structure formation is being able to follow the evolution of haloes in time. To do this, we use merger trees (e.g. [Lacey & Cole, 1993](#)), which track haloes back through the simulation. Moving backwards in time, haloes that exist today divide up into progenitors, where the progenitor that takes most of the halo's mass is the main progenitor.

Throughout this thesis, we use the **consistent-trees** package ([Behroozi et al., 2013b](#)), which models the gravitational dynamics of haloes to estimate positions and velocities of haloes throughout cosmic time, then comparing this to the actual haloes found in the simulations. As a first guess, **consistent-trees** requires particle-based merger trees, which give a rough estimate of halo ancestry between simulation snapshots, by assigning a halo's descendant as the one which hosts the largest number of the ancestor's particles. In order to use **consistent-trees** with **AHF** data, we use the conversion tools supplied with **AHF**. For a thorough comparison of merger tree tools, see [Srisawat et al. \(2013\)](#).

A useful measure of the growth of haloes is the mass accretion history $M(z)/M(z_0)$, where $M(z_0)$ is the mass of a halo at some time z_0 and $M(z)$ is the mass of that halo's

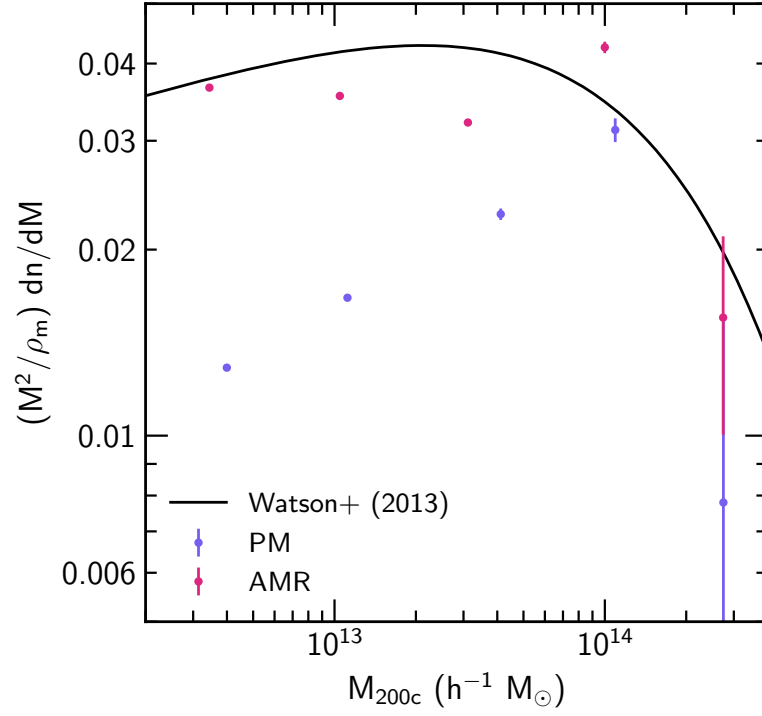


Figure 1.6: Halo multiplicity function at $z = 0$ for a test 128^3 *RAMSES* simulation, for the PM (purple) and AMR (pink) cases. Also shown is the fitting function of [Watson et al. \(2013\)](#). Haloes are identified using *AHF* for an overdensity $\Delta = 200$ with respect to the critical density ρ_{cr} .

progenitor at some earlier time $z > z_0$. As with the halo mass functions, theoretical models exist in the literature to make predictions for the mass accretion histories of haloes. Some models involve producing functional forms before fitting to simulations, like [McBride et al. \(2009\)](#) who fit to the Millennium simulation or [van den Bosch et al. \(2014\)](#) who fit to the Bolshoi simulations. [Correa et al. \(2015\)](#) produce an analytic model to relate the growth rate to the initial linear matter power spectrum. The mass accretion fits often have some dependence on the final mass $M(z_0)$, so when comparing to populations of haloes in simulations we will bin the haloes in mass and compute the mean mass accretion history $\langle M(z)/M(z_0) \rangle$ of all haloes in that bin.

Chapter 2

Relative baryon-dark matter velocities in cosmological zoom simulations

This work was begun by David Sullivan, Ilian T. Iliev, Anastasia Fialkov and Keri L. Dixon, but I have significantly redeveloped parts of the methodology and performed all the simulations and analysis.

This chapter is mostly adapted from *Relative baryon-dark matter velocities in cosmological zoom simulations* by [Conaboy, Iliev, Fialkov, Dixon & Sullivan \(2022a\)](#), submitted to Monthly Notices of the Royal Astronomical Society.

2.1 Introduction

The cosmic microwave background (CMB) radiation carries an image of the Universe at the moment of recombination, when the first neutral atoms formed at $z_{\text{rec}} \sim 1000$. Prior to recombination, photons and baryons were tightly coupled and oscillated as a single plasma. These oscillations, referred to as the baryon acoustic oscillations (BAO), are observed today as fluctuations of the CMB temperature (e.g. [Planck Collaboration et al., 2020](#)). At the moment of the baryons decoupling, the oscillations were also imprinted in the distribution of baryons, resulting in over and underdense regions. The initially tiny perturbations grew under the effect of gravity and are detected today in the distribution of galaxies on the largest cosmological scales (e.g. [Alam et al., 2017](#)).

Plasma oscillations did not only shape the post-recombination distribution of baryons, but also affected their velocities ([Sunyaev & Zeldovich, 1970](#)). [Tseliakhovich & Hirata](#)

(2010) were the first to point out that the BAO pattern is imprinted in the magnitude of the relative velocity between baryons and dark matter, because the latter was not coupled to the primordial plasma at the time of recombination. At decoupling, the relative velocity had a root-mean-square (RMS) of $\langle v_{\text{bc}}^2 \rangle^{\frac{1}{2}} \approx 30 \text{ km s}^{-1}$, or $\sim 10^{-4}c$ with c the speed of light. Over scales smaller than a few Mpc, the relative velocity is coherent, while the correlation length is of order a few hundred Mpc (Tseliakhovich & Hirata, 2010). At recombination the sound speed of the baryonic fluid dropped from being relativistic, $\sim c/\sqrt{3}$, to the thermal velocities of hydrogen atoms, $\sim 2 \times 10^{-5}c$, which is much smaller than the RMS value of v_{bc} . Therefore, on average, at decoupling baryons were travelling with supersonic velocities relative to the underlying potential wells generated by dark matter haloes (Tseliakhovich & Hirata, 2010). The relative velocity remained supersonic all the way down to $z \sim 15$ with a Mach number $\mathcal{M}_{\text{bc}} \approx 1.7$ over the redshift range $15 \lesssim z \lesssim 150$, sourcing shocks and entropy generation (Tseliakhovich & Hirata, 2010; O’Leary & McQuinn, 2012). The amplitude of the velocity field decayed with time as $(1+z)$, and thus the effect weakened as the Universe expanded. For instance, the signature of v_{bc} in the low- z three-point correlation function of BOSS CMASS galaxies was found to be negligible (e.g. Slepian et al., 2018).

In the post-recombination Universe, growth of structure on large cosmological scales is generally described by linear perturbation theory, which follows the evolution of density and velocity fields to the leading order in perturbations. Despite being formally second-order contributions, terms that involve the supersonic relative velocity can actually be as large as the first order terms. Moreover, on scales below the coherence scale, v_{bc} is position-independent and the second-order terms become effectively linear (Tseliakhovich & Hirata, 2010). Using such a ‘quasi-linear’ approach, analytical methods were employed to explore implications of v_{bc} in the cosmological context. Supersonic relative velocities modulate the abundance of minihaloes and their gas content on the BAO scale (e.g. Tseliakhovich & Hirata, 2010; Tseliakhovich et al., 2011; Fialkov et al., 2012; Ahn, 2016; Ahn & Smith, 2018), affecting fluctuations of the 21-cm signal of neutral hydrogen (e.g. Dalal et al., 2010; McQuinn & O’Leary, 2012; Visbal et al., 2012; Fialkov et al., 2013; Cohen et al., 2016; Fialkov et al., 2018; Muñoz, 2019; Muñoz et al., 2022).

Numerical simulations were used to explore non-linear effects of v_{bc} on scales well below its coherence scale. Such simulations typically employ boxes of several comoving Mpc or less and assume a position-independent velocity field. These simulations demonstrated that v_{bc} suppresses formation of small dark matter haloes (Naoz et al., 2012, 2013; O’Leary

& McQuinn, 2012), induces shocks (O’Leary & McQuinn, 2012), affects the formation of first stars (e.g. Maio et al., 2011; Stacy et al., 2011; Greif et al., 2011; Schauer et al., 2019, 2021) and black holes (e.g. Hirano et al., 2017; Schauer et al., 2017), and even helps shaping globular clusters (Naoz & Narayan, 2014; Chiou et al., 2019, 2021; Druschke et al., 2020).

Finally, a hybrid approach was used to incorporate the non-linear effects into the large-scale cosmological picture by tiling regions of fixed v_{bc} together (e.g. Visbal et al., 2012; Fialkov et al., 2013). In such studies, the distribution of v_{bc} on scales larger than the ‘pixel’ size was generated from the corresponding density field using the continuity equation, while star formation in each ‘pixel’ was calibrated to numerical simulations (Maio et al., 2011; Stacy et al., 2011; Greif et al., 2011; Naoz et al., 2012, 2013). This method was applied to the 21-cm signal of neutral hydrogen revealing enhanced BAO patterns (Visbal et al., 2012; Fialkov et al., 2013).

To fully capture the non-linear effect of v_{bc} in the cosmological context, it is necessary to properly include the velocity effect in the initial conditions of N -body and hydrodynamical simulations. Such a task would require an accurate non-linear treatment of dark matter, baryons, and radiation, starting at z_{rec} and following the growth of structure all the way down to the lowest simulated redshift. This treatment is not possible due to the large dynamical range: the amplitude of density fluctuations at recombination is smaller than the precision of many commonly used integration schemes. Today, state-of-the-art numerical simulations are typically initialised at $z_{\text{ini}} \sim 200$ with fields that do not reflect the relative velocity motion, thus missing the effect.

Recently, Ahn & Smith (2018) introduced a new cosmological initial condition generator BCCOMICS, based on a code that solves the quasi-linear equations between z_{rec} and z_{ini} for fixed values of large-scale density, δ , and v_{bc} at decoupling (Ahn, 2016). Next, the solver is applied to a larger cosmic volume divided in regions of fixed δ and v_{bc} . The code simulates the growth of small-scale structure inside density peaks and voids, by treating each patch of fixed δ and v_{bc} as a separate universe. Even though the eventual goal is to provide initial conditions for large-scale (few hundred Mpc) hydrodynamical adaptive mesh refinement (AMR) simulations, the current version of BCCOMICS was tested only on a suite of N -body and hydrodynamics simulations with box sizes of 1 – 4 Mpc at fixed values of v_{bc} and δ . The effect of v_{bc} and δ on the abundance of small haloes was estimated, and, in some cases, qualitative disagreement with prior works was reported. The authors intend to address this discrepancy as well as render the method applicable

to AMR simulations in their future work.

Here we take an independent approach and develop a new initial conditions generator. The basic principle is similar to BCCOMICS in that our code, as well, compensates for the lacking effect of v_{bc} between z_{rec} and $z_{\text{ini}} = 200$. After this compensation, the effect of v_{bc} from $z_{\text{ini}} = 200$ is naturally included by the simulation, through initialising the simulations with separate transfer functions for the baryon and dark matter velocities. We do not account for the large-scale effect of δ ; however, at the redshift of 200, the density correction is expected to be tiny (Ahn & Smith, 2018). Our methodology employs the widely used code MUSIC (Hahn & Abel, 2011) to generate high-resolution ‘zoom’ initial conditions (Bertschinger, 2001) in large cosmic volumes and by design is well-matched to AMR simulations. We demonstrate the performance by generating initial conditions in a $400 h^{-1}$ Mpc box before extracting a $100 h^{-1}$ Mpc subbox, which is used to run a simulation from $z_{\text{ini}} = 200$ to the final redshift of 11.2 with the AMR code RAMSES (Teyssier, 2002). We explore the performance by computing the effects of v_{bc} on the halo mass function, baryon fraction, and star formation. The paper is organised as follows: in § 2.2, we recap the theoretical background and discuss why large simulation box sizes are needed; in § 2.3.4, we discuss the simulation setup and our methodology for incorporating the effect of the v_{bc} through a scale-dependent bias parameter $b(k, v_{bc})$; in § 2.A.2 we present some tests of our module for solving the evolution equations, as well as a comparison to previous works; in § 2.4.2, we present the results of a first demonstration of our methodology and discuss the findings in § 2.5 and § 2.6; finally, in § 2.B we present a discussion on the effect of contamination on the HMF. Throughout this paper, we assume a flat Λ CDM cosmology consistent with the Planck 2018 results (Planck Collaboration et al., 2020), with parameters: $\Omega_m = 0.314$, $\Omega_\Lambda = 0.686$, $\Omega_b = 0.049$, $n_s = 0.965$, $\sigma_8 = 0.812$ and $h = 0.673^1$.

¹Wherever units are expressed in terms of h , it can be taken to be this value.

2.2 Theory

Writing Equation (1.2.18) and (1.2.19) for pressureless dark matter (denoted by ‘c’) and baryons (denoted by ‘b’), we obtain

$$\begin{aligned}
\frac{\partial \delta_c}{\partial t} + \frac{\mathbf{v}_c \cdot \nabla \delta_c}{a} &= -\frac{(1 + \delta_c) \nabla \cdot \mathbf{v}_c}{a}, \\
\frac{\partial \delta_b}{\partial t} + \frac{\mathbf{v}_b \cdot \nabla \delta_b}{a} &= -\frac{(1 + \delta_b) \nabla \cdot \mathbf{v}_b}{a}, \\
\frac{\partial \mathbf{v}_c}{\partial t} + \frac{(\mathbf{v}_c \cdot \nabla) \mathbf{v}_c}{a} &= -\frac{\nabla \phi}{a} - H \mathbf{v}_c, \\
\frac{\partial \mathbf{v}_b}{\partial t} + \frac{(\mathbf{v}_b \cdot \nabla) \mathbf{v}_b}{a} &= -\frac{\nabla \phi}{a} - H \mathbf{v}_b - \frac{\nabla p}{a \bar{\rho}_b (1 + \delta_b)},
\end{aligned} \tag{2.2.1}$$

$$\nabla^2 \phi = 4\pi G a^2 (\bar{\rho}_c \delta_c + \bar{\rho}_b \delta_b),$$

where we have not made the assumption that p is solely a function of ρ , as we did in Equation (1.2.21) and (1.2.22). Using this definition of the sound speed along with the ideal gas law Now splitting the velocities into a background bulk flow $\mathbf{v}^{(0)}$ and perturbations $\mathbf{u}$ such that $\mathbf{v} = \mathbf{v}^{(0)} + \mathbf{u}$, and discarding terms that are negligible or involve products of perturbations, we get

$$\begin{aligned}
\frac{\partial \delta_c}{\partial t} + \frac{\mathbf{v}_c^{(0)} \cdot \nabla \delta_c}{a} &= -\frac{\nabla \cdot \mathbf{u}_c}{a}, \\
\frac{\partial \delta_b}{\partial t} + \frac{\mathbf{v}_b^{(0)} \cdot \nabla \delta_b}{a} &= -\frac{\nabla \cdot \mathbf{u}_b}{a}, \\
\frac{\partial \mathbf{u}_c}{\partial t} + \frac{\mathbf{v}_c^{(0)} \cdot \nabla \mathbf{u}_c}{a} &= -\frac{\nabla \phi}{a} - H \mathbf{u}_c, \\
\frac{\partial \mathbf{u}_b}{\partial t} + \frac{\mathbf{v}_b^{(0)} \cdot \nabla \mathbf{u}_b}{a} &= -\frac{\nabla \phi}{a} - H \mathbf{u}_b - \frac{\nabla p}{a \bar{\rho}_b}.
\end{aligned} \tag{2.2.2}$$

Moving now to the rest frame of the dark matter (this differs slightly to the method of Tseliakhovich & Hirata (2010), who instead transform to the baryon rest frame) we have

$$\begin{aligned}
\mathbf{v}_c^{(0)'} &= 0, \\
\mathbf{v}_b^{(0)'} &= \mathbf{v}_b^{(0)} - \mathbf{v}_c^{(0)} = \mathbf{v}_{bc},
\end{aligned} \tag{2.2.3}$$

which we can substitute into Equations (2.2.2) to give

$$\begin{aligned}
\frac{\partial \delta_c}{\partial t} &= -\frac{\nabla \cdot \mathbf{u}_c}{a}, \\
\frac{\partial \delta_b}{\partial t} + \frac{\mathbf{v}_{bc} \cdot \nabla \delta_b}{a} &= -\frac{\nabla \cdot \mathbf{u}_b}{a}, \\
\frac{\partial \mathbf{u}_c}{\partial t} &= -\frac{\nabla \phi}{a} - H \mathbf{u}_c, \\
\frac{\partial \mathbf{u}_b}{\partial t} + \frac{\mathbf{v}_{bc} \cdot \nabla \mathbf{u}_b}{a} &= -\frac{\nabla \phi}{a} - H \mathbf{u}_b - \frac{\nabla p}{a \bar{\rho}_b}.
\end{aligned} \tag{2.2.4}$$

The importance of gas pressure on the growth of density modes was stressed by Naoz & Barkana (2005, 2007), and we follow them in solving an extra equation to track fluctuations in the baryon temperature δ_T . Turning to the pressure term in the equation for baryon velocity, we can write the gradient in terms of the baryon density ρ_b and temperature T as

$$\nabla p = \nabla \rho_b \frac{\partial p}{\partial \rho_b} + \nabla T \frac{\partial p}{\partial T} \tag{2.2.5}$$

and use the ideal gas law

$$p = \frac{k_B}{\mu m_p} \rho_b T, \tag{2.2.6}$$

where k_B is the Boltzmann constant, m_p the mass of the proton and $\mu = 1.22$ the mean molecular weight of the baryons in units of m_p , to calculate the derivatives in Equation (2.2.5)

$$\nabla p = \frac{k_B}{\mu m_p} (T \nabla \rho_b + \rho_b \nabla T). \tag{2.2.7}$$

Now writing the gradients in terms of perturbed quantities gives

$$\nabla \rho_b = \nabla [\bar{\rho}_b (1 + \delta_b)] = \bar{\rho}_b \nabla \delta_b \tag{2.2.8}$$

$$\nabla T = \nabla [\bar{T} (1 + \delta_T)] = \bar{T} \nabla \delta_T, \tag{2.2.9}$$

where the bars indicate average quantities, and substituting back into Equation (2.2.7) gives

$$\nabla p = \frac{k_B}{\mu m_p} [\bar{T} (1 + \delta_T) \bar{\rho}_b \nabla \delta_b + \bar{\rho}_b (1 + \delta_b) \bar{T} \nabla \delta_T] \tag{2.2.10}$$

which, ignoring negligible terms, yields

$$\frac{\nabla p}{a \bar{\rho}_b} = \frac{k_B \bar{T}}{\mu m_p} \frac{1}{a} (\nabla \delta_b + \nabla \delta_T). \tag{2.2.11}$$

Transforming into Fourier space, we can use the relation $\nabla f(\mathbf{x}) \rightarrow i\mathbf{k}f(\mathbf{k})$ (as we did in § 1.2.2) to write Equation (2.2.11) as

$$\frac{k_B \bar{T}}{\mu m_p} \frac{i\mathbf{k}}{a} (\delta_b + \delta_T) \quad (2.2.12)$$

and the Poisson equation as

$$-k^2 \phi = 4\pi G a^2 (\bar{\rho}_c \delta_c + \bar{\rho}_b \delta_b). \quad (2.2.13)$$

Now, we rearrange Equation (1.2.11) to give

$$4\pi G = \frac{3H^2}{2\rho_{cr}} \quad (2.2.14)$$

and substitute into Equation (2.2.13)

$$\phi = -\frac{3H^2 a^2}{2k^2} (\Omega_c \delta_c + \Omega_b \delta_b) \quad (2.2.15)$$

where we have used Equation (1.2.12) to write $\bar{\rho}_i/\rho_{cr} = \Omega_i$. Next, we write the velocities in terms of the velocity divergence θ as

$$\mathbf{u} = -\frac{ia\mathbf{k}}{k^2} \theta \quad (2.2.16)$$

and take the time derivative

$$\frac{\partial \mathbf{u}}{\partial t} = \frac{-i\mathbf{k}}{k^2} \left(a \frac{\partial \theta}{\partial t} + \theta \frac{\partial a}{\partial t} \right). \quad (2.2.17)$$

All of which substituted into Equations (2.2.4) gives, after some rearrangement,

$$\begin{aligned} \frac{\partial \delta_c}{\partial t} &= -\theta_c, \\ \frac{\partial \delta_b}{\partial t} &= -\frac{i\mathbf{v}_{bc} \cdot \mathbf{k}}{a} \delta_b - \theta_b, \\ \frac{\partial \theta_c}{\partial t} &= -\frac{3H^2}{2} (\Omega_c \delta_c + \Omega_b \delta_b) - 2H\theta_c, \\ \frac{\partial \theta_b}{\partial t} &= -\frac{3H^2}{2} (\Omega_c \delta_c + \Omega_b \delta_b) - 2H\theta_b - \frac{i\mathbf{v}_{bc} \cdot \mathbf{k}}{a} \theta_b + \frac{k_B \bar{T}}{\mu m_p} \frac{k^2}{a^2} (\delta_b + \delta_T) \end{aligned} \quad (2.2.18)$$

We follow Bovy & Dvorkin (2013) and Ahn (2016) in neglecting tracking fluctuations in photon density and temperature within the evolution equations, since they are subdominant at most of our scales and redshifts of interest. The equation for the temperature fluctuations then becomes

$$\frac{\partial \delta_T}{\partial t} = \frac{2}{3} \frac{\partial \delta_b}{\partial t} - \frac{x_e(t)}{a^4 t_\gamma} \frac{\bar{T}_\gamma}{\bar{T}} \delta_T, \quad (2.2.19)$$

where

$$t_\gamma^{-1} = \frac{8}{3} \rho_\gamma^0 \frac{\sigma_{Tc}}{m_e} = 8.55 \times 10^{-13} \text{ yr}^{-1}, \quad (2.2.20)$$

$T_\gamma = 2.726 \text{ K}/a$ is the mean photon temperature and $x_e(t)$ is the electron fraction out of the total number density of gas particles at time t . Both $x_e(t)$ and $\bar{T}$ are calculated using **recfast++** (Seager et al., 1999; Chluba et al., 2010; Chluba & Thomas, 2011). The initial conditions for δ_T are set as in Naoz & Barkana (2005), by requiring that $\partial(\delta_T - \delta_{T_\gamma})/\partial t = 0$ at the initial redshift $z = 1000$, where $\partial\delta_{T_\gamma}/\partial t$ is taken from CAMB (Lewis et al., 2000). This final set of equations to be solved is then

$$\begin{aligned} \frac{\partial\delta_c}{\partial t} &= -\theta_c, \\ \frac{\partial\delta_b}{\partial t} &= -\frac{\mathbf{v}_{bc} \cdot \mathbf{k}}{a} \delta_b - \theta_b, \\ \frac{\partial\theta_c}{\partial t} &= -\frac{3H^2}{2} (\Omega_c \delta_c + \Omega_b \delta_b) - 2H\theta_c, \\ \frac{\partial\theta_b}{\partial t} &= -\frac{3H^2}{2} (\Omega_c \delta_c + \Omega_b \delta_b) - 2H\theta_b - \frac{\mathbf{v}_{bc} \cdot \mathbf{k}}{a} \theta_b + \frac{k_B \bar{T}}{\mu m_p} \frac{k^2}{a^2} (\delta_b + \delta_T), \\ \frac{\partial\delta_T}{\partial t} &= \frac{2}{3} \frac{\partial\delta_b}{\partial t} - \frac{x_e(t)}{a^4 t_\gamma} \frac{\bar{T}_\gamma}{\bar{T}} \delta_T. \end{aligned} \quad (2.2.21)$$

Tselikhovich & Hirata (2010) showed that most of the contributions to the variance of the v_{bc} come from scales between $0.005 h \text{ Mpc}^{-1}$ and $0.5 h \text{ Mpc}^{-1}$. In a similar fashion to Pontzen et al. (2020), we can compute the RMS v_{bc} inside a box of size L by integrating the power spectrum of v_{bc} fluctuations from the fundamental mode of the box $k_{\min} = 2\pi/L$ to infinity. The mean square v_{bc} in a box of size L is given by

$$\langle v_{bc}^2 \rangle_L = \int_{2\pi/L}^{\infty} dk \frac{\Delta_{v_{bc}}^2}{k} \quad (2.2.22)$$

where $\Delta_{v_{bc}}^2$ is the dimensionless power spectrum of the v_{bc} , taken from CAMB. In theory, the upper limit of the integral in Equation (2.2.22) should be the maximum wavenumber of the box, dictated by the number of simulation elements. In practice, however, any upper limit $k_{\max} \gg 0.5 h \text{ Mpc}^{-1}$ is sufficient, since the v_{bc} power spectrum drops off rapidly above this value. Figure 2.1 shows the RMS v_{bc} , calculated as the square root of Equation (2.2.22), where the oscillatory nature of $\Delta_{v_{bc}}^2$ at low- k (cf. Figure 1 in Tselikhovich & Hirata, 2010) is clearly visible. From Figure 2.1 we can see that even in a box size of $100 h^{-1} \text{ Mpc}$, we do not capture all of the scales relevant to the v_{bc} . The curve only begins to plateau around $\sim 400 h^{-1} \text{ Mpc}$, and so using a box size smaller than this means

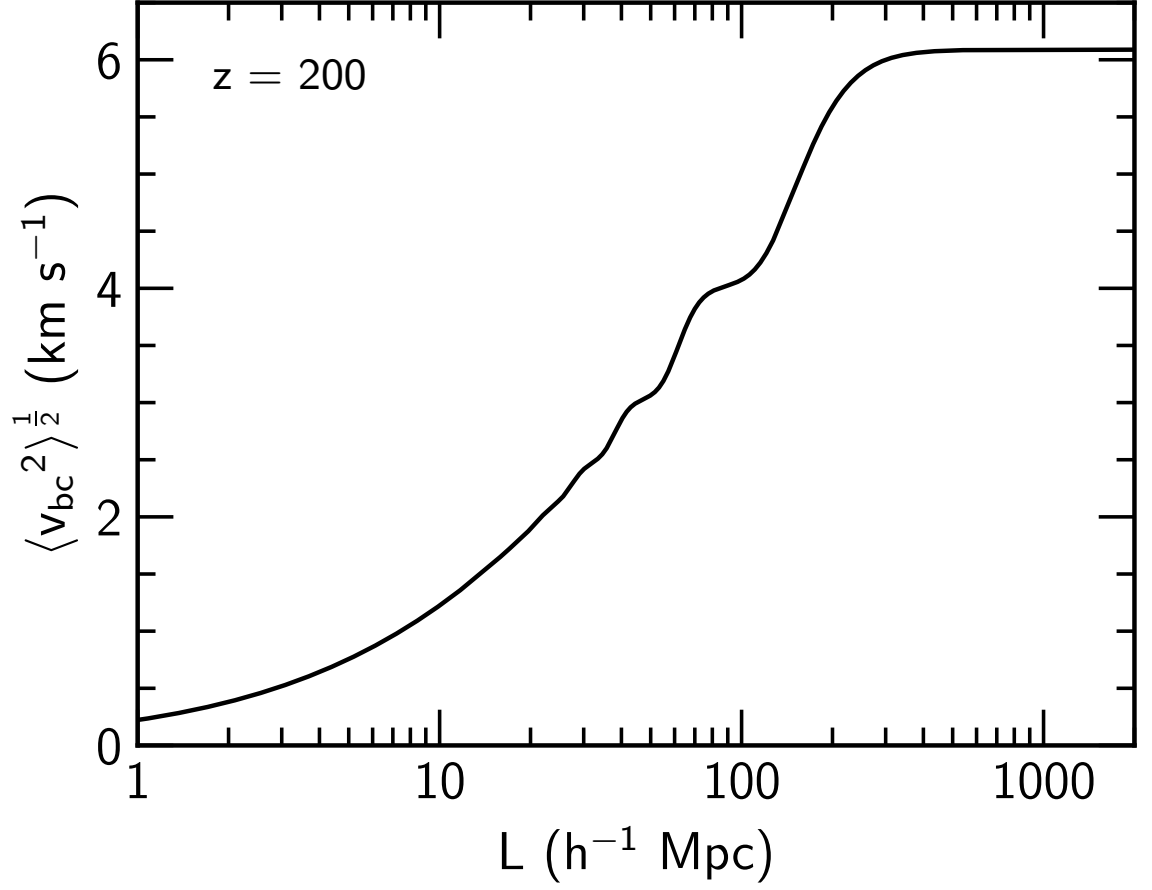


Figure 2.1: RMS v_{bc} at $z = 200$ as a function of box size, calculated by integrating the v_{bc} power spectrum from $2\pi/L$ to $3365 h \text{ Mpc}^{-1}$. The v_{bc} power spectrum is computed for the cosmological parameters listed in § 2.1.

that we may miss out on some of the effect, for example by not sampling extreme values of the v_{bc} . Simultaneously simulating this large scale box and the very high-resolution zoom region needed to observe the effect would be computationally infeasible. In § 2.3.2 we discuss our solution to this problem.

2.3 Methods

2.3.1 Simulations

We follow the evolution of dark matter, gas, and stars in the cosmological context using **RAMSES**², which employs a second-order Godunov method to solve the equations of hydrodynamics. Gas states are computed at cell interfaces using the Harten-Lax-van Leer-contact Riemann solver, with a MinMod slope limiter. Dark matter and stars are modelled as a collisionless N -body system, described by the Vlasov-Poisson equations. Grid refinement is performed whenever a cell contains more than eight high-resolution dark matter particles, or has the equivalent amount of baryonic mass scaled by Ω_b/Ω_m . We set the maximum AMR level to be $\ell_{\max} = 23$ and allow free refinement from the coarsest level $\ell_{\min} = 8$ to $\ell = 21$, beyond which grid hold-back prevents higher-resolution AMR grids being released, meaning that the finest comoving resolution achieved is $47.7 h^{-1}$ pc. Releasing higher levels of AMR grids at specified steps in scale factor (‘grid hold-back’) is a technique employed in **RAMSES** to ensure that the *physical* (as opposed to comoving) resolution remains roughly constant over an entire simulation, which is desirable for e.g. ensuring that cells at high redshift do not over-refine and end up containing too little mass to form stars. [Snaith et al. \(2018\)](#) performed a detailed study into the effects of grid hold-back on simulation properties, finding, among other things, that the sudden release of high-resolution grids can lead to spikes in the star formation rate.

Star formation is allowed whenever the gas density of a cell is greater than $n_{\star} = 1 \text{ cm}^{-3}$ in units of the number density of hydrogen atoms and when the local overdensity is greater than $200\rho_{\text{cr}}$, where the latter condition prevents spurious star formation at extremely high-redshift. We impose a polytropic temperature function with index $g_{\star} = 2$ and $T_0 = 1050 \text{ K}$, which ensures that the Jeans length is always resolved by at least eight cells. We do not rigorously calibrate the star formation parameters to reproduce any stellar mass-halo mass relation, since we are interested only in the differences between simulations. Star particles, which represent a population of stars, form with a mass of $108.0 h^{-1} M_{\odot}$. Supernova

²The version used here is commit `aa56bc01` from the `master` branch. Note that older versions of **RAMSES** may not use separate fields for dark matter and baryon velocities by default.

feedback is included using the kinetic feedback model of [Dubois & Teyssier \(2008\)](#), with a mass fraction $\eta_{\text{SN}} = 0.1$ and a metal yield of 0.1. A star particle goes supernova after 10 Myr. We allow gas cooling and follow the advection of metals. We do not include molecular hydrogen in this simulation so, to attempt to compensate for this missing cooling channel, we initialise the zoom region with a metallicity of $Z = 10^{-3} Z_{\odot}$, where $Z_{\odot} = 0.02$ in RAMSES.

2.3.2 Initial conditions

As described in § 2.2, large box sizes of $\gtrsim 400 h^{-1}$ Mpc are required in order to capture all of the scales pertaining to v_{bc} . By performing calibration runs, we found that very high resolution (a cell size of $\Delta x \lesssim 2 h^{-1}$ kpc) is needed in the ICs in order to properly resolve the effect. To this end, we employ ‘zoom’ initial conditions (ICs), generating density and velocity fields at $z_{\text{ini}} = 200$ first in a $400 h^{-1}$ Mpc box using MUSIC ([Hahn & Abel, 2011](#)). The ICs are refined from the base level $\ell_{\text{min}} = 10$ (1024^3) up to $\ell = 18$ (262144^3 effective) in a cube of side length $543 h^{-1}$ kpc at the finest level. Since the zoom region is very small compared to the box size, we use extra padding between zoom levels, increasing the number of padding cells on each side for each dimension from the typical value of 4 to 32. We use transfer functions from CAMB ([Lewis et al., 2000](#)), which gives distinct density and velocity fields for the baryons and dark matter.

In order to make the simulation tractable, we extract a $100 h^{-1}$ Mpc ($\ell_{\text{min}} = 8$, 256^3) base grid from the $400 h^{-1}$ Mpc ($\ell_{\text{min}} = 10$, 1024^3) box and use this as our coarsest level, meaning that the maximum refinement level in the zoom region also drops two levels from $\ell = 18$ to $\ell = 16$ (65536^3 effective). This amounts to using periodic boundary conditions on a box that is now no longer periodic and, as a result, some very large-scale modes present

Table 2.1: The sets of ICs used for the main zoom simulation. The columns list the name of each case, which velocity fields are used for the baryons ($\mathbf{v}_{\text{b}}$), whether the baryon fields have been modified and the magnitude of v_{bc} at $z = 1000$ ($v_{\text{bc,rec}}$), and $z = 200$ ($v_{\text{bc,ini}}$) in km s^{-1} . If a value is present for $v_{\text{bc,ini}}$, but not $v_{\text{bc,rec}}$, then v_{bc} is only included from the start time of the simulation.

Case	$\mathbf{v}_{\text{b}}$	Modified?	$v_{\text{bc,rec}}$	$v_{\text{bc,ini}}$ (km s^{-1})
no v_{bc}	$\mathbf{v}_{\text{c}}$	no	0.0	0.0
$v_{\text{bc-ini}}$	$\mathbf{v}_{\text{b}}$	no	0.0	20.09
$v_{\text{bc-rec}}$	$\mathbf{v}_{\text{b}}$	yes	100.07	20.09

in the initial conditions will not be accurately reproduced in the simulation, since the simulation box size is smaller. Further, structures near the edge of the new base grid will also be inaccurately reproduced, since now when particles leave one side of the box, they re-enter in a totally unrelated patch of the universe. While our choice of boundary conditions may introduce some error, this error will be common to all the sets of simulations and so will wash out when comparing between the runs. Errors around the sub-box edges will also have little impact, since we are concerned with a sub- h^{-1} Mpc zoom region in the centre of the box. This compromise is necessary in order to be able to sample the relative velocity from the large box.

We selected a region for zoom-in with $v_{\text{bc,ini}} = 20.09 \text{ km s}^{-1}$ at $z = 200$, corresponding to $v_{\text{bc,rec}} = 100.07 \text{ km s}^{-1}$, or $\sim 3.3\sigma_{v_{\text{bc}}}$, at recombination. Given that the relative velocities follow a Maxwell-Boltzmann distribution (e.g. [Tsaliakhovich et al., 2011](#)), we can estimate how rare a patch of the universe with this v_{bc} is by integrating over the distribution. Switching variable from v_{bc} to $\beta = v_{\text{bc}}/\sigma_{v_{\text{bc}}}$ we find

$$P(> 3.3) = \int_{3.3}^{\infty} d\beta P(\beta) \quad (2.3.1)$$

$$= 3.8 \times 10^{-7}, \quad (2.3.2)$$

meaning there should be roughly one $3 h^{-1}$ Mpc patch in our $400 h^{-1}$ Mpc box with $\beta > 3.3$. In contrast, for $\beta = 2$ we find $P(> 2) = 7.4 \times 10^{-3}$, which corresponds to $\sim 10^4$ $3 h^{-1}$ Mpc patches in our $400 h^{-1}$ Mpc box. While this value of v_{bc} is rare, it is likely to exist given a large enough box, and therefore is an interesting single case study to demonstrate the effect of v_{bc} in our methodology. Lower values of v_{bc} lead to a weaker effect on structure and star formation, though these lower values are more important for studies on the spatial fluctuations of v_{bc} , since they are more prevalent.

Table 2.1 details the sets of ICs used in this work. The no v_{bc} case is often used in cosmological simulations, for example when using transfer functions that do not have separate amplitudes for the baryon and dark matter velocity fields (in fact, it is the default behaviour for older versions of **RAMSES**, where the dark matter velocity field is used to initialise both the dark matter and baryon velocities). The $v_{\text{bc}}\text{-ini}$ case is where the simulation is initialised using separate transfer functions for the baryon and dark matter velocity fields, such as by generating ICs using **MUSIC** with transfer functions from **CAMB**. In this case, v_{bc} is included from the start time of the simulation z_{ini} , but the effect of v_{bc} on density and velocity perturbations between recombination and z_{ini} is missed. In the final, and most realistic, case, $v_{\text{bc}}\text{-rec}$, we include the contributions from v_{bc} across all z

by computing a bias factor which is applied to the ICs. The methodology for computing the bias factor is detailed in § 2.3.3.

2.3.3 Bias factor

Using transfer functions that have distinct amplitudes for the baryon and dark matter velocity fluctuations naturally yields the v_{bc} field at the start time of the simulation z_{ini} . First, we interpolate the dark matter particle velocities onto the same grid as the baryons, then take the difference of these two fields to calculate the magnitude as $v_{bc} = |\mathbf{v}_b - \mathbf{v}_c|$. A $0.39 h^{-1}$ Mpc thick slice through the resultant v_{bc} field is shown in Figure 2.2.

With the v_{bc} field in hand, we split our ICs into cubic patches, aiming for a patch extent of $0.5 h^{-1}$ Mpc, though the actual extent depends upon how many patches can be fit in each level of the **grafic** files. The size of these patches is chosen to be smaller than the scale over which v_{bc} is coherent (Tseliaxhovich & Hirata, 2010). Within each patch, the average value of v_{bc} is calculated and used as v_{bc} in equations (2.2.4). The initial values for equations (2.2.4) are set using the transfer functions from CAMB at $z = 1000$, and the equations are integrated from $z = 1000$ to $z = 200$ using the LSODA ordinary differential equation solver. Equations (2.2.4) are solved for the average patch value of v_{bc} and also for $v_{bc} = 0 \text{ km s}^{-1}$, which yields power spectra for the baryon perturbations both with and without v_{bc} . We use these power spectra to calculate a ‘bias’ factor at $z_{\text{ini}} = 200$ that depends both upon scale k and the magnitude of the relative velocity v_{bc}

$$b(k, v_{bc}) = \left[\frac{P(k, v_{bc})}{P(k, v_{bc} = 0)} \right]^{\frac{1}{2}}, \quad (2.3.3)$$

where the square root arises from $P \propto |\delta^2|$. In Figure 2.3, we show the bias factor for the baryon and dark matter densities (δ_b and δ_c) and velocities (v_b and v_c), computed for the average v_{bc} in our zoom region. The strongest suppression is seen in the baryons and in particular the baryon density, while the dark matter is hardly affected. We do not expect the oscillatory features in $b(k, v_{bc})$ at the very small scales to have much, if any, impact since the power spectrum of fluctuations in the baryon density contrast begins to fall rapidly for $k \gtrsim 300 h \text{ Mpc}^{-1}$, while for the velocity most of the power is at much larger scales. Ali-Haïmoud et al. (2014) also found oscillatory features in the small-scale baryon perturbations, and we have checked that we find similar oscillations for typical values of v_{bc} and also find that increasing the magnitude of v_{bc} increases the frequency of oscillations for the larger-scale ($\sim 100 h \text{ Mpc}^{-1}$) modes too.

This factor is then convolved with the Fourier transform of the corresponding patch

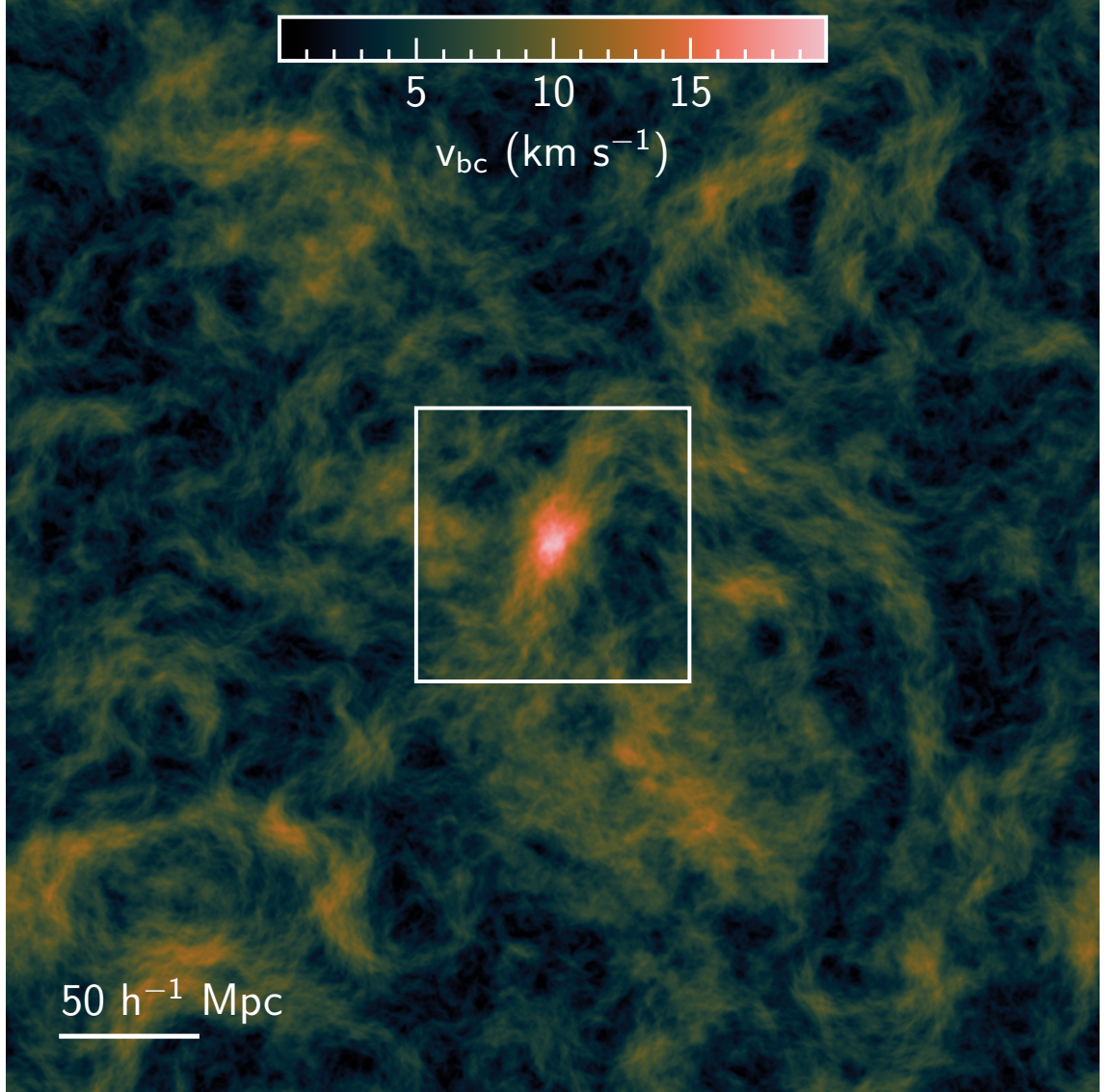


Figure 2.2: A slice through the large-scale $v_{bc} = |\mathbf{v}_b - \mathbf{v}_c|$ field in the full $400 h^{-1} \text{ Mpc}$ initial conditions at $z_{ini} = 200$. Each pixel corresponds to a cell width of $0.39 h^{-1} \text{ Mpc}$ and the slice has a thickness of one cell width. Also shown (white square) is the position of the extracted $100 h^{-1} \text{ Mpc}$ subbox, centred on the peak v_{bc} in the ICs. The zoom region is located in the centre of the subbox. The colour shows the magnitude of the v_{bc} at $z_{ini} = 200$, where light pink is high v_{bc} and dark blue is low v_{bc} .

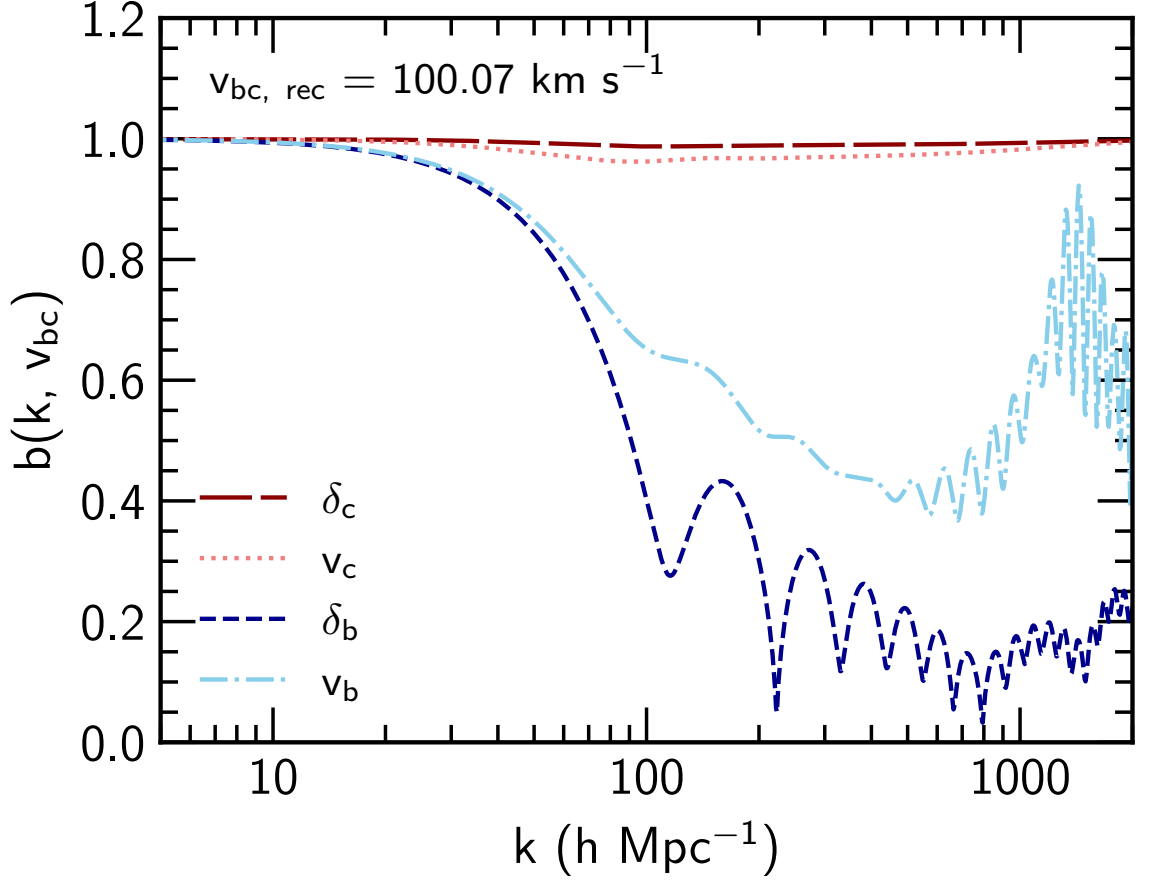


Figure 2.3: The bias factors $b(k, v_{bc})$ at $z_{\text{ini}} = 200$ for the average v_{bc} in the zoom region, scaled back to its value at recombination $v_{bc, \text{rec}} = 100.07 \text{ km s}^{-1}$, which is a $\sim 3.3\sigma_{v_{bc}}$ value. We show $b(k, v_{bc})$ for baryon and dark matter overdensities and peculiar velocities. These are the bias factors that are applied to the perturbations in the zoom region. Note how the perturbations in the baryon overdensity (dark blue, short-dashed) are strongly suppressed for $k > 40 \text{ h Mpc}^{-1}$, while the perturbations in the dark matter overdensity (dark red, long-dashed) are largely unaffected, to the few per cent level. Note that we show $b(k, v_{bc})$ for the peculiar velocities for the full range of k , but the velocity field is dominated by large-scale (small- k) modes. Therefore, $b(k, v_{bc})$ will have little if any impact on small scales (large- k).

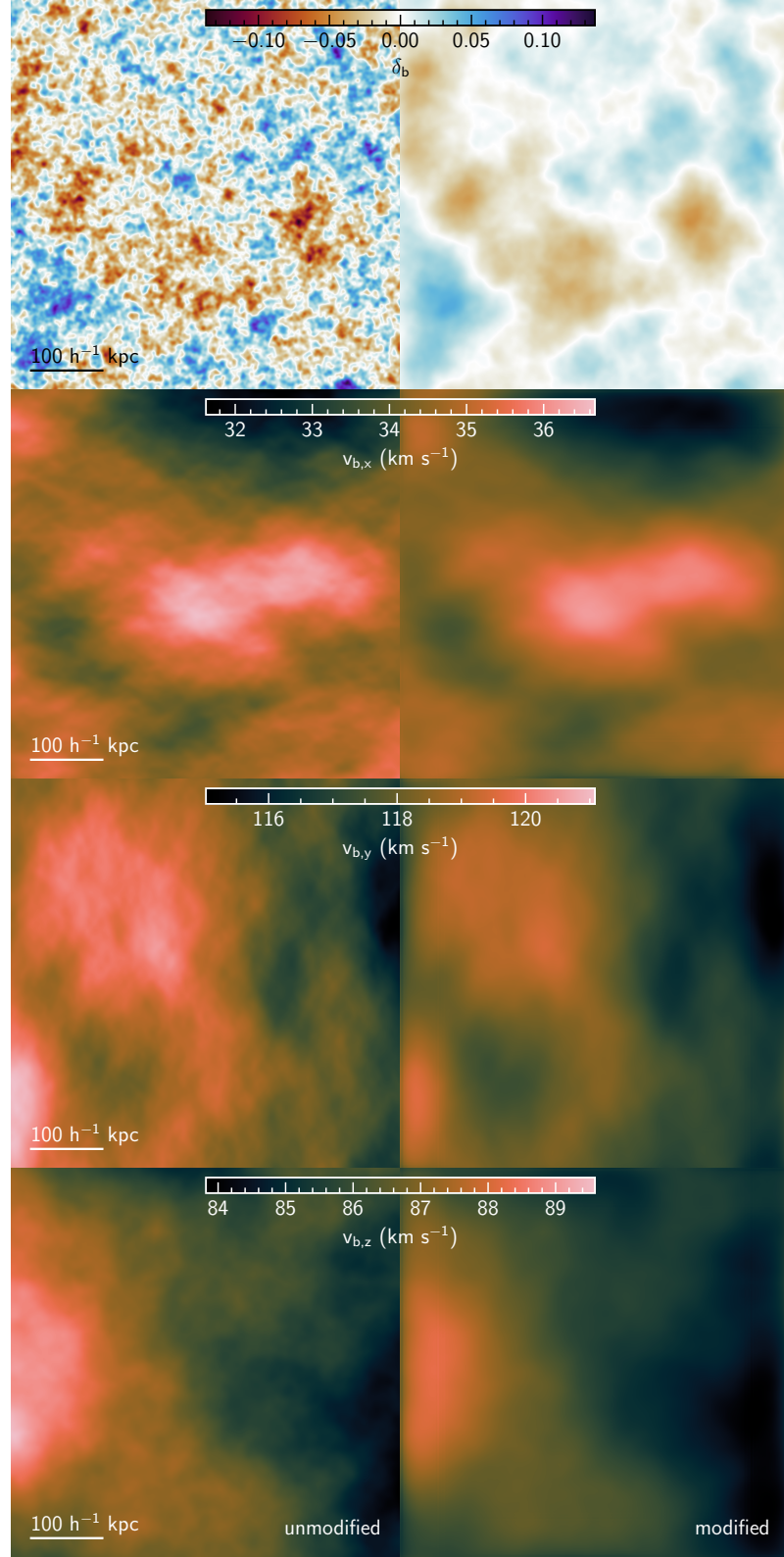


Figure 2.4: Slices of the unmodified (left column) and modified (right column) baryon overdensity (top row), peculiar velocity in the x -direction (second row), y -direction (third row) and z -direction (bottom row) in the high-resolution zoom region, of side length $543 h^{-1} \text{ kpc}$. Each pixel corresponds to a cell width of $1.53 h^{-1} \text{ kpc}$ and the slice has a thickness of one cell width. The effect of applying $b(k, v_{bc})$ can be clearly seen in the baryon overdensity, in that it washes out the small-scale fluctuations. The effect is less pronounced in the peculiar velocities, which are dominated by large scale modes.

of baryon overdensity

$$\hat{\delta}_b(k, v_{bc}) = b(k, v_{bc}) \cdot \delta_b(k) \quad (2.3.4)$$

to give individual patches of biased overdensity $\hat{\delta}_b$, which are then stitched together to generate the v_{bc} -rec set of ICs. In this way, the bias factor compensates for the suppression of baryon perturbations between $z = 1000$ and z_{ini} that is missing if v_{bc} is included only from z_{ini} . We only modify the baryons, since as discussed earlier, they are much more strongly affected than the dark matter, as can be seen from Figure 2.3.

We deal with the peculiar velocity field for the baryons in a similar way, by first converting the velocity divergence to peculiar velocities as $\mathbf{v}_b(k) = -ia\mathbf{k}\theta_b(k)/k^2$. Note again that we do not include directionality when solving the evolution equations, and therefore, the bias factor is applied to each direction of $\mathbf{v}_b$ equally. In reality, there would be preferential directions for the bias factor, depending on the direction of $\mathbf{v}_{bc}$, but we defer that implementation.

Figure 2.4 shows a $1.53 h^{-1}$ kpc thick slice through the highest resolution level of the zoom ICs directly from MUSIC (‘unmodified’, left column) and after the bias factor $b(k, v_{bc})$ has been applied (‘modified’, right column). For δ_b (top row), the unmodified ICs contain a lot of small-scale structure, which is almost totally washed out after applying $b(k, v_{bc})$. Most of what remains is in the form of lower amplitude, larger scale fluctuations. For $v_{b,i}$ (bottom rows)³, there is less small-scale structure to begin with, since the peculiar velocity fields are dominated by large scales. The effect of $b(k, v_{bc})$ on $v_{b,i}$ is therefore much less striking than on the δ_b , with the main effect being smoothing and a slight reduction in amplitude.

2.3.4 Haloes

After the ICs have been correctly initialised with v_{bc} , we can characterise the effect of v_{bc} on structure formation, principally by exploring how haloes are affected. Haloes are identified using AHF (Gill et al., 2004; Knollmann & Knebe, 2009), which supports multi-resolution datasets and calculates baryonic properties of haloes. In order to use AHF with a RAMSES dataset, we use the supplied `ramses2gadget` tool to convert leaf cells of the AMR hierarchy into gas pseudoparticles placed at the centre of each cell. We ignore the internal energy of the gas and do not allow AHF to perform any unbinding, as this has been shown to remove most of the gas from haloes in a manner that is highly dependent upon the

³Note that we show the v_b for each direction for completeness, but the effect is independent of direction in our methodology.

choice of halo finder (Knebe et al., 2013). We define the halo overdensity with respect to the critical density ρ_{cr} , such that the average density inside the halo is $200\rho_{\text{cr}}$.

Guided by the resolution of Naoz & Barkana (2007), we perform our analysis on haloes that have ≥ 500 particles, as they found that this is the level at which the baryon fraction is resolved with a scatter of ~ 20 per cent when compared to higher resolution simulations.

We only use haloes comprised entirely of high-resolution dark matter particles, since contaminant low-resolution particles can disrupt the dynamics of haloes (Oñorbe et al., 2014). Due to the small size of the zoom region, it is often the case that haloes which were initially solely composed of high-resolution particles can become contaminated by low-resolution particles as the simulation progresses. If contaminated haloes are removed at each timestep, then haloes can ‘disappear’ if they become contaminated between one timestep and the next. To counter this effect, we generate merger trees using **consistent-trees** (Behroozi et al., 2013b) and only keep haloes that have never been contaminated at any point in the simulation. When exploring the effect on halo properties, such as when looking at their gas content, we go one step further and match haloes between the simulations. We do this using AHF’s **MergerTree** tool to correlate the particle IDs between each run. This allows us to isolate the effect on identical haloes, as opposed to also capturing the impact on the global population of haloes.

2.4 Results

In this section we discuss the impact of v_{bc} on the halo baryon fraction and star formation. We do not present results on the impact on the HMF due to halo contamination, and present a discussion of our reasoning for not doing so in § 2.B.

2.4.1 Baryon fraction

We allow star formation in these runs, so the total baryon fraction of a given halo is defined as

$$f_{\text{b}} = \frac{M_{\text{g}} + M_{\star}}{M_{\text{d}} + M_{\text{g}} + M_{\star}}, \quad (2.4.1)$$

where M_{g} is the gas, $M_{\star}$ the stellar, and M_{d} the dark matter mass in each halo. We upweight the best resolved (i.e. most massive) haloes by calculating the mass-weighted average baryon fraction as

$$\langle f_{\text{b}} \rangle_M = \frac{\sum_i f_{\text{b},i} M_i}{\sum_i M_i} \quad (2.4.2)$$

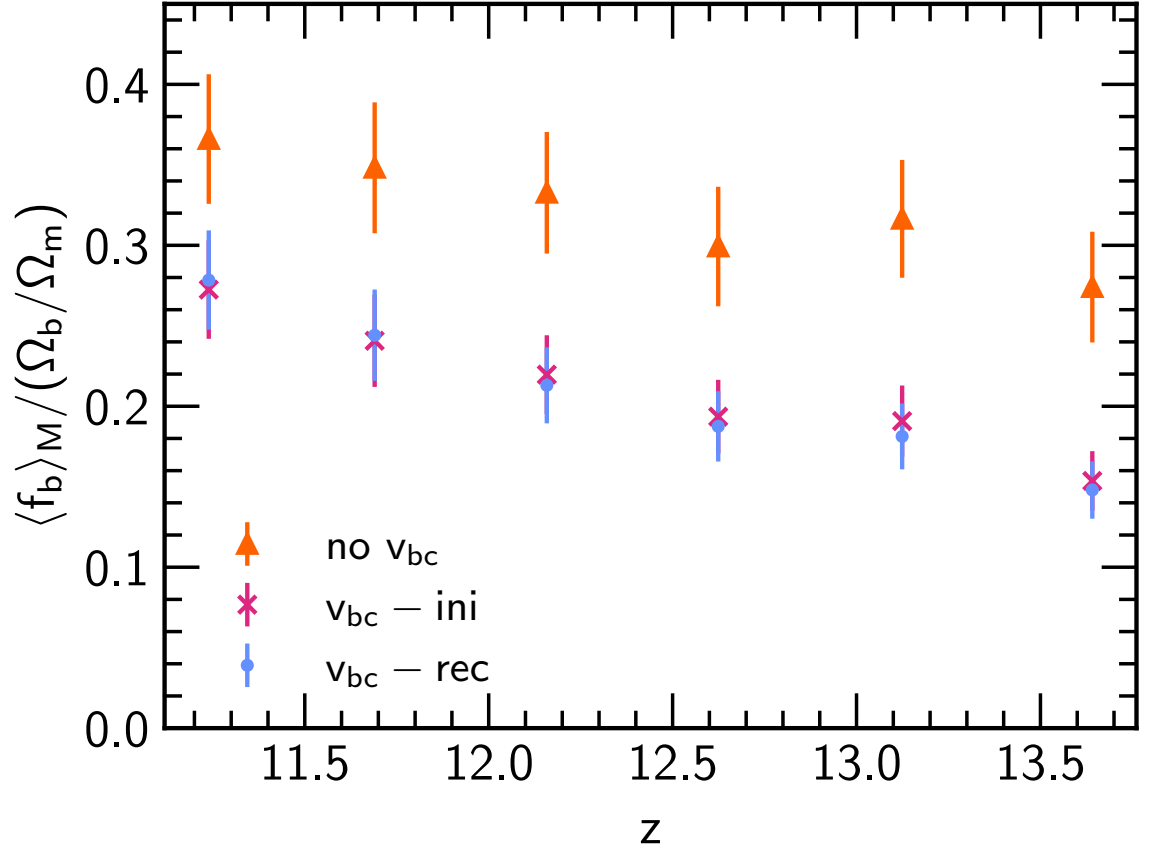


Figure 2.5: Mass-weighted average baryon fraction f_b as a function of redshift z , normalised to the cosmic mean $\bar{f}_b = \Omega_b / \Omega_m$. The average is shown for all z where more than 30 haloes have formed. The errorbars show the 1σ standard deviation as calculated using Equation (2.4.3).

and the associated mass-weighted standard deviation as

$$\sigma_M = \left(\frac{\sum_i f_{b,i}^2 M_i}{\sum_i M_i} - \langle f_b \rangle_M^2 \right)^{\frac{1}{2}}, \quad (2.4.3)$$

where the sum is over all haloes that satisfy the conditions in § 2.3.4. Figure 2.5 shows $\langle f_b \rangle_M$ and associated 1σ errorbars as function of z . We show each z where ≥ 30 haloes have formed that satisfy the criteria in § 2.3.4, starting from $z = 13.6$ where we are able to match 38 haloes between the three cases. The gas fraction is suppressed at all z for the v_{bc} -ini and v_{bc} -rec cases compared to the no v_{bc} case. At earlier z , the suppression is stronger, though even by the final snapshot at $z = 11.2$, $\langle f_b \rangle_M$ for both the v_{bc} -rec and v_{bc} -ini cases are not within 1σ of the no v_{bc} case. Notably, at all z , $\langle f_b \rangle_M$ in v_{bc} -ini and v_{bc} -rec cases are almost indistinguishable from, and certainly consistent with, one another.

2.4.2 Star formation

In Figure 2.6, we show the cumulative $M_\star$ formed in the simulation, not accounting for mass loss due to supernovae, and the corresponding number of stellar particles $N_\star$, which each have a mass of $108.0 h^{-1} M_\odot$. In each case, all of the star particles in the simulation formed inside a single halo. In total, 29 star particles formed by $z = 11.2$ in the no v_{bc} case, 10 in the v_{bc} -ini case, and 7 in the v_{bc} -rec case. This hierarchy persists across all z , with more star particles having formed in the no v_{bc} case than in the v_{bc} -ini case and fewer still in the v_{bc} -rec case.

In the following, all times quoted in Myr are measured relative to the Big Bang. The very first star particle forms in the no v_{bc} case at 338.9 Myr ($z = 12.8$), for the v_{bc} -ini case at 368.2 Myr ($z = 12.0$) and for the v_{bc} -rec case at 377.8 Myr ($z = 11.8$). From these formation times, we find that there is a delay in primordial star formation of 29.3 Myr for the v_{bc} -ini and 38.9 Myr for the v_{bc} -rec cases, compared to the no v_{bc} case. However, star formation in RAMSES is stochastic, so the formation of the very first star particle is perhaps not the best indicator of when star formation is fully underway. If we instead look at the time when a simulation had formed five star particles, we find that this threshold was reached by 372.5 Myr ($z = 11.9$) for the no v_{bc} case, by 385.8 Myr ($z = 11.6$) for the v_{bc} -ini case, and 398.0 Myr ($z = 11.4$) for the v_{bc} -rec case. Again, from these formation times we find a delay in star formation of 13.3 and 25.5 Myr for the v_{bc} -ini and v_{bc} -rec cases, respectively.

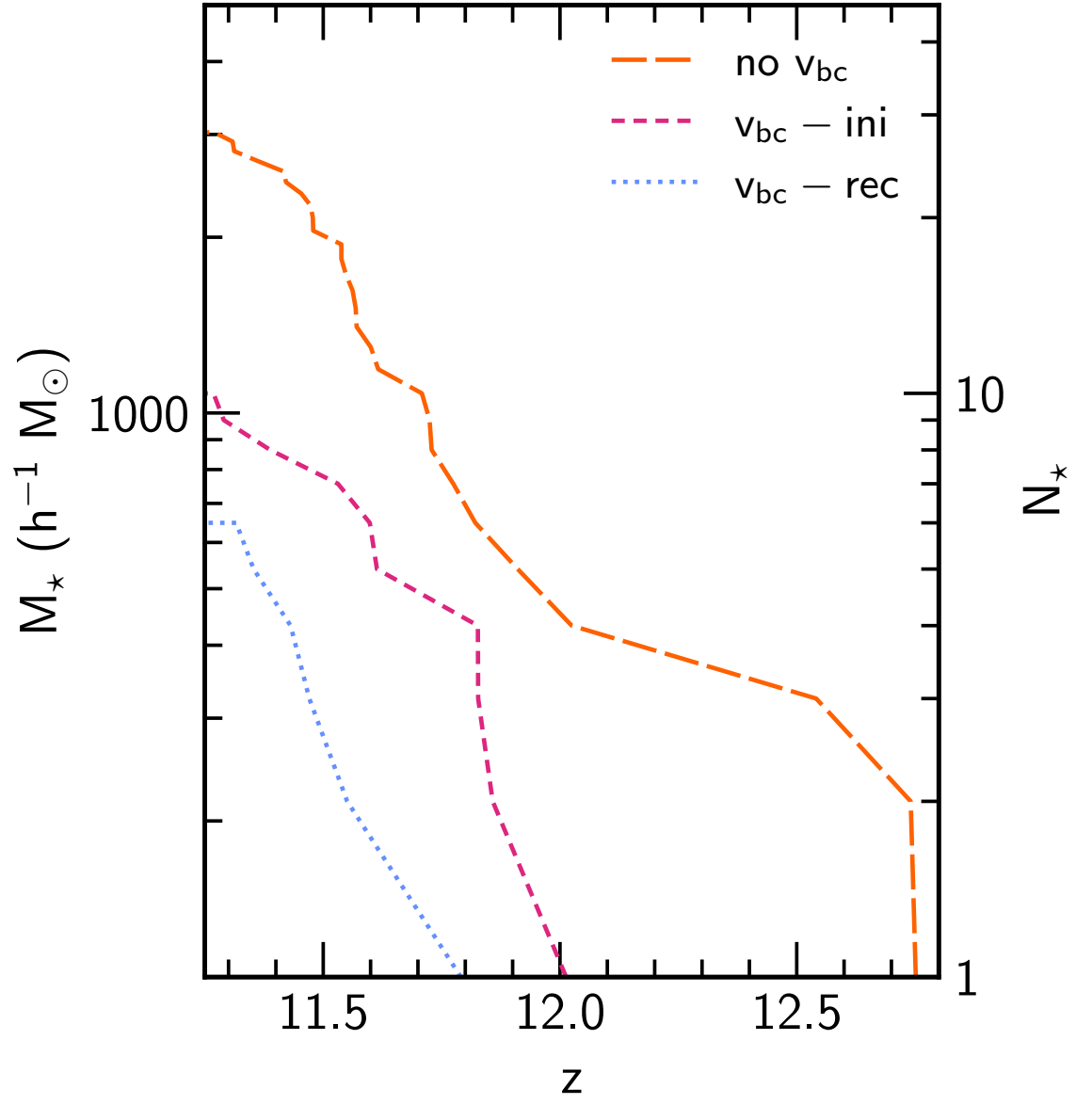


Figure 2.6: Cumulative stellar mass M_* formed as function of redshift z . Also shown is the corresponding number of stellar particles N_* .

2.5 Discussion

Including v_{bc} significantly affects the baryon fraction f_b , where we see that the mass-weighted baryon fraction $\langle f_b \rangle_M$ is suppressed at all redshifts in both cases, with the suppression stronger at higher redshift. Even by $z = 11.2$, the v_{bc} -ini and v_{bc} -rec cases are still not in agreement with the no v_{bc} case, though the difference between the two populations has decreased. Again, this is likely due to the decay in the magnitude of v_{bc} , which allows the haloes to accrete more gas. Interestingly, $\langle f_b \rangle_M$ is almost indistinguishable between the v_{bc} -ini and v_{bc} -rec cases. This effect is in qualitative agreement with previous studies.

This decrement in baryon fraction for the v_{bc} -ini and v_{bc} -rec cases is reflected in the cumulative stellar mass formed, as fewer star particles formed in both cases than in the no v_{bc} case. Not only do they form fewer star particles, they also start forming star particles later since the effect of v_{bc} is to wash out the peaks (and troughs) in the baryon density contrast, meaning that it takes longer for gas to reach the densities required for star formation. The delay in the formation of the first (fifth) star particle is 29.3 Myr (13.3 Myr) for the v_{bc} -ini case and 38.9 Myr (25.5 Myr) for the v_{bc} -rec case. From [Schaerer \(2002\)](#), we find that these delays are all of the order of the lifetime of a $9 M_\odot$ first-generation Population (Pop) III star, which has a lifetime of 20.02 Myr (Table 3 in [Schaerer, 2002](#)). More massive Pop III stars have even shorter lifetimes, for example a $120 M_\odot$ Pop III star lives for only 2.52 Myr. Pop III stars form from initially pristine gas, and their death pollutes their immediate surroundings with metals, introducing new cooling channels into the high-redshift Universe. Any delay in this introduction of metals will delay the transition between Pop III to Pop II (i.e. from metal-enriched gas), which can, for example, affect the 21 cm signal ([Magg et al., 2022](#)). In our case, though we do not form Pop III stars, chemical enrichment is still vitally important for star formation to get properly underway, particularly as all of the star particles form in the same halo.

Despite there being almost no difference in $\langle f_b \rangle_M$ between the v_{bc} -ini and v_{bc} -rec cases at most redshifts, there is a clear hierarchy in the amount of stars formed – no v_{bc} forms the most, v_{bc} -ini forms fewer, and v_{bc} -rec forms the least, albeit on the order of a few star particles. This effect is expected, since the bias factor washes out baryonic density peaks, and there are slightly more haloes (i.e. star formation locations) present in the v_{bc} -ini case than in the v_{bc} -rec case.

2.6 Conclusions

We have performed the first cosmological zoom simulations that self-consistently sample the relative baryon-dark matter velocity v_{bc} from a large $400 h^{-1}$ Mpc box. This relative velocity naturally arises when simulations are initialised using transfer functions that have separate amplitudes for the baryon and dark matter velocities, and we have shown that a box roughly as large as this is required to properly sample all of the scales associated with the relative velocity. However, solely initialising simulations in this manner misses out on the effect of the relative velocities from $z = 1000$ to the start time of the simulation, z_{ini} . We developed a methodology that compensates for the effect of v_{bc} on baryon density and velocity perturbations by computing a ‘bias’ factor $b(k, v_{bc})$, which is convolved with the ICs. We verified that our methodology performs as expected by comparing to previous works (see Appendix 2.A.2).

As a first demonstration of our methodology, we applied it to an extremely high-resolution zoom region in a $100 h^{-1}$ Mpc subbox, extracted from the main $400 h^{-1}$ Mpc box. The zoom region is centred on the region with the largest relative velocity in the $400 h^{-1}$ Mpc box, which has an RMS value of $v_{bc} = 100.07 \text{ km s}^{-1}$ at $z = 1000$, corresponding to $\sim 3.3\sigma_{v_{bc}}$. We find qualitative agreement with previous works, namely a reduction in halo baryon fraction and a delay in the onset of star formation for high-redshift, low-mass haloes. The strength of the effect decreases with redshift, but the two simulations still exhibit some differences by $z = 11.2$. We find that the delay in the onset of star formation is of the order of the lifetime of a $\sim 9 M_{\odot}$ Pop III star. We also test the effect of incorporating the bias factor by running a simulation that includes the relative velocity from the start time of the simulation only. In this case, we find that the suppression of the halo mass function is slightly weakened and more stars are formed when compared to the simulation that includes the bias factor, but there is almost no change in the average baryon fraction, except at the earliest redshift.

In this work, we have demonstrated our methodology for self-consistently sampling the relative velocity in cosmological zoom simulations. Since this methodology self-consistently samples the *spatially-fluctuating* relative velocity using transfer functions produced by a linear Boltzmann solver (in this case, CAMB), it is of use for modelling the inhomogeneous effects of v_{bc} , such as the effect on chemical enrichment from the suppression of the formation of the first stars. The effect that the fluctuation of the relative velocity over space can have important implications beyond small-scale structure formation, impacting e.g. the power spectrum of 21 cm fluctuations.

Future work will involve simulating larger and more varied patches of the universe, to get a rounder view of the impact of the varying magnitude of v_{bc} in different environments. In addition to improving the sampling, improvements could also be made to the modelling of high- z physics by including: molecular hydrogen cooling; Lyman-Werner radiation; Pop III star formation; and photoheating and ionisation, all of which play a vital role in shaping high- z galaxies.

Our code for producing these compensated ICs is publicly available⁴, and we hope will be of use for studying this effect in the full cosmological context.

⁴<https://github.com/lconaboy/drft>

Appendix

2.A Tests

Other studies have looked at the effect of the v_{bc} on high-redshift structure formation in different contexts, affording us an opportunity to compare and verify our method when set up in similar circumstances.

2.A.1 `py_vbc`

Originally, this project built upon the excellent ICs generator **CICsASS** released by [O’Leary & McQuinn \(2012\)](#), which included a module for producing transfer functions including v_{bc} . Integration into our method was problematic as **CICsASS** would end up writing lots of tiny files, which is not ideal for HPC file systems where there are often limits on the number of files that can be stored. In the end, we decided to repackage **CICsASS** to allow for easier incorporation into our method. This is the module that we use to evolve the transfer functions calculated with **CAMB** from $z = 1000$ down to the start time of the simulation z_{ini} . We verified that our module faithfully reproduced the results of **CICsASS** by performing some tests.

Interpolations

To solve the evolution equations, **CICsASS** takes information from other codes, namely gas temperature $T(z)$ and electron fraction $x_e(z)$ from **RECFAST** ([Seager et al., 1999](#); [Chluba et al., 2010](#); [Chluba & Thomas, 2011](#)) and transfer functions $T(k)$ from **CAMB** ([Lewis et al., 2000](#)), which are used to set the ICs. **CICsASS** uses **GSL** interpolation routines, whereas we use those available in **scipy**. Figure 2.7 shows the interpolation of temperature and electron fraction over redshift z and Figure 2.8 shows the interpolation of the transfer functions over wavenumber k , and their finite difference derivatives. We find good agreement over all interpolations.

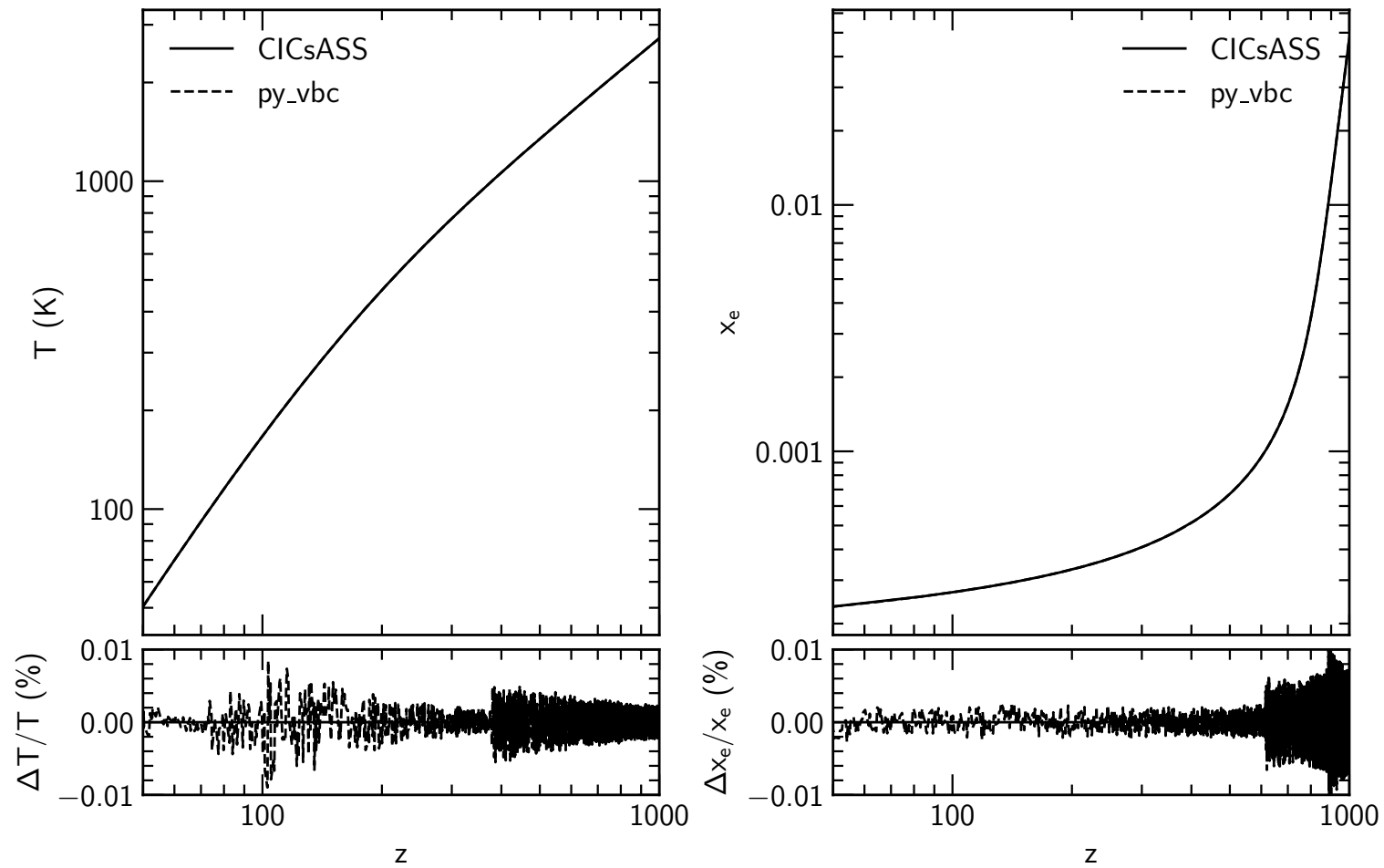


Figure 2.7: Left top: interpolated temperature as a function of redshift, as calculated by RECFast, for CICsASS (solid) and py_vbc(dashed). Left bottom: fractional difference between CICsASS and py_vbc relative to the CICsASS interpolation. Right: same as left, but for electron fraction.

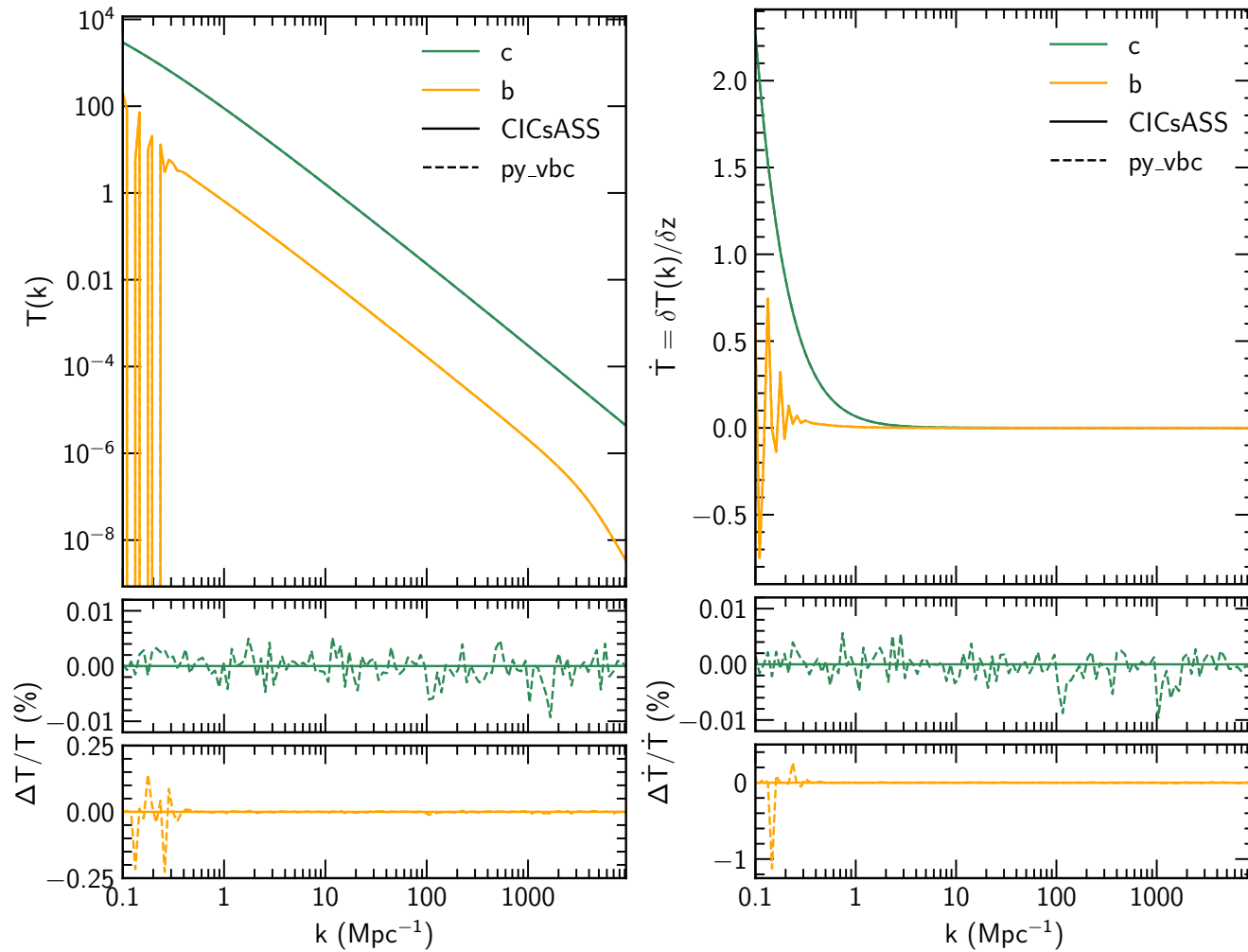


Figure 2.8: Left top: interpolated CAMB transfer functions at $z = 1000$ for dark matter (green) and baryons (orange), produced by `CICsASS` (solid) and `py_vbc` (dashed). Left bottom: fractional difference between `CICsASS` and `py_vbc` relative to the `CICsASS` interpolation. Right: same as left but for the derivative of the the transfer functions, calculated at $z = 1000$ by taking a finite difference over the redshift range $z \pm 3$.

Evolution

Once we ascertained that the the code is being set up in the same fashion, we tested the results of the code. Figure 2.9 shows the result of integrating the evolution equations from $z = 1000$ to $z = 50$ in the case $v_{bc} = 0 \text{ km s}^{-1}$. For the dark matter we find excellent agreement at all scales, while for the baryons we get excellent agreement up to the largest scales whereupon we see some divergence. We note that the perturbations in the baryons are very small at the point of divergence, so the absolute difference is also small.

2.A.2 Comparison to previous works

We run a series of test simulations set up as in Naoz et al. (2012, 2013), one of the first studies to explore the effect of v_{bc} on the halo mass function and gas fraction of haloes using fully numerical cosmological simulations in boxes with side lengths $< 1 \text{ Mpc}$. The specific case shown here has a base resolution $\ell_{\min} = 9$ (512^3 dark matter particles and, initially, cells), in a $471.1 h^{-1} \text{ kpc}$ periodic box. The simulations in Naoz et al. (2012, 2013) were performed using the SPH code GADGET2 (Springel, 2005), while we use the AMR code RAMSES. We allow the AMR grid to refine freely up to $\ell_{\max} = 14$, corresponding to a maximum comoving resolution of $28.9 h^{-1} \text{ pc}$, comparable to the gravitational softening length of $45.8 h^{-1} \text{ pc}$ comoving used in Naoz et al. (2012). We use our fiducial cosmology (§ 2.3.1), whereas Naoz et al. (2012) used a cosmology consistent with Komatsu et al. (2009) with parameters: $\Omega_m = 0.28$, $\Omega_\Lambda = 0.72$, $\Omega_b = 0.046$, $h = 0.7^5$ and a boosted $\sigma_8 = 1.4$. We adopt the boosted $\sigma_8 = 1.4$ as used in the original studies. We initialise the simulations at $z_{\text{ini}} = 200^6$ both with and without a relative velocity of $1.7\sigma_{v_{bc}} = 10 \text{ km s}^{-1}$ at z_{ini} . We also compute and apply the bias factor $b(k, v_{bc})$ to the baryonic component of the ICs, while the Naoz et al. (2012) simulations are initialised by computing transfer functions which explicitly include the effect of the v_{bc} . Following Naoz et al. (2012) we set both of the velocity fields to that of the dark matter and apply the v_{bc} to the x -component of the baryon velocity as

$$\begin{pmatrix} v_{b,x} \\ v_{b,y} \\ v_{b,z} \end{pmatrix} = \begin{pmatrix} v_{c,x} + v_{bc} \\ v_{c,y} \\ v_{c,z} \end{pmatrix}. \quad (2.A.1)$$

⁵When lengths and masses are quoted in units of h , we use $h = 0.673$ from our choice of cosmology.

⁶The Naoz et al. (2012) simulations are actually initialised at $z_{\text{ini}} = 199$ but the v_{bc} would only have decreased by 0.5 per cent in this time, so we ignore this difference.

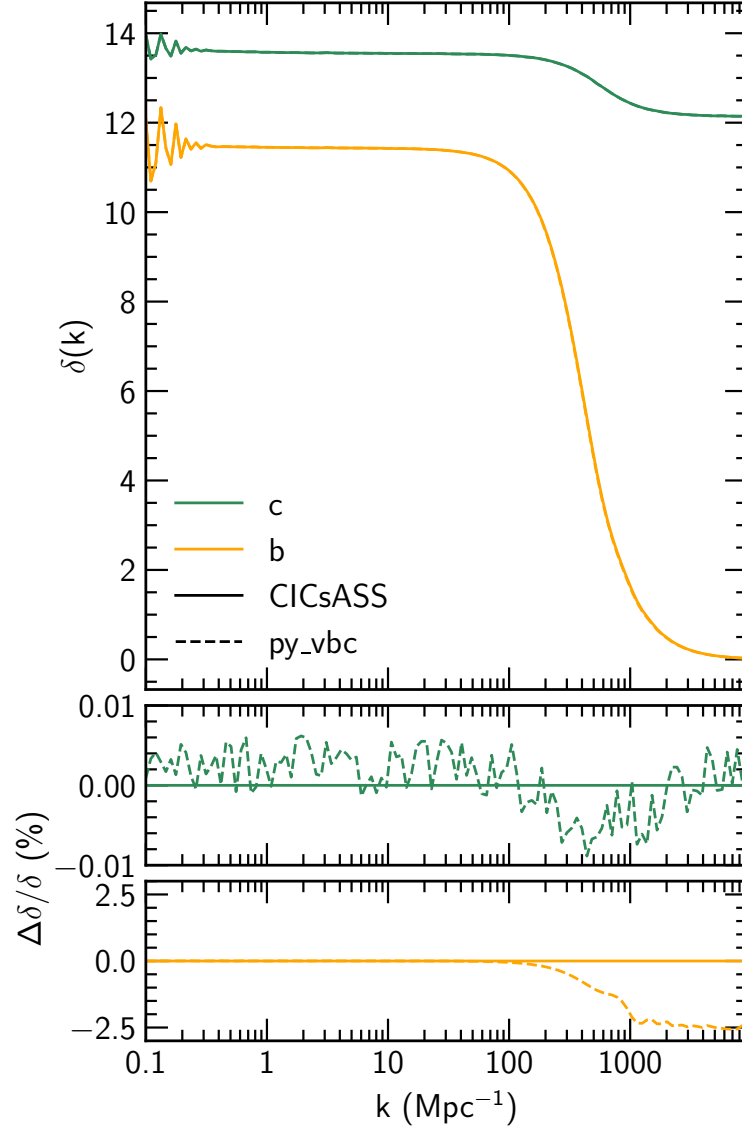


Figure 2.9: Top: perturbations in dark matter (green) and baryon (orange) density perturbations evolved from $z = 1000$ to $z = 50$, using `CICsASS` (solid) and `py_vbc` (dashed). Bottom: fractional difference in dark matter (upper) and baryon (lower) result compared to `CICsASS`.

Including the v_{bc} in this manner is justified by the box size being much smaller than the coherence scale of the v_{bc} . We do not allow star formation in these runs. Haloes are identified as described in § 2.3.4, noting that although [Naoz et al. \(2012\)](#) define their halo overdensity with respect to the background matter density $\bar{\rho}_m$, we are working in the period of matter domination the difference will be small.

To calculate the effect of the v_{bc} we compare to simulations without v_{bc} , where the velocity field of the baryons is equal to that of the dark matter. In order to quantify this effect, we calculate the fractional difference of a quantity A as

$$\Delta_A = \frac{A_{v_{bc}} - A_{no\ v_{bc}}}{A_{no\ v_{bc}}}. \quad (2.A.2)$$

First, we look at the effect on the cumulative halo mass function $N(> M)$, as in [Naoz et al. \(2012\)](#). Figure 2.10 shows the decrement in $N(> M)$ for the case with v_{bc} compared to the case without, both for our simulations and for the [Naoz et al. \(2012\)](#) run. We see qualitatively similar behaviour, observing a decrement between ~ 0 per cent and -50 per cent at all redshifts shown and for almost all masses below the M where $N(> M) = 10\ (h^{-1}\text{ Mpc})^{-3}$. However, the overall shape of our Δ_N is slightly different to [Naoz et al. \(2012\)](#); we match well below $\sim 3 \times 10^5\ h^{-1}\text{ M}_\odot$ but show more relative suppression above this mass. This discrepancy is due, at least in part, to the different simulation codes used and the different white noise fields in the initial conditions. One further significant source of difference is the cosmologies used. To see the effect of cosmology on the halo mass function we use the fitting formula of [Watson et al. \(2013\)](#), which is a fit to N -body simulations spanning many orders of magnitude in mass resolution and box size, and covers the redshift range $z = 30 - 0$ thus making it a good choice for this high- z comparison. Figure 2.11 shows the difference expected at $z = 15$ by comparing the [Watson et al. \(2013\)](#) $N(> M)$ mass functions for the different cosmologies (cyan solid). From this, we would expect the [Naoz et al. \(2012\)](#) simulation to have ~ 6 per cent more haloes with $M > 3 \times 10^5\ h^{-1}\text{ M}_\odot$. This increase in the number of haloes increases with mass and for $M > 1 \times 10^7\ h^{-1}\text{ M}_\odot$, we would expect ~ 24 per cent more haloes in the [Naoz et al. \(2012\)](#) simulation. Indeed this is borne out by the simulations (navy dashed), which show that the [Naoz et al. \(2012\)](#) simulations do produce more haloes at all masses. At higher masses Δ_N diverges as the absolute number of haloes becomes small. We also use a different halo finding method to [Naoz et al. \(2012\)](#), which is likely to introduce some differences into the halo masses.

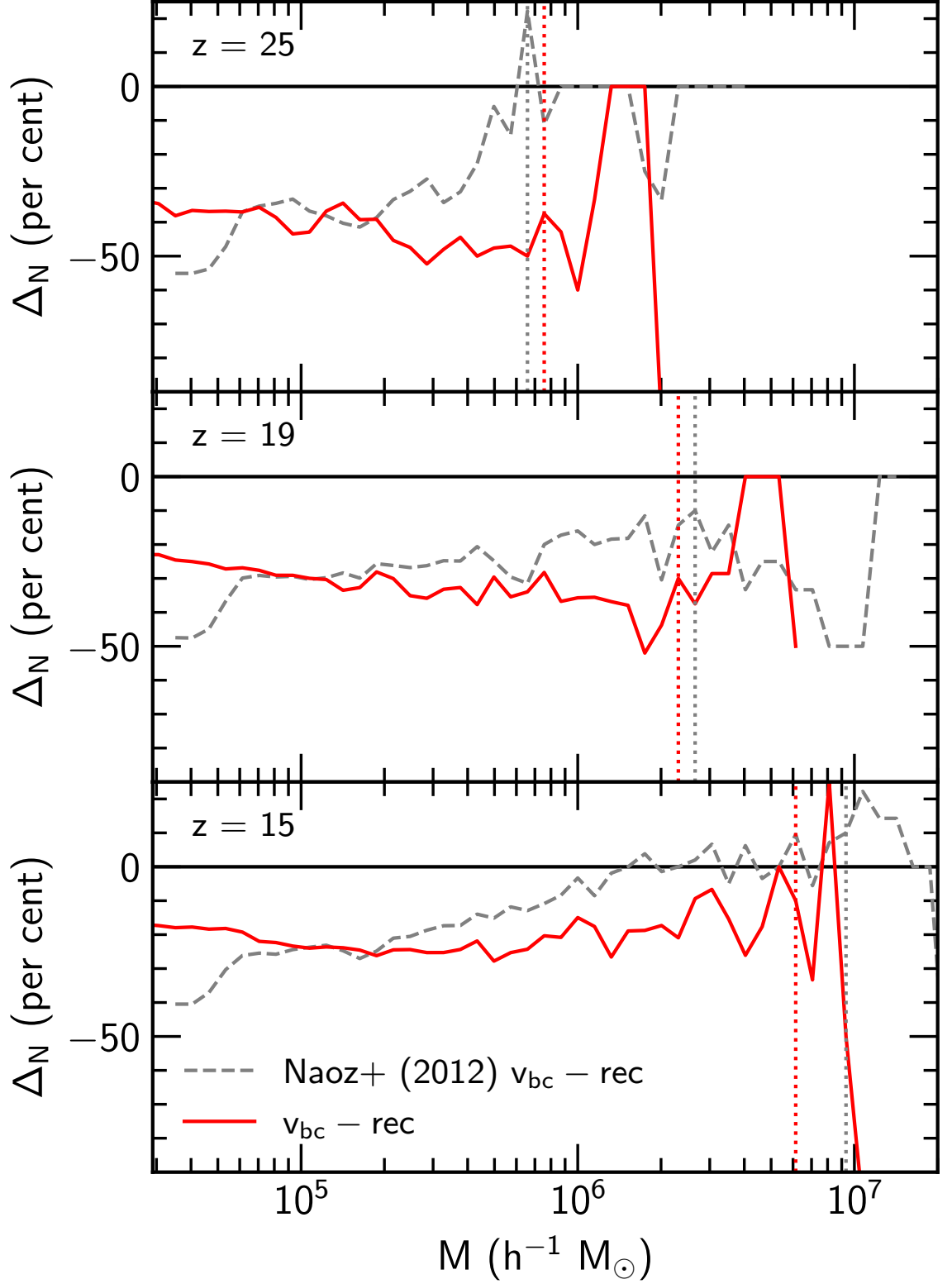


Figure 2.10: The fractional difference Δ_N in halo mass function $N(> M)$ for the $v_{bc,ini} = 10 \text{ km s}^{-1}$ case, calculated with Equation (2.A.2). We show Δ_N at $z = 25$ (top), 19 (centre) and $z = 15$ (bottom) for our simulations (red solid) and for the [Naoz et al. \(2012\)](#) work (grey dashed). The dotted lines indicate where $N(> M)$ drops to $10 (h^{-1} \text{ Mpc})^{-3}$ for each set of simulations.

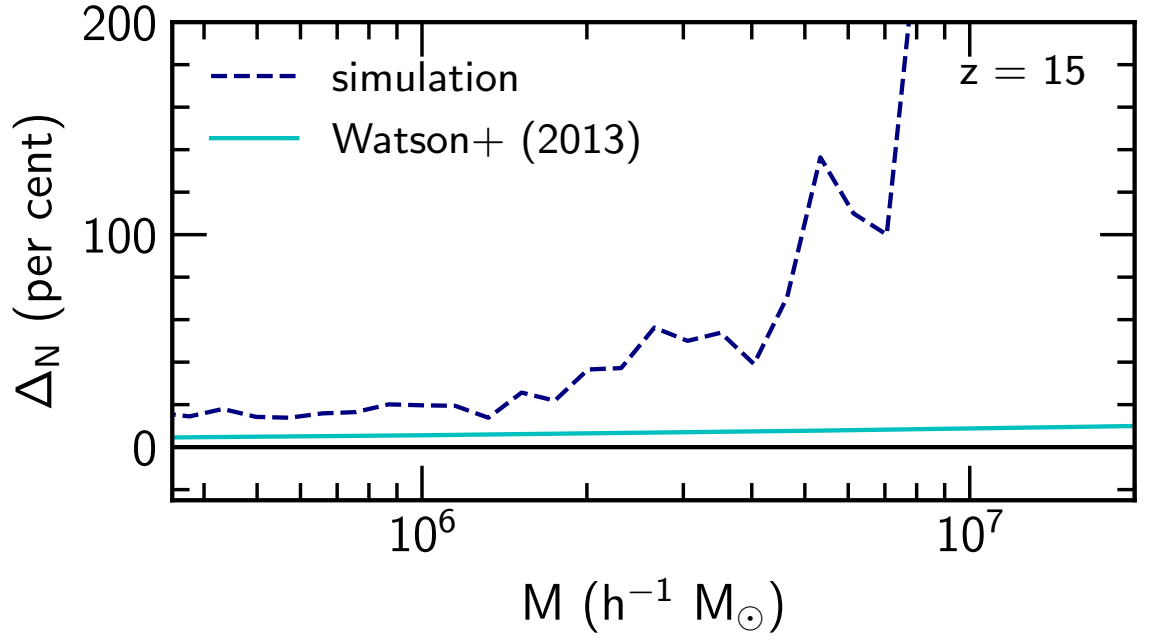


Figure 2.11: Comparison of the fractional difference Δ_N in halo mass function $N(> M)$ between our simulations and the simulations from [Naoz et al. \(2012\)](#) (dark blue short-dashed) and between the analytic [Watson et al. \(2013\)](#) curve for the cosmology used in our work and the one used in [Naoz et al. \(2012\)](#) (cyan solid). The decrement is calculated as $\Delta_N = (N_1 - N_0)/N_0$, where N_0 are the data corresponding to our work and N_1 to [Naoz et al. \(2012\)](#), so $\Delta_N > 0$ means there are more haloes in [Naoz et al. \(2012\)](#).

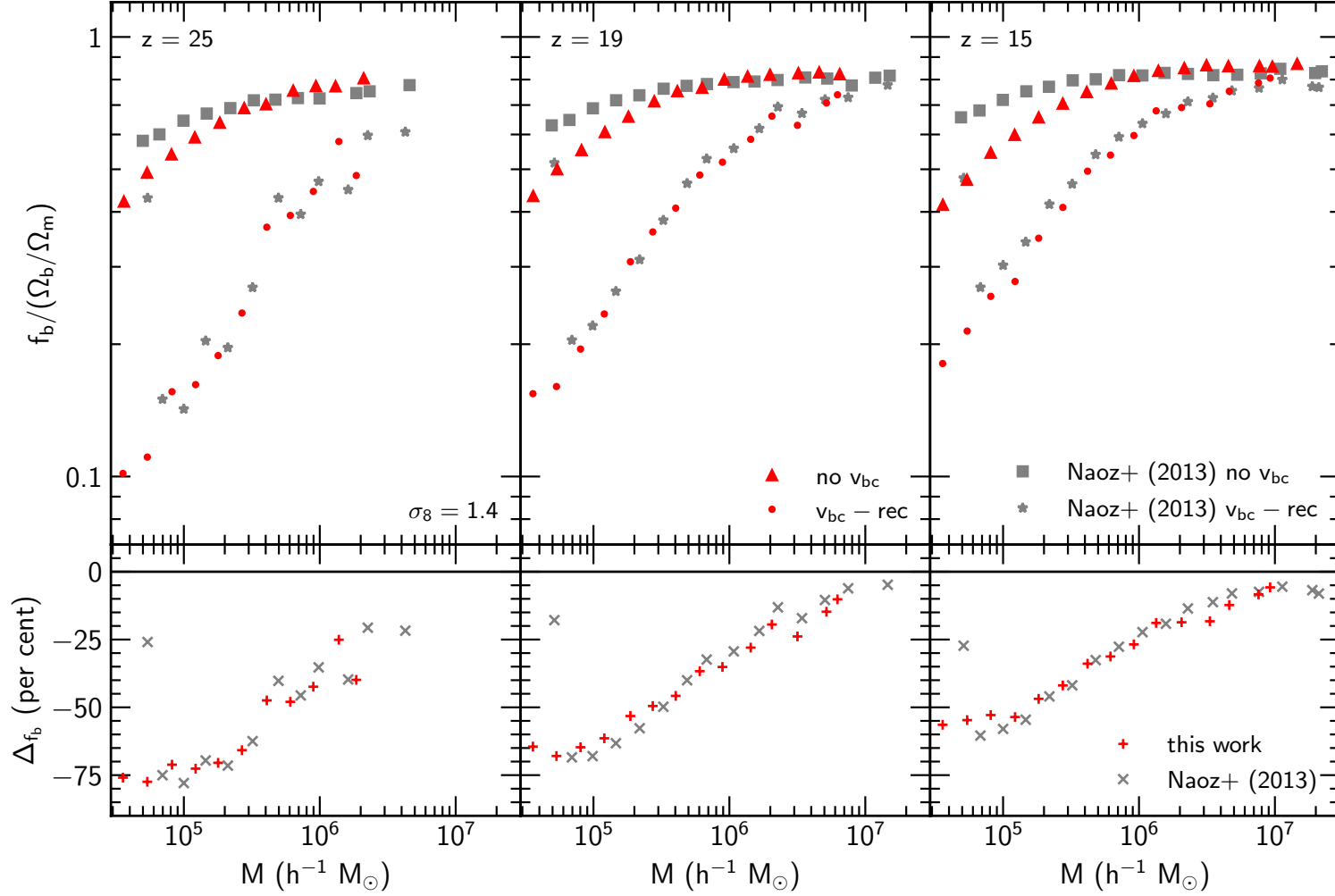


Figure 2.12: Binned baryon fraction f_b (top panels) and relative fractional difference Δf_b between each run with v_{bc} to the run without, calculated with Equation (2.A.2) (bottom panels). We show data from our simulations (red triangles, points and plusses) and from the Naoz et al. (2013) work (grey squares, stars and crosses). The panels show $z = 25$ (left), 19 (centre) and 15 (right).

Next, we turn our attention to the gas fraction of haloes, as studied in [Naoz et al. \(2013\)](#). Since we do not include star formation in these runs, the baryon fraction is simply the halo gas mass divided by the total halo mass

$$f_b = \frac{M_g}{M_g + M_d}. \quad (2.A.3)$$

Figure 2.12 shows the binned gas fractions (top panel) for our and for the [Naoz et al. \(2013\)](#) simulations, each normalised to the cosmic mean $\bar{f}_b = \Omega_b/\Omega_m$ for the appropriate cosmology, and the decrement (bottom panel) as defined in Equation (2.A.2). We take the midpoint of the mass bin to be the mean of all the mass values in that bin. The binned gas fractions for [Naoz et al. \(2013\)](#) are slightly higher than in this work, though they exhibit roughly the same mass dependence. The agreement between the two simulations for the decrement is striking – they have an extremely similar mass dependence. There is some difference in the binned baryon fractions, in particular we find slightly more suppression at lower masses. This is likely due to differences in code used since, as mentioned previously, [Naoz et al. \(2013\)](#) used GADGET2 ([Springel, 2005](#)), where we use RAMSES. There are well documented differences between Lagrangian (e.g. SPH) and Eulerian (e.g. AMR) codes (e.g. [Agertz et al., 2007](#)), and indeed it has been shown that numerical diffusion due to baryon-grid relative velocities can artificially smooth densities in Eulerian codes ([Pontzen et al., 2020](#)). In any case, we are not interested in comparing the merits of different codes, so by calculating the difference between the runs with and without v_{bc} we can remove artefacts due to the choice of code.

2.B Contamination and the halo mass function

While zoom simulations offer an excellent compromise between scale and resolution, they are not without their limitations. Particle masses increase by a factor of eight for each step down in resolution and so it is essential to ensure that structures made up of a mix of low- and high-resolution particles are not included in any analysis, since the radically different masses can severely affect the dynamics of the structures (see [Oñorbe et al., 2014](#), for a good discussion of this effect). When structures are made up of a mix of particle resolutions in this fashion, we say they are ‘contaminated’. Contamination occurs when low-resolution particles (which are present outside the zoom region), enter the zoom region and become bound to high-resolution haloes (or vice versa). Using a very small zoom region means we are at high risk of contamination, since coarse particles do not have to travel very far to contaminate a high-resolution structure. The tiny zoom volume also makes mitigating

the effects of contamination more difficult, since we cannot now simply cut out a smaller uncontaminated region from the main zoom region. When exploring the effect of v_{bc} on baryon fraction and star formation, we can avoid the effects of contamination by comparing the baryon fraction of haloes which are never contaminated and matched between the sets of simulations, thereby exploring the effect on individual haloes. When exploring the effect on *populations* of haloes, such as the HMF, this approach breaks down. In this appendix we demonstrate why this approach to contamination does not work for the HMF and discuss the impact on this work.

Forgetting for a moment the problem of contamination, we can construct mass functions from the raw halo catalogues produced by **AHF**, which we will denote by $N_{\text{all}}(> M)$. In Figure 2.13 we show the ratio of $N_{\text{all}}(> M)$ for the v_{bc} -ini and v_{bc} -rec cases compared to the no v_{bc} case at three redshifts. At all redshifts and almost all masses shown, the HMF for the cases with v_{bc} are consistent with no difference, except at $z = 14.2$ and below $10^6 h^{-1} M_{\odot}$ and at $10^7 h^{-1} M_{\odot}$ for the v_{bc} -rec case. This suppression is less strong than that reported in Naoz et al. (2012), for example, though drawing any conclusion about the effect of v_{bc} on the HMF from Figure 2.13 should be avoided since that HMF includes contaminated haloes and haloes formed outside of the zoom region—we show this HMF mainly for comparison to the HMF produced from the clean catalogue.

Next, we clean the catalogue by removing all haloes that are, have ever been, or will ever be contaminated in the simulation. To do this, we compute merger trees using **consistent-trees** and, at the final snapshot, identify and remove any haloes with a contaminated lineage. In this way, we not only ensure that no contaminated haloes are present at a given snapshot, but also that haloes do not ‘disappear’ on account of becoming contaminated between one snapshot and the next. Figure 2.14 shows the ratio of HMFs (cf. Figure 2.13) for this cleaned catalogue, $N_{\text{clean}}(> M)$, again normalised to the no v_{bc} case and for the same redshifts as in Figure 2.13. Where before there was almost no difference between the HMFs for the cases with and without v_{bc} , there is now a huge difference between the v_{bc} -rec and no v_{bc} case, while there remains almost no difference between the v_{bc} -ini and no v_{bc} case.

The result presented in Figure 2.13 may seem counterintuitive—why should suppressing fluctuations in the initial baryon density contrast in the ICs result in such a huge difference in halo abundance, when compared to the case also run with v_{bc} but no initial suppression? The answer lies in the way the halo catalogues are cleaned. Looking now to Figures 2.15, 2.16 and 2.17, we can see the difference between the original and cleaned

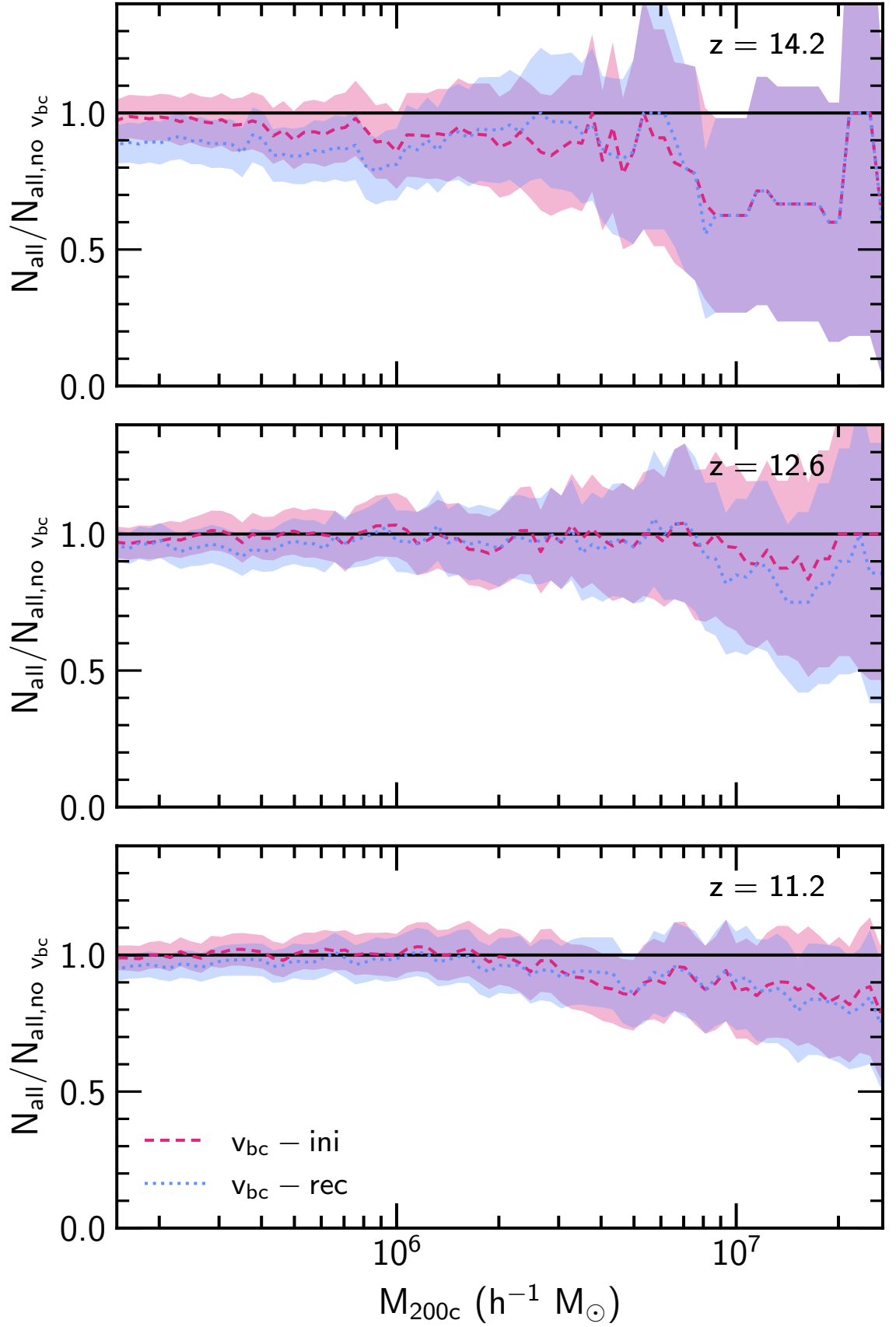


Figure 2.13: The HMF for the v_{bc} -ini (pink dotted) and v_{bc} -rec (blue dashed) runs, normalised to the no v_{bc} run. All haloes found by AHF are used here, regardless of contamination. From top to bottom, we show the ratio at $z =$. Shaded region indicates the 1σ Poisson uncertainty, computed as $\sqrt{N(>M)}$.

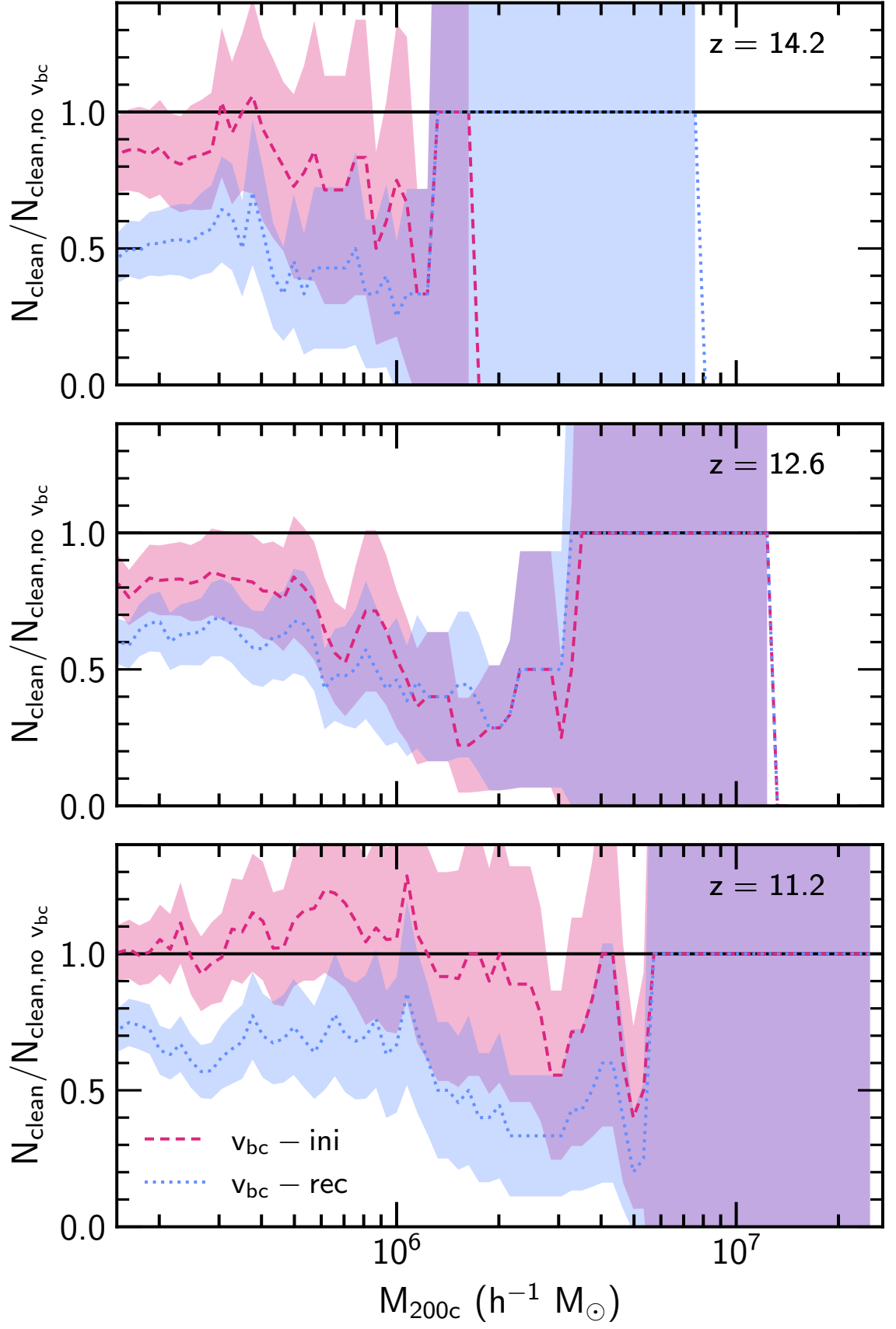


Figure 2.14: As in Figure 2.13, but this time using only the cleaned catalogue, the construction of which is described in § 2.B.

catalogues at $z = 14.2, 12.6$ and 11.2 , respectively. In particular, comparing the fraction of haloes retained $N_{\text{clean}}(> M)/N_{\text{all}}(> M)$ for each run (bottom panels), we see that a different fraction of haloes are kept for each run, with the $v_{\text{bc}}\text{-rec}$ case consistently having the most removed, which is reflected in the apparent suppression for the $v_{\text{bc}}\text{-rec}$ case seen in Figure 2.14. It is also worth noting that at $z = 11.2$ (Figure 2.17), over most of the mass range $\lesssim 10^6 h^{-1} M_{\odot}$, the $v_{\text{bc}}\text{-ini}$ case has fewer haloes removed than the no v_{bc} case, explaining the apparent boost in $N_{\text{clean}}(> M)$ for $v_{\text{bc}}\text{-ini}$ in the bottom panel of Figure 2.14 (though the two cases are still consistent with no difference).

In summary, the differences between the HMF for each case seen in Figure 2.14 are not a result of suppression due to v_{bc} , but are artificially introduced through neglecting the impact of removing a different fraction of contaminated haloes for each run. Due to limitations imposed by our very small zoom region, we are unable to perform a fairer removal of contaminated haloes (e.g. through imposing a position-based cut) and as such forgo a study of the effect of v_{bc} on the HMF for this simulation. Future works that use our methodology to explore the impact of v_{bc} in a larger zoom region should have no such trouble, and we present this discussion as a cautionary tale in dealing with contaminated haloes.

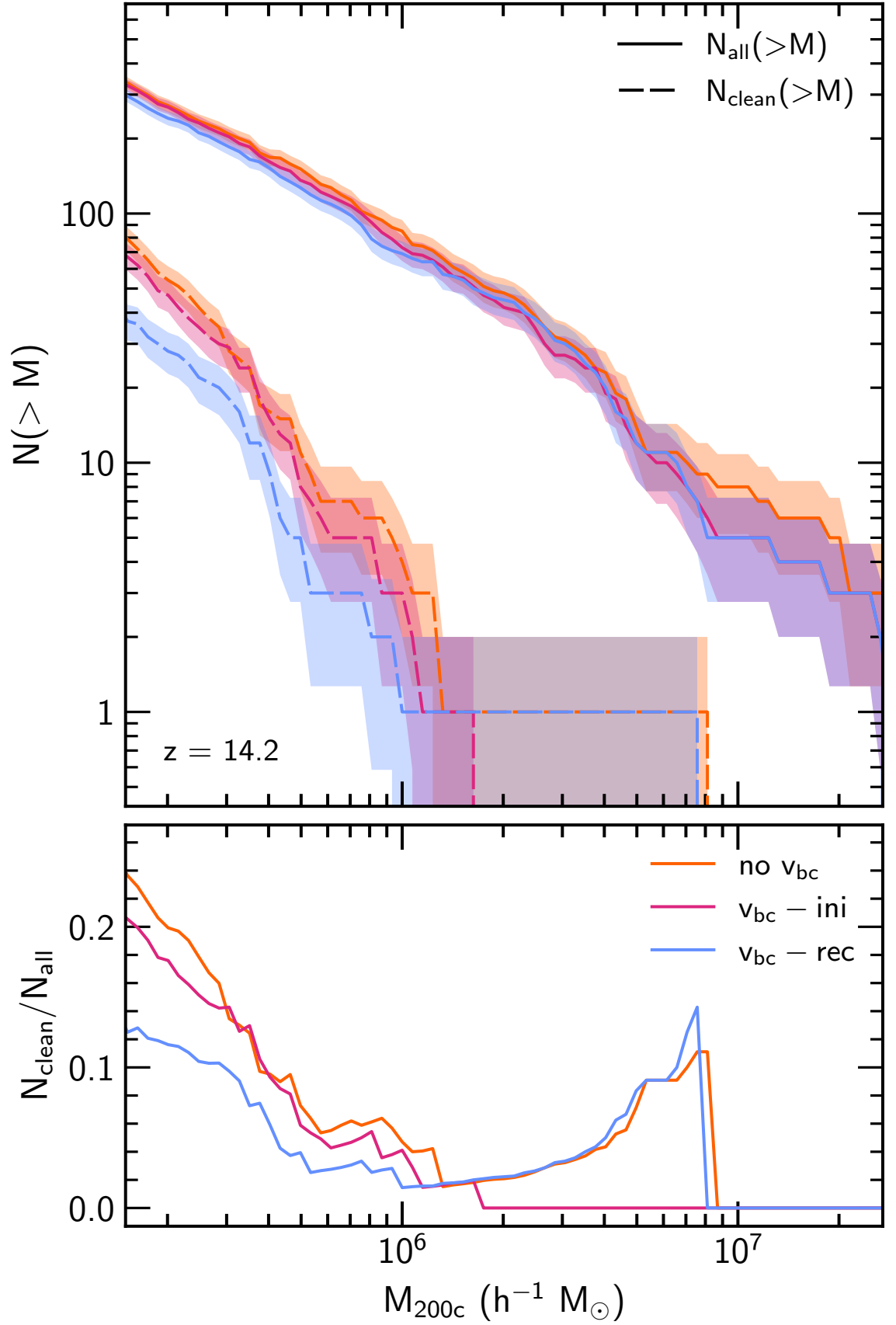


Figure 2.15: Top: HMFs computed directly from the AHF catalogues (solid lines) and from the cleaned catalogues (long-dashed lines) for $z = 14.2$. Shaded regions indicate the 1σ Poisson uncertainty, computed as $\sqrt{N(>M)}$. Bottom: the ratio of the cleaned to all HMFs for each of the three cases.

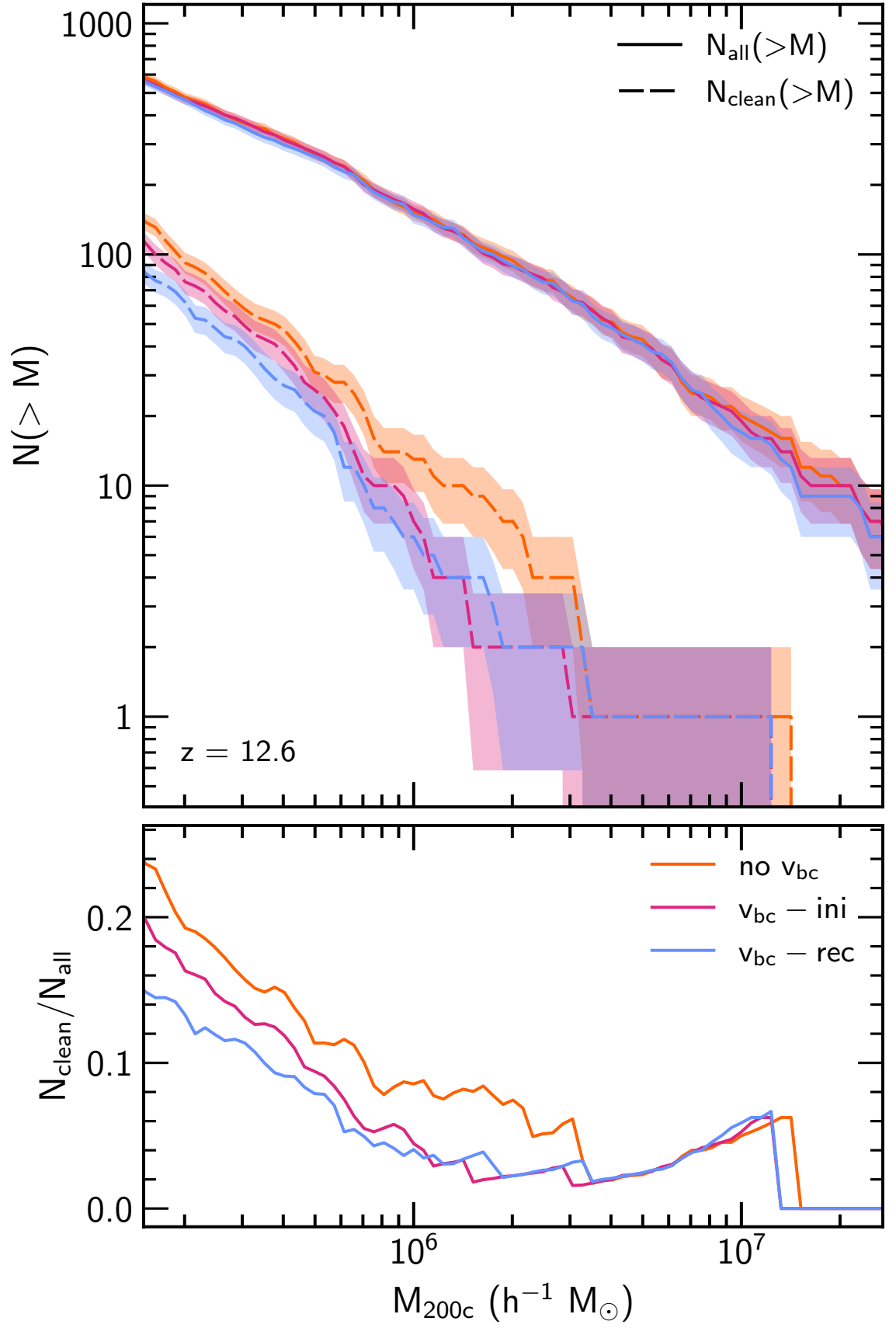


Figure 2.16: As in Figure 2.15 but for $z = 12.6$.

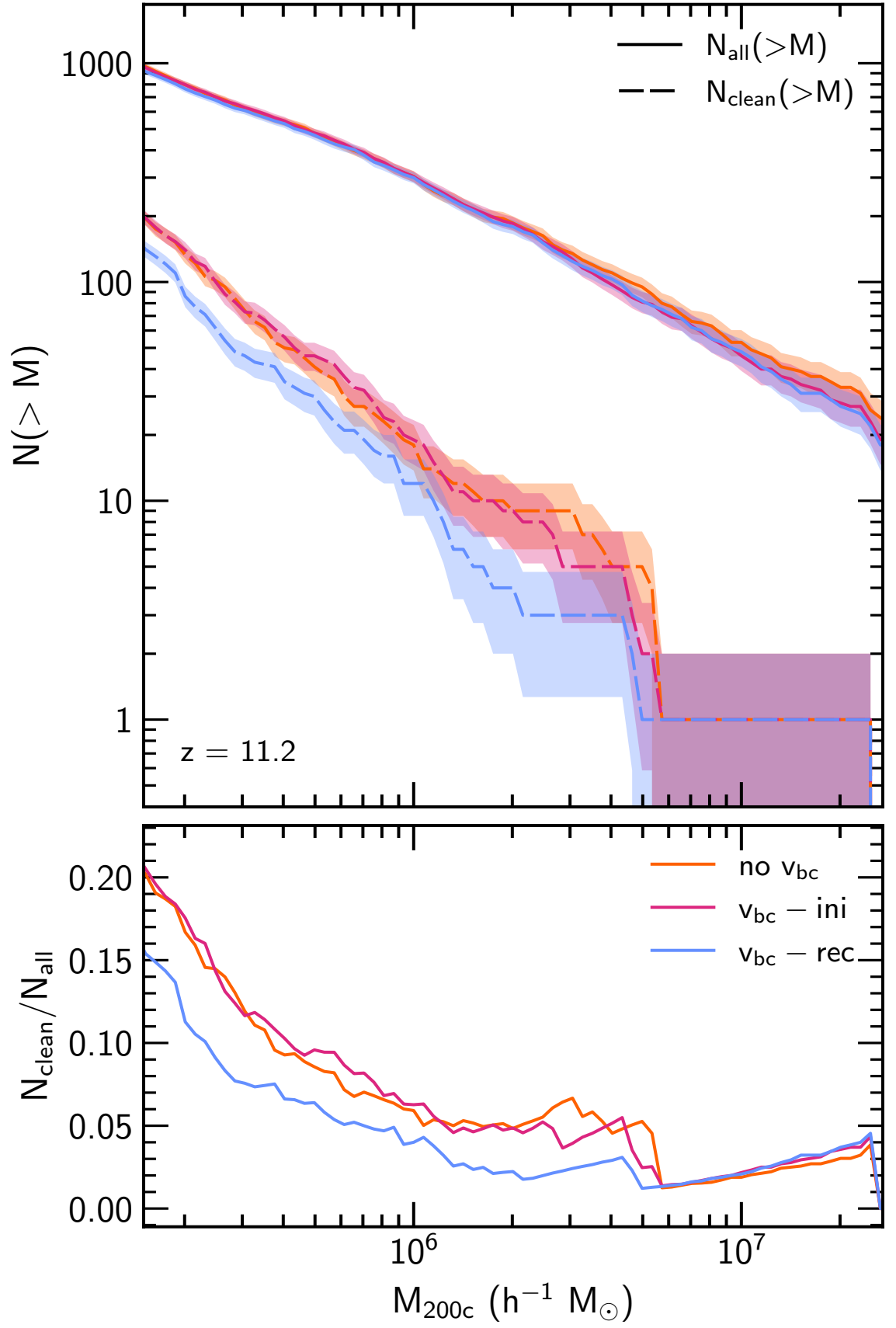


Figure 2.17: As in Figure 2.15 but for $z = 11.2$.

Chapter 3

Reionisation of the local universe in the HESTIA suite

This work was carried out in collaboration with Sergey Pilipenko, Ilian T. Iliev and Noam I. Libeskind. Sergey Pilipenko produced the white noise fields for the initial conditions and assisted with running the `ginnugagap` code. The original constrained initial conditions were generated as part of the HESTIA project. I ran all the simulations and performed the analysis.

This chapter is adapted from *Reionisation of the local universe in the Hestia suite* by [Conaboy, Iliev & Libeskind \(2022b\)](#), submitted to the John von Neumann Institute for Computing (NIC) Symposium 2022.

3.1 Introduction

Our Milky Way (MW) galaxy resides within a group of galaxies called the Local Group (LG). Of this LG, the Andromeda galaxy (M31) is our nearest large neighbour having a mass of similar magnitude to the MW. The next largest galaxy is the Triangulum galaxy (M33) and following this are the Large and Small Magellanic Clouds and a whole host of faint dwarf galaxies (for a comprehensive review of the LG see [van den Bergh, 2000](#)). Outside the LG, we reach the larger galaxies Centaurus A and M83, and the galaxy cluster Virgo. All of these galaxies, groups and clusters then form one overarching structure, the supercluster Laniakea ([Tully et al., 2014](#)).

By dint of its proximity to us, the near-field, made up of the LG and surrounding galaxies, is the best-studied cosmological region in the universe. This makes the near-field a prime testbed for cosmological models, and indeed many ‘tensions’ have arisen over

the years between predictions from numerical simulations of Λ CDM and observations of the LG (for a comprehensive review of the small-scale challenges see [Bullock & Boylan-Kolchin, 2017](#)). Most of the tensions originally came from dark matter-only simulations, and baryonic solutions have been proposed for lots of them (e.g. [Sawala et al., 2016](#)). Some curiosities still persist, for instance the ‘planes of satellites’ problem ([Kroupa et al., 2005](#); [Pawlowski, 2018](#)), where observations of 11 of the MW’s brightest satellites appear to lie in a plane across the orbital poles ([Lynden-Bell, 1976](#)). This configuration is thought by some to be incompatible with Λ CDM, though some have claimed it is not that unusual at all and, at least partly, down to chance ([Sawala et al., 2022](#)). Whatever the answer, the near-field has certainly proved useful in testing our understanding of the universe.

Constrained simulations allow us to reproduce the large-scale structure surrounding the LG (e.g. the Virgo cluster), while at the same time forming objects which closely match the properties of galaxies within the LG. Such simulations are constrained using observations of the galaxies’ positions and velocities in the local Universe. Previous works have used constrained simulations from the CLUES project to explore the effect of reionisation on the progenitors of the LG, modelling the radiative transfer in large ($64 h^{-1}$ Mpc) boxes with post-processed ray-tracing ([Iliev et al., 2011](#); [Dixon et al., 2018](#)) and fully-coupled radiation-hydrodynamics with fixed ([Ocvirk et al., 2016, 2020](#)) and adaptive ([Aubert et al., 2018](#)) resolution. The [Iliev et al. \(2011\)](#) and [Dixon et al. \(2018\)](#) studies were based on N -body simulations of the LG and surrounding clusters, with radiation coming from sources assigned to haloes and the radiative transfer computed over the smoothed density field. Their setup focused on the large scales and allowed different source models to be explored. The [Ocvirk et al. \(2016, 2020\)](#) studies involved, again, large-scale simulations, this time evolving the matter and radiation together on a high-resolution mesh (4096^3 particles and cells), but were unable to use adaptive mesh refinement (AMR) due to aggressive optimisations of the code. [Aubert et al. \(2018\)](#) performed similar simulations to [Ocvirk et al. \(2016, 2020\)](#) and this time was able to use AMR, but at the expense of poorer mass resolution (using 2048^3 particles and, initially, cells).

The constrained simulation used for this study is the HESTIA (High-resolution Environmental Simulations of The Immediate Area, [Libeskind et al., 2020](#)) suite, which accurately model the environmental dependence of the LG. This is in contrast to many previous simulations of the LG, which focused solely on finding pairs of $\sim 10^{12} M_{\odot}$ haloes whose properties resemble that of the LG (e.g. [Sawala et al., 2016](#)). Some galaxy properties have been shown to have an environmental dependence (e.g. [Dressler, 1980](#), showed that

elliptical and lenticular galaxies tend to reside in higher density environments, while for spirals the reverse is true), and so constrained simulations increasingly try to match to larger-scale surroundings as well as the local galaxy properties (in addition to the HESTIA project, there is now also the SIBELIUS suite [Sawala et al., 2022](#)).

The overarching goal of this project is to produce extremely high-resolution, cosmological, fully-coupled radiation-hydrodynamical simulations of the LG of galaxies using the AMR code `RAMSES-RT`, allowing us to explore the effect of reionisation on the population of satellite and dwarf galaxies in unprecedented detail. When completed, these will be the highest-resolution fully-coupled radiation-hydrodynamics constrained simulation of the Local Group. Such high resolution is required as it is low-mass haloes that are most affected by reionisation, on account of their shallower potential wells, with photoheating impacting their ability to form stars (e.g. [Efstathiou, 1992](#)). Using such well-resolved simulations will also allow us to accurately connect the galaxies that make up the $z = 0$ LG with their high- z progenitors and study the effect of reionisation on the aforementioned small-scale tensions.

This chapter details part of the work to realise this project, which is still ongoing. We demonstrate that we are able to successfully produce a set of working `RAMSES` ICs from the original HESTIA suite (which were in the `AREPO` format), by comparing the $z = 0$ LG properties at a range of resolutions. Then, we detail the preliminary done work on calibrating the code parameters to produce realistic reionisation histories. Future work stemming from this chapter will be to continue the calibration work, and eventually run extremely high-resolution simulations of the LG throughout the EoR.

3.2 Methods

3.3 HESTIA constrained simulations

The initial conditions (ICs) for the HESTIA suite ([Libeskind et al., 2020](#)) were produced through substantial effort from the CLUES collaboration, for a discussion on the background to their production, see § 1.4.7. The peculiar velocities used in Equation (1.4.16) were taken from the CosmicFlows-2 catalogue ([Tully et al., 2013](#)). Various techniques were used to ensure that the data were unaffected by non-linear contamination, such as by collapsing all objects within a larger bound structure into a single data point, to mitigate the impact of non-linear small-scale motions ([Sorce, 2015](#)).

In this work, we restrict our analysis to the ‘09_18’ set of ICs, where the first number

corresponds to the seed for the large scales of the white noise fields and the second to the seed for the small scales.

3.4 Initial conditions

The ICs we use for these simulations were originally designed for use with the **AREPO** code (Weinberger et al., 2020), so have undergone conversion to be used in a **RAMSES** zoom simulation. Here we describe the technical details.

Our simulations are performed in a $100 h^{-1}$ Mpc box at a base resolution of 256^3 dark matter particles and cells. Small-scale information, necessary for the formation of the LG, is included through the use of a zoom region, where a region of the simulation box initially has higher resolution than the base level. The size and shape of this zoom region varies with the level of resolution, since higher resolution means more particles and cells, and hence a higher computational cost. At the highest level in the zoom region, the effective resolution is 16384^3 (this would be the resolution if you simulated the entire box at this level), which means the zoom particles have a mass 262144 times smaller than the coarse particles.

To determine the location and extent of the zoom region, we first run a full dark matter-only constrained realisation with 512^3 particles down to $z = 0$. Using 512^3 particles means we have eight times better mass resolution than the base resolution and can resolve the MW and M31 with a few thousand particles, as opposed to a few hundred. From the 512^3 simulation, we identify the approximate location of the LG and its Lagrangian region. The Lagrangian region is the area which contains all of the particles that eventually reside in a specified region around the LG (this is resolution dependent Oñorbe et al., 2014); it is determined by tracking back the positions of particles from $z = 0$ to the start time of the simulation $z = 99$. The size of the region around the LG varies from a $5 h^{-1}$ Mpc sphere centred on the midpoint of the MW and M31 for the lowest resolution, to the union of two $2.5 h^{-1}$ Mpc spheres centred on the MW and M31 for the highest resolution. With the Lagrangian region in hand, we generate a refinement mask which marks out the region that will contain the high-resolution particles.

Generating such a mask for **RAMSES** is not trivial and there is precious little documentation on producing working zoom ICs. We produced a working code for generating cubic zoom ICs, but these are the least efficient type of ICs, since you end up simulating a much larger region than is strictly necessary (Lagrangian regions are rarely cubic, and resemble more closely an amoeba). In order to use more efficient zoom ICs, we modified part of

the IC code MUSIC (Hahn & Abel, 2011) to write out working convex hull masks in the RAMSES-readable `grafic` format. A convex hull is the smallest convex volume (i.e. has no indents) that can be generated given a set of points that defines a Lagrangian region.

The phases of the white noise fields from the original HESTIA work are stored as HDF5 files from which the density and velocity fields are then produced by the `ginnugagap` code¹.

3.4.1 Simulations

We use the adaptive mesh refinement (AMR) code RAMSES (Teyssier, 2002) to follow the evolution of dark matter, gas, and stars within the cosmological context. Ionising radiation from stars is modelled using the publicly available radiative transfer (RT) extension RAMSES-RT (Rosdahl et al., 2013), which solves the radiation-hydrodynamics equations on the same AMR grid as the gas and so self-consistently includes the backreaction of radiation on the gas. Comparing resolution between RAMSES and AREPO (the code HESTIA ICs were originally designed for Weinberger et al., 2020) is not simple, since AREPO is a moving-mesh code where RAMSES is an AMR code. The softening length in the original AREPO runs was $\epsilon = 220$ pc, and the Plummer force is exact above 2.8ϵ , so we opt for a roughly equivalent force resolution by setting a minimum cell size of $\Delta x = 570$ pc, where the RAMSES force resolution is $\sim 1.5\Delta x$ (cf. Figure 1 Teyssier, 2002).

As described in § 1.4.9, in the simulations containing gas and radiation, as well as dark matter, we allow star formation in any gas cell where i) the hydrogen number density is above some threshold n_* , ii) the local overdensity is $200\rho_{\text{cr}}$ and iii) the temperature of the gas is below 2×10^4 K (see § 1.4.9 for a discussion of these criteria). Whenever a gas cell satisfies the above three criteria, star particles (each representing a population of stars) are produced stochastically, according to a Poisson process. We test three different values of $n_* = 0.1, 1$ and 10 cm^{-3} , in units of the number density of hydrogen atoms. Feedback from supernovae is included through the kinetic feedback model (Dubois & Teyssier, 2008) where we choose all of the feedback to be in the kinetic mode, with supernova mass fraction $\eta_{\text{SN}} = 0.2$, a metal yield of 0.1 and a high mass-loading factor $\eta_w = 10$.

3.4.2 Structure finding

As in the original HESTIA work, we use the AHF code (Gill et al., 2004; Knollmann & Knebe, 2009) to build catalogues of the dark matter haloes in the simulation. When a simulation includes hydrodynamics and star formation, AHF also uses the gas and stellar

¹<https://github.com/spilipenko/ginnungagap>

mass when computing halo masses. Halo masses are calculated as the mass within a sphere which encloses a mean density of $200\rho_{\text{cr}}$. In order to use **RAMSES** outputs with **AHF**, we use the supplied **ramses2gadget** code to convert the outputs into the **GADGET-2** format. For runs containing only dark matter, the difference is minor since both codes use particles to model the dark matter—the particles are just rewritten in a slightly different format. Things are slightly more involved for runs with hydrodynamics—here the leaf cells of the AMR hierarchy are converted into pseudoparticles, deposited at the centre of the cell.

To follow the evolution of haloes in time, we construct merger trees using **consistent-trees** (Behroozi et al., 2013a). This choice of merger tree code is in contrast to the original HESTIA analysis, which used the **MergerTree** code supplied with **AHF**. We choose to use **consistent-trees** over **MergerTree** since the former does gravitational consistency checks and does not solely rely on particle membership to determine halo descendants, as the latter does (for a detailed comparison of the two algorithms, see Srisawat et al., 2013). In order to facilitate comparison with the merger trees computed for this work, we reanalyse some HESTIA simulations with **consistent-trees**. To convert our **AHF** outputs into the **consistent-trees** format, we use the conversion tools supplied with **consistent-trees**, which calculates an initial guess for halo descendants based on particle membership between snapshots.

3.4.3 Cosmographic criteria

To identify LG candidates from our $z = 0$ snapshot we apply the cosmographic criteria listed in the original HESTIA paper, which are a set of constraints on the local large-scale structure, as well as the properties of the LG itself. The constraints we impose are:

- the Virgo candidate must have $M > 2 \times 10^{14} M_{\odot}$,
- the Virgo candidate must form within 7.5 Mpc of its expected location,
- there must be no other Virgo candidate within 20 Mpc of the LG,
- the LG candidate must form within 5 Mpc of its expected location,
- the LG candidate must form within 3.5 Mpc of the true distance to Virgo,
- the masses of the MW and M31 must be between $8 \times 10^{11} M_{\odot}$ and $3 \times 10^{12} M_{\odot}$,
- the MW (the smaller mass halo) must be no less than half the size of M31,
- the LG haloes must be between 0.5 and 1.2 Mpc apart,

- there must be no other halo more massive than the MW within 2 Mpc of the LG midpoint,
- the haloes must be infalling, $v_{\text{rad}} < 0$.

3.5 Results and discussion

Different simulation methods produce different results, each method having their own strengths and weaknesses (e.g. [Agertz et al., 2007](#)). The original HESTIA simulations were carried out using the moving mesh code **AREPO**, whereas in this study we use the adaptive mesh refinement code **RAMSES** – so the first steps were to demonstrate convergence between the two codes. To begin with, we ran a series of dark matter-only simulations at increasing resolution allowing us to fine-tune the refinement mask in the initial conditions to yield good agreement with the original runs.

Figure 3.1 shows the LG produced by these simulations, identified using the criteria in § 3.4.3, where the large halo in the centre-left of each panel is the MW, and the halo in the centre-right is M31. The top panel of Figure 3.1 shows the result at an effective resolution (the total number of particles if the entire box were simulated at the zoom resolution) of 4096^3 in the zoom region, while the bottom panel shows the result of increasing this to an effective resolution of 16384^3 . At the higher resolution, more structure can develop on the smallest scales (i.e. lowest masses) which does not exist in the lower resolution runs. We are also able to resolve the dynamics of the LG with increased accuracy, as can be seen in Table 3.5 where we show the fractional difference in halo properties between this work and the original HESTIA runs, with increasing resolution giving a better match. Note that during this process we found that, through a subtle bug, the ICs for the original 16384^3

Effective resolution	Δd_{sep} (%)	ΔM_{M31} (%)	ΔM_{MW} (%)
4096^3	-22.20	-2.61	-3.26
16384^{3*}	-21.48	0.06	-2.41

Table 3.1: The DMO runs used to verify our ICs and compare to the original HESTIA runs, where the effective resolution is the same for this work and HESTIA*. We calculate the fractional difference between our new runs and the HESTIA runs as $\Delta = (x_{\text{new}} - x_{\text{HESTIA}})/x_{\text{HESTIA}}$. d_{sep} is the separation between MW and M31. M_{M31} is the mass of M31. M_{MW} is the mass of the MW. *The 16384^3 run does not have a counterpart in the original HESTIA suite, so we compare to the nearest available resolution, 8192^3 .

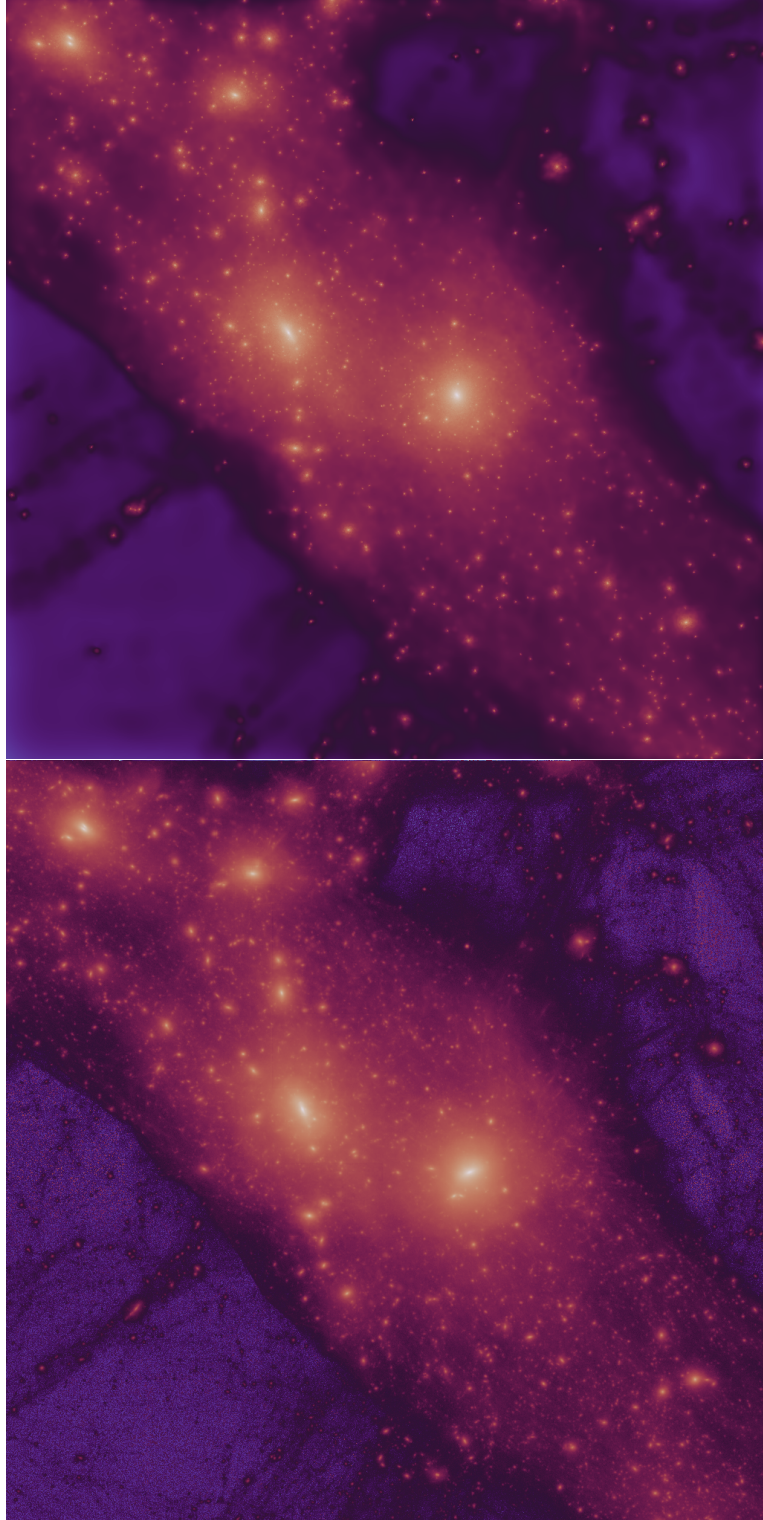


Figure 3.1: Projected dark matter density at $z = 0$, showing the result of going from 4096^3 (top) to 16384^3 (bottom) effective resolution on the simulated LG (each centre). With the higher resolution, more structure is able to develop on the smallest scales and on the larger scales more particles means we can resolve the internal dynamics in exquisite detail. The projection is of a sphere of radius $1 h^{-1}$ Mpc centred on the midpoint of the LG.

dark matter-only HESTIA runs had inadvertently been produced using the incorrect density and velocity fields, rendering them unusable. Therefore, to compare with our 16384^3 runs we use the 8192^3 HESTIA runs.

Once we have identified the LG at $z = 0$ in our simulations, we must trace these haloes back in time to find where they were during the EoR. To do this, we compute merger trees, as described in § 3.4.2. Merger trees allow us to trace halo properties, such as mass and position, back through cosmic time. Figure 3.2 shows the growth of the LG in this work (in the 16384^3 run) and in the original HESTIA suite (in the 8192^3 run), compared to some analytic predictions. We find excellent agreement between this work and the original work, allowing for some expected deviation due to differing simulation codes and resolution, as well as slight differences in the size, shape and location of the initial refinement mask.

Next, we run a set of mid-resolution test simulations, with an effective resolution of 4096^3 , but now including gas and radiation. In these test simulations, we vary the density threshold for star formation n_* , as described in § 3.4.1, to calibrate the simulations to produce a realistic reionisation history. Varying the ease with which star particles can form (through the density threshold) offers a way to alter the pace of reionisation, since star particles produce the photons which ionise the gas and so fewer stars means later reionisation. Star particles can only form inside the high-resolution region surrounding the LG, so we look at this region when computing quantities related to ionisation. Figure 3.3 shows the average fraction of ionised hydrogen x_{HII} in a $2 h^{-1}$ Mpc sphere surrounding the midpoint of the LG, estimated by calculating the midpoint of the main progenitors of the MW and M31 using the high-resolution merger trees. We show the three different star formation thresholds and the average ionised fraction calculated using a mass and volume weighting. Using a lower density threshold means that reionisation ends earlier because star particles are more easily formed and thus more ionising photons are produced. Reionisation is expected to be complete by $z \sim 5.5$ (though for the volume size we consider here there can be a lot of scatter around this, see Iliev et al. (2006a)), so for only one of the thresholds, $n_* = 0.1 \text{ cm}^{-3}$, does reionisation appear to really get underway. This is still quite late, as previous simulations predict that MW and M31 should reionise by $z \sim 8 - 9$ (e.g. Ocavirk et al., 2020). It is possible that this is due to a lack of external radiation (since stars only form inside the zoom region) but, again, previous works (e.g. Dixon et al., 2018; Aubert et al., 2018) predict that the LG reionises internally. Therefore, this late reionisation is likely an issue of star formation and feedback calibration.

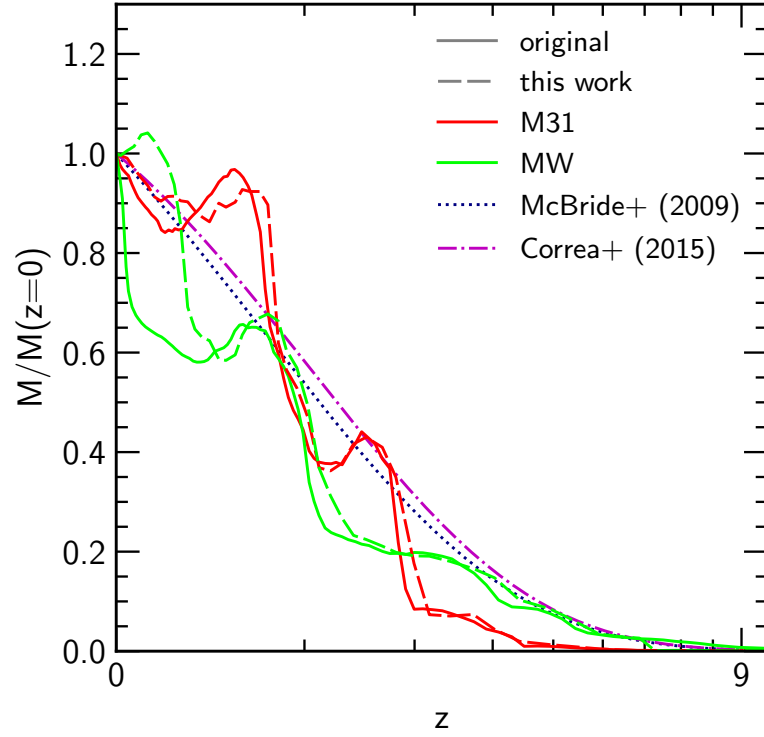


Figure 3.2: The halo mass M of M31 (red) and MW (green) as a function of z , normalised to the final halo mass $M(z=0)$ for the new (long-dashed) and the original HESTIA (solid) simulations. Also shown are the analytic models of McBride et al. (2009) (blue dotted) and Correa et al. (2015) (purple dot-dashed).

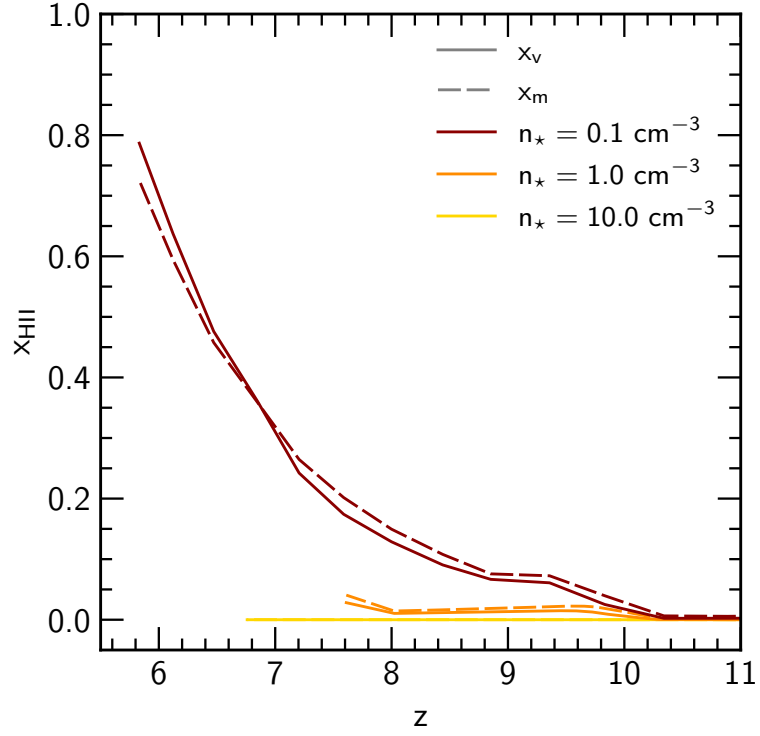


Figure 3.3: Hydrogen ionised fraction x_{HII} in a series of mid-resolution test simulations, with an effective resolution of 4096^3 . The ionised fraction is averaged over a $2 h^{-1}$ Mpc sphere, centred on the midpoint of the LG and weighted by the computational cell volume (x_v , solid) or the mass within each computational cell (x_m , long-dashed). The position of the midpoint is determined at each timestep from the high-resolution 16384^3 merger trees. We show three different star formation thresholds $n_* = 0.1$ (red), 1 (orange) and 10 (yellow) cm^{-3} , as detailed in § 3.4.1.

3.6 Conclusions

We have demonstrated excellent agreement between our RAMSES AMR resimulations and the original constrained realisation suite HESTIA, both in the final properties of the LG and in their temporal evolution. Confident that we can accurately reproduce the expected structure at $z = 0$, we were able to produce precursor radiation-hydrodynamics tests in order to calibrate star formation parameters. From here, we are now able to produce the highest resolution radiation-hydrodynamics simulations of the LG, affording us the opportunity to explore the effect of reionisation on our local neighbourhood in exquisite detail. These extremely high-resolution simulations will afford an unprecedented view of the LG, allowing us to unravel the effect that the formation of the earliest stars had on, for example, the star formation history and dwarf galaxies of the LG.

One drawback of employing the RAMSES-RT code is that, since the simulation is focused on a high-resolution zoom region, the star formation criteria must be calibrated to the resolution of the zoom. Star formation routines are highly dependent upon resolution, and the resolution achieved in the zoom region will not be reached in the coarse region outside the zoom. Therefore, stars will not form outside the region described by the zoom mask and we will not include radiation external to the LG, for example from the Virgo cluster. One solution to this could be to run companion simulations, focused on the larger scales, with star formation parameters calibrated to produce stars in this coarse region. Then, it would be possible to compare the two sets of simulations to see in which simulation a given region reaches a specific ionisation fraction first. The difficulty then, is being able to link the coarse and zoom simulations, which have inherently different star formation criteria.

Chapter 4

Growth of structure from interacting dark matter initial conditions

The initial conditions for this work were produced by Sergey Pilipenko and Gustavo Yepes, using the input $P(k)$ produced by Julia Stadler and Celine Boehm. The simulations were run by Ilian T. Iliev. I ran the halo finder and merger tree code and performed the analysis of the resulting data products.

4.1 Introduction

Typical cosmological models assume that $\sim 85\%$ of the matter in the universe is in the form of collisionless cold (has small thermal velocities $v \ll c$) dark (does not interact electromagnetically) matter (CDM). CDM is predicted to form structure in a hierarchical fashion, with larger structures forming later from smaller initial structures (e.g. [Press & Schechter, 1974](#)). These structures can span many orders of magnitude in mass, from Earth-mass haloes to galaxy clusters ([Wang et al., 2020](#)). Low-mass haloes ($M \lesssim 10^9 h^{-1} M_\odot$), which host the first galaxies, are thought to be the initial drivers of reionisation (e.g. [Ocvirk et al., 2021](#)). Consequently, it is important to consider any process that could affect the formation of such small-scale structures.

Potential small-scale shortcomings of the CDM model, such as the ‘missing satellites’ problem ([Bullock & Boylan-Kolchin, 2017](#)), where the observed number of LG satellites is far smaller than predicted from dark matter simulations, have spurred the consideration

of alternative dark matter models, such as warm, fuzzy and self-interacting dark matter¹. One such alternative model considers CDM that has non-negligible interactions between dark matter and photons in the early universe (Boehm et al., 2014), called ‘ γ CDM’. These interactions lead to a damped, oscillatory suppression of the smallest scales ($k > 1 \, h \, \text{Mpc}^{-1}$) in the linear matter power spectrum (see Figure 4.1). The oscillations in Figure 4.1 arise in a similar fashion to the baryon acoustic oscillations, occurring when dark matter is coupled to radiation, preventing gravitational collapse and leading to the propagation of acoustic waves (often called ‘dark acoustic oscillations’) (Boehm et al., 2002; Cyr-Racine et al., 2014; Schaeffer & Schneider, 2021). Using the Planck 2015 data (Planck Collaboration et al., 2016), Stadler & Boehm (2018) place a conservative upper limit on the cross-section of dark matter-photon interactions of

$$\sigma_{\text{DM}-\gamma} \leq 2.25 \times 10^{-4} \sigma_{\text{T}} \left(\frac{m_{\text{DM}}}{100 \, \text{GeV}} \right) \quad (4.1.1)$$

where σ_{T} is the Thomson cross-section and m_{DM} is the dark matter particle mass.

In this section we explore the effect of initialising a simulation with the γ CDM model, by comparing to a standard CDM simulation, whose ICs are produced using the same Gaussian random field such that the only difference between the two simulations is the input power spectrum. We explore the effect on the matter power spectrum, halo mass function and halo mass accretion history.

4.2 Methods

4.2.1 Initial conditions

The input power spectra $P(k)$ for the ICs are computed using CLASS (Blas et al., 2011), modified to allow for dark matter–photon interactions and a nonzero dark matter sound speed, as described in Stadler & Boehm (2018)². Figure 4.1 shows the power spectra at $z = 0$, in their dimensionless form

$$\Delta^2(k) = \frac{k^3 P(k)}{2\pi^2}. \quad (4.2.1)$$

Power spectra were computed for a standard CDM model (i.e. non-interacting DM, hereafter CDM) and for the case with dark matter–photon interactions (hereafter γ CDM). The strength of the interaction is characterised by the cross-section for dark matter-photon

¹Exotic dark matter models are not the only route to alleviating such a tension, for example Sawala et al. (2016) propose a resolution using baryonic physics.

²The modified code is publicly available at https://github.com/bufeo/class_v2.6_gcdm.

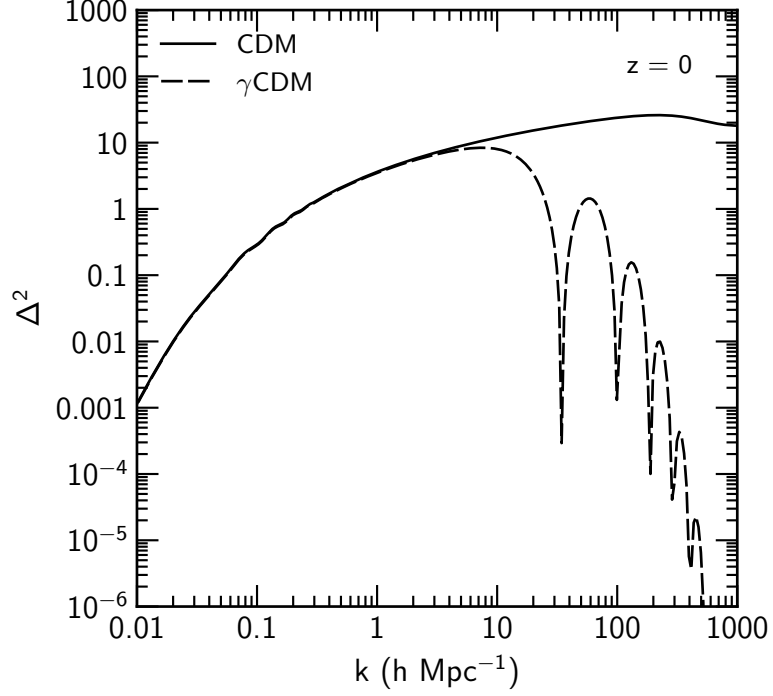


Figure 4.1: Input dimensionless power spectra for the γ CDM and CDM cases, at $z = 0$.

scattering $\sigma_{\text{DM}-\gamma}$. In turn, this cross-section can be parametrised in dimensionless form as (see Equation (1) in [Stadler & Boehm, 2018](#))

$$u_{\text{DM}-\gamma} = \frac{\sigma_{\text{DM}-\gamma}}{\sigma_{\text{T}}} \left(\frac{100 \text{ GeV}}{m_{\text{DM}}} \right). \quad (4.2.2)$$

For these simulations, $u_{\text{DM}-\gamma} = 10^{-7}$, well below the upper limit proposed by [Stadler & Boehm \(2018\)](#). For this run, the dark matter sound speed is zero, corresponding to a DM particle with mass $m_{\text{DM}} \gtrsim 1 \text{ GeV}/c^2$ (cf. Figure 3 in [Stadler & Boehm 2018](#)), where the inequality arises because the dark matter sound speed is inversely proportional to m_{DM} (cf. Equation (25) in [Stadler & Boehm 2018](#)). We defer to [Stadler & Boehm \(2018\)](#) for further details on computing $P(k)$ in the γ CDM case.

For each case, the ICs are generated with identical white noise fields, so the only difference is the power spectrum that is convolved with the field. In this way, we can ensure that any differences between the simulations are due entirely to the different ICs.

The ICs are generated at $z = 120$ assuming a flat cosmology consistent with the Planck 2013 results ([Planck Collaboration et al., 2014](#)), with parameters: $\Omega_{\text{m}} = 0.318$, $\Omega_{\Lambda} = 0.682$, $\Omega_{\text{b}} = 0.049$, $h = 0.678$, $\sigma_8 = 0.833$ and $n_s = 0.9611$.

4.2.2 Simulations

The simulations are run using the N -body particle-particle–particle-mesh code CUBEP³M (Harnois-Déraps et al., 2013). The particle-mesh solver computes long-range gravity forces and the particle-particle solver computes short-range forces. A box size of $100 h^{-1}$ Mpc is used, containing 4096^3 particles, meaning haloes of mass $6.4 \times 10^7 h^{-1} M_{\odot}$ are resolved with 50 particles. We do not include radiation in these simulations, since the interaction rate between CDM and radiation is negligible at the redshifts we consider here ($z < 120$).

The ICs are a constrained realisation produced by the CLUES collaboration, designed to reproduce the LG (MW and M31) and surrounding environment (e.g. Virgo) to high accuracy. At this resolution, the simulations are prohibitively expensive to run to $z = 0$, and so are stopped at the end of reionisation $z = 6$. A companion set of zoom simulations, starting from the same white noise phases but with a high-resolution region only on the LG, has been run to $z = 0$, allowing the progenitors of the $z = 0$ MW and M31 to be tracked back in time. We defer a study of the LG for now, opting to consider the global effect of the different dark matter models. The constrained nature of the simulations should have no more impact on our results than if this were a random realisation.

4.2.3 Power spectra

CUBEP³M computes the power spectrum $P(k)$ of the density contrast field

$$\delta(\mathbf{x}) = \frac{\rho(\mathbf{x}) - \rho_m}{\rho_m} \quad (4.2.3)$$

at a given redshift z on-the-fly, using the coarse mesh of the simulation. To calculate $\delta(\mathbf{x})$, the dark matter particle mass is first assigned on to a regular mesh. The interpolation method used to assign the mass, in this case cloud-in-cell (CIC), can introduce artefacts, which can be removed by deconvolving the assignment kernel (Hockney & Eastwood, 1981). This is done automatically by CUBEP³M. Next, the density contrast is transformed into Fourier space to give $\delta(\mathbf{k})$, which yields the power spectrum $P(k) = \langle |\delta(\mathbf{k})|^2 \rangle$, spherically-averaged over k .

4.2.4 Haloes

To identify structure in the simulations, we postprocess the output particle data using the halo finder **rockstar** (Behroozi et al., 2013a), which uses position and velocity information to identify haloes in phase space. Halo masses are calculated as the mass within a sphere that has an overdensity $\Delta = 200$, with respect to the critical density ρ_{cr} , where only dark

matter particles that `rockstar` determines to be bound are included in the calculation of halo properties. `rockstar` also makes a first attempt at constructing merger trees, assigning a given halo’s descendant as the halo in the next timestep that has the largest number of particles in common.

We follow the formation and growth of haloes with merger trees, computed using `consistent-trees` (Behroozi et al., 2013b). `consistent-trees` takes the particle-based merger trees produced by `rockstar`, and estimates the gravitational dynamics of haloes to improve the consistency of the trees. We use the halo catalogues produced by `consistent-trees`, which also determines whether a given structure is a host or subhalo, to compute the halo mass function.

The halo mass function dn/dM is constructed by binning haloes by mass and dividing by the bin width and box volume. We use mass bins of constant width in log space, of width $\Delta\log_{10}(M/h^{-1} \text{ M}_{\odot}) = 0.2$ (bin widths of $\Delta\log_{10}(M/h^{-1} \text{ M}_{\odot}) = 0.5$ or smaller were found to introduce negligible error into the mass function reconstruction by Lukić et al., 2007). We take the mean halo mass of all haloes in that bin to be the bin centre. Only host haloes are used to compute the halo mass function, though the mass of a host is inclusive of all the substructure contained within it. Analysis of the merger trees is done using the `ytree` package (Smith & Lang, 2019).

4.3 Results

In this section we explore the effect of initialising the simulations with γ CDM ICs, by comparing to the simulation initialised with standard CDM ICs. We explore the effect on the matter power spectrum, the halo mass function and the mass accretion history (MAH) of haloes.

4.3.1 Power spectra

To quantify the difference in power between the two simulations, we can look at the ratio of the power spectra at fixed z , shown in Figure 4.2. We can see that at $z = 119.4$ the power spectra ratio follows in the input ratio quite closely, although there is already some sign of a reduction in suppression at the low- k end. By $z = 12.9$ the oscillatory nature of the suppression is barely visible and by $z = 10.1$ it is not visible at all. If we fix the scale at $k = 10.0 \text{ h Mpc}^{-1}$ we find that at $z = 119.4$, the power spectrum in the γ CDM case is 0.69 times that of the CDM case, but by $z = 6.0$ this suppression is reduced to 0.91. By $z = 6.0$ the γ CDM power spectrum more closely follows the CDM spectrum, though the

small scales ($k \gtrsim 20 \ h \text{ Mpc}^{-1}$) still show strong deviation.

Now in Figure 4.3 we play the opposite game and fix the ratio, asking what is the first (lowest) k for which this ratio occurs at a given z . As expected from Figure 4.2 we find that the suppression by a given ratio monotonically shifts to higher k as z decreases. The rate at which the suppression is shifted to higher k also appears to increase for $z \lesssim 10$.

4.3.2 Halo mass function

In Figure 4.4 we show the halo multiplicity function for the CDM (top, points) and γ CDM (bottom, crosses) cases, with the analytic [Watson et al. \(2013\)](#) curve (solid) calculated using the CDM input $P(k)$. We find good agreement between the CDM data and the theoretical mass function at almost all masses at $z = 6.0$, for low masses at $z = 8.1$ and a suppression for earlier redshifts. The γ CDM data exhibit similar behaviour to the CDM data for haloes with $\gtrsim 10^{10} \ h^{-1} \text{ M}_\odot$, but are strongly suppressed for smaller haloes. At $z = 20.1$, where we would not expect to find any haloes above $10^{10} \ h^{-1} \text{ M}_\odot$ in our simulation box, there are no haloes with more than 50 particles in the γ CDM case, whereas there are haloes in the CDM case albeit suppressed by at most a factor of ~ 5 compared to the theoretical prediction.

In Figure 4.5 we show the ratio of dn/dM for the γ CDM case to the CDM case. Here, the low-mass suppression is clearly seen, with most of the reduction in haloes occurring below $\sim 10^{10} \ h^{-1} \text{ M}_\odot$. There remains some suppression at the highest masses, though much less than at lower masses. Note that we plot the ratio against the mean mass for γ CDM haloes in that mass bin, which means that here we are only sensitive to changes in the binned mass function dn/dM , not the masses of haloes in that bin. Hence, by comparing to Figure 4.4 by eye, it may appear that the ratio of dn/dM should be slightly below one for the highest mass bins for $z = 10.1, 8.1$ and 6.0 , not exactly one as Figure 4.5 suggests. In fact, the dn/dM are exactly equal in these cases, it is only the mean mass of haloes in the bin that are slightly different.

4.3.3 Mass accretion history

We now turn our attention to the effect of using γ CDM ICs on the growth of dark matter haloes. We characterise the growth of haloes by tracking the main progenitor branch back through time, normalising the mass at each redshift $M(z)$ to the final mass $M_0 = M(z = 6.0)$, thus calculating the mass accretion history (MAH) of a halo as $M(z)/M_0$. We bin the haloes by their final mass, calculating the average MAH $\langle M(z)/M_0 \rangle$ as the mean of

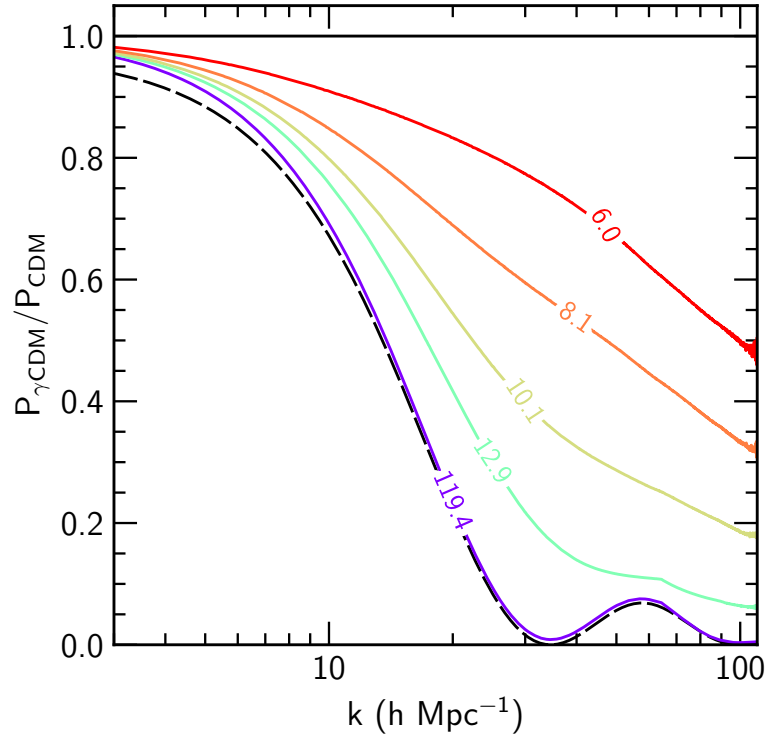


Figure 4.2: Ratio of the matter power spectrum $P(k)$ in the γ CDM simulations to the CDM simulations at $z = 119.4$ (purple), 12.9 (green), 10.1 (yellow), 8.1 (orange) and 6.0 (red). Also shown is the ratio of the input power spectra at $z = 120.0$ (black dashed).

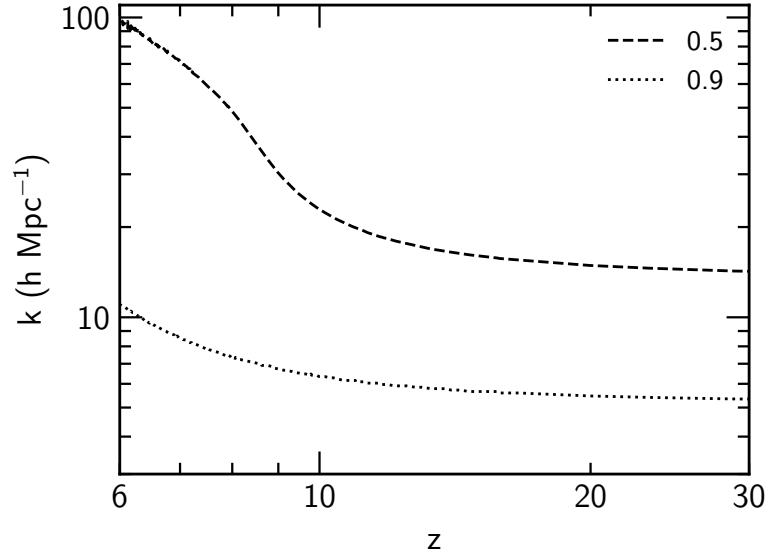


Figure 4.3: Scale k at which the γ CDM power spectrum is suppressed by a specified factor, compared to the CDM power spectrum (cf. Figure 4.2) as a function of redshift z .

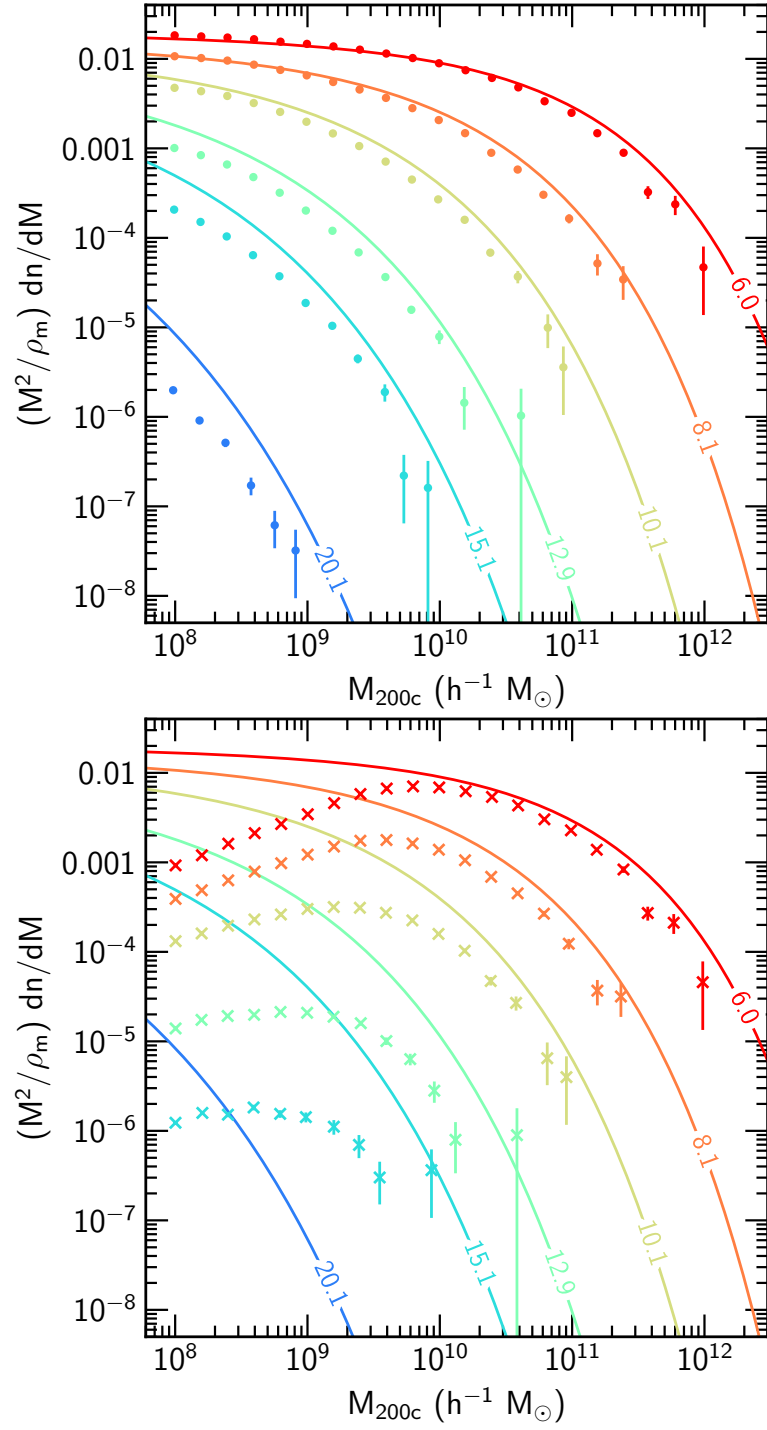


Figure 4.4: Halo multiplicity function for the CDM (top, points) and γ CDM (bottom, crosses) cases, at $z = 20.1$ (dark blue), 15.1 (light blue), 12.9 (green), 10.1 (yellow), 8.1 (orange) and 6.0 (red). Also shown is the analytic [Watson et al. \(2013\)](#) curve, calculated at each z using the input CDM $P(k)$ in both cases.

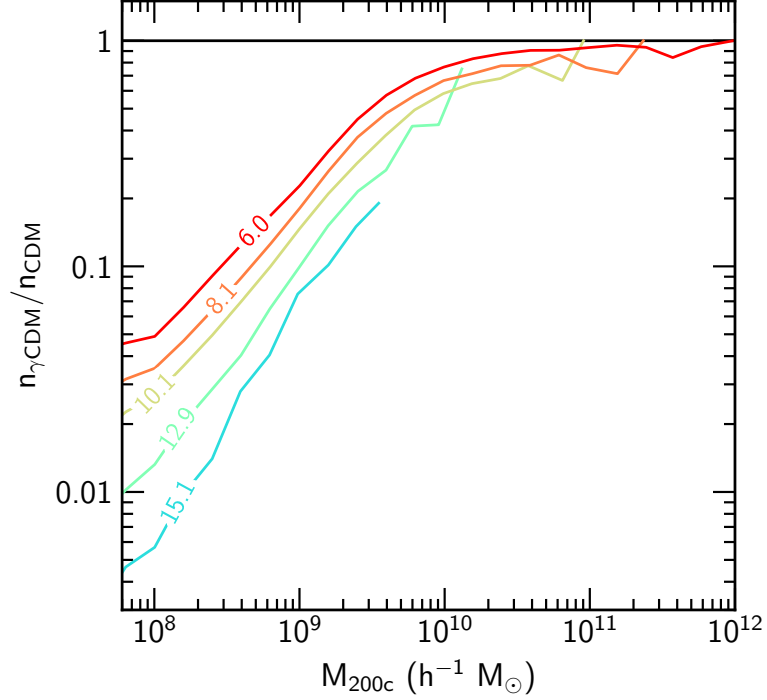


Figure 4.5: Ratio of halo mass function dn/dM for the γ CDM case to the CDM case at $z = 15.1$ (light blue), 12.9 (green), 10.1 (yellow), 8.1 (orange) and 6.0 (red).

all the MAHs in the bin. We compute theoretical MAHs using the model presented in [van den Bosch et al. \(2014\)](#), which solves for the MAH using the universal time coordinate presented in that study and a fitting formula calibrated to the Bolshoi simulations ([Klypin et al., 2011](#)) at $z \leq 2$ and a semi-analytic model at higher z . For the theoretical MAHs, we take M_0 to be the midpoint of the mass bin.

Figure 4.6 shows the MAH for the full range of redshifts for which a halo remains above the resolution limit. The CDM case exhibits excellent agreement with the theoretical prediction at $z < 10$, deviating above this redshift due to resolution issue – it is only possible to accurately track a halo back to a certain fraction of its final mass since at some point you will run out of particles with which to make up your halo. In the γ CDM case, the first haloes always form later than their CDM counterparts. This delayed formation means that the mass accretion of the γ CDM case lags behind that of the CDM case, with the γ CDM haloes accreting more of their mass later on than the CDM haloes.

This can be more clearly seen in Figure 4.7 where we show the mean MAH again, this time for the redshift range $6 \leq z \leq 10$ on a linear scale. The agreement between the CDM case and the [van den Bosch et al. \(2014\)](#) prediction can be more clearly seen here, as can the increase in the rate of accretion at $z \lesssim 8$.

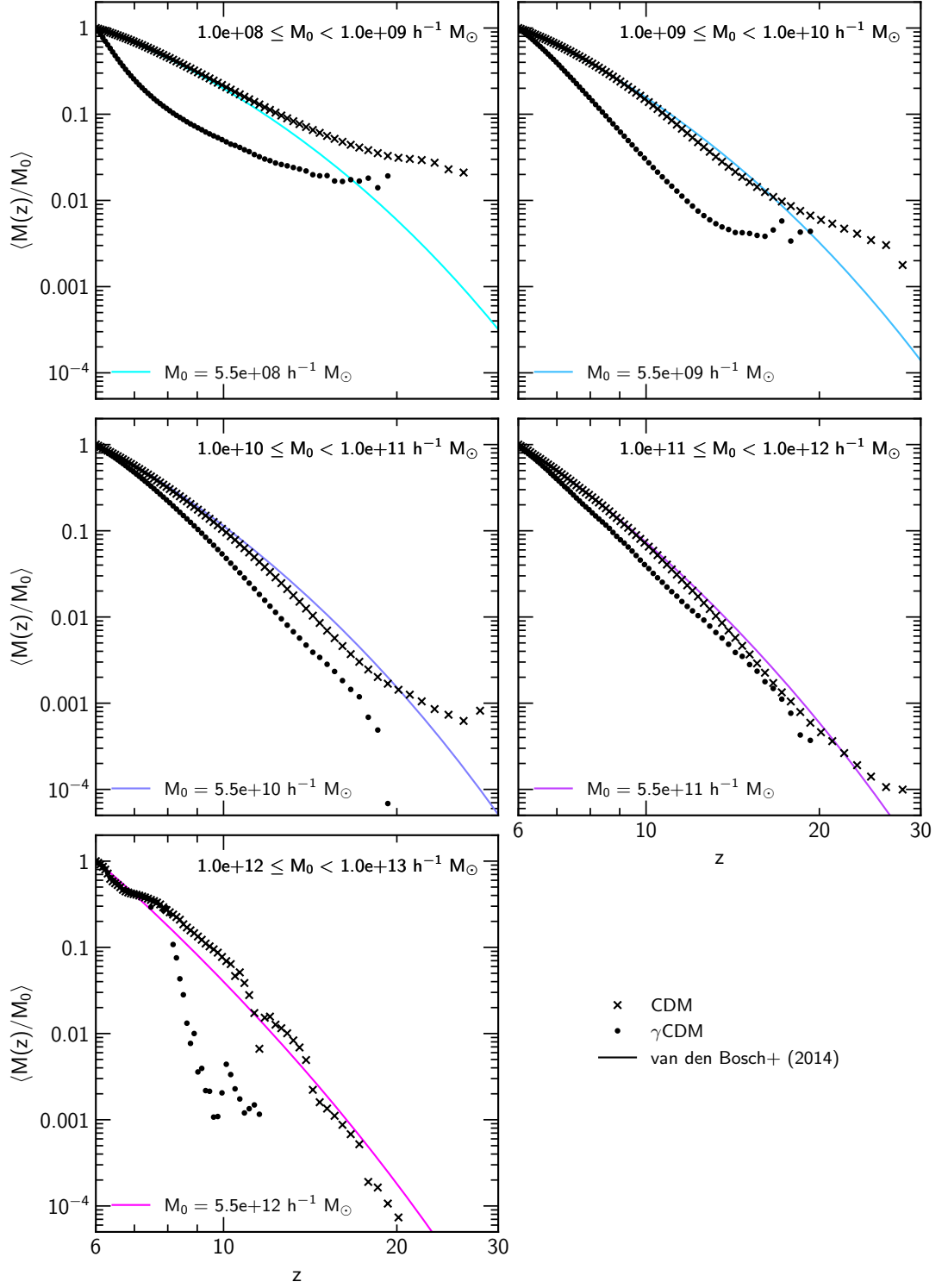


Figure 4.6: MAHs for the main progenitor binned by the final mass at $z = 6.0$, M_0 , calculated from the CDM (crosses) and the γ CDM (points) simulations. The mass at each redshift $M(z)$ is normalised by the final mass M_0 and we take the mean at each z over all haloes in the bin. For each bin, we also show the mean MAH from [van den Bosch et al. \(2014\)](#) for a halo with a typical mass for that bin (solid).

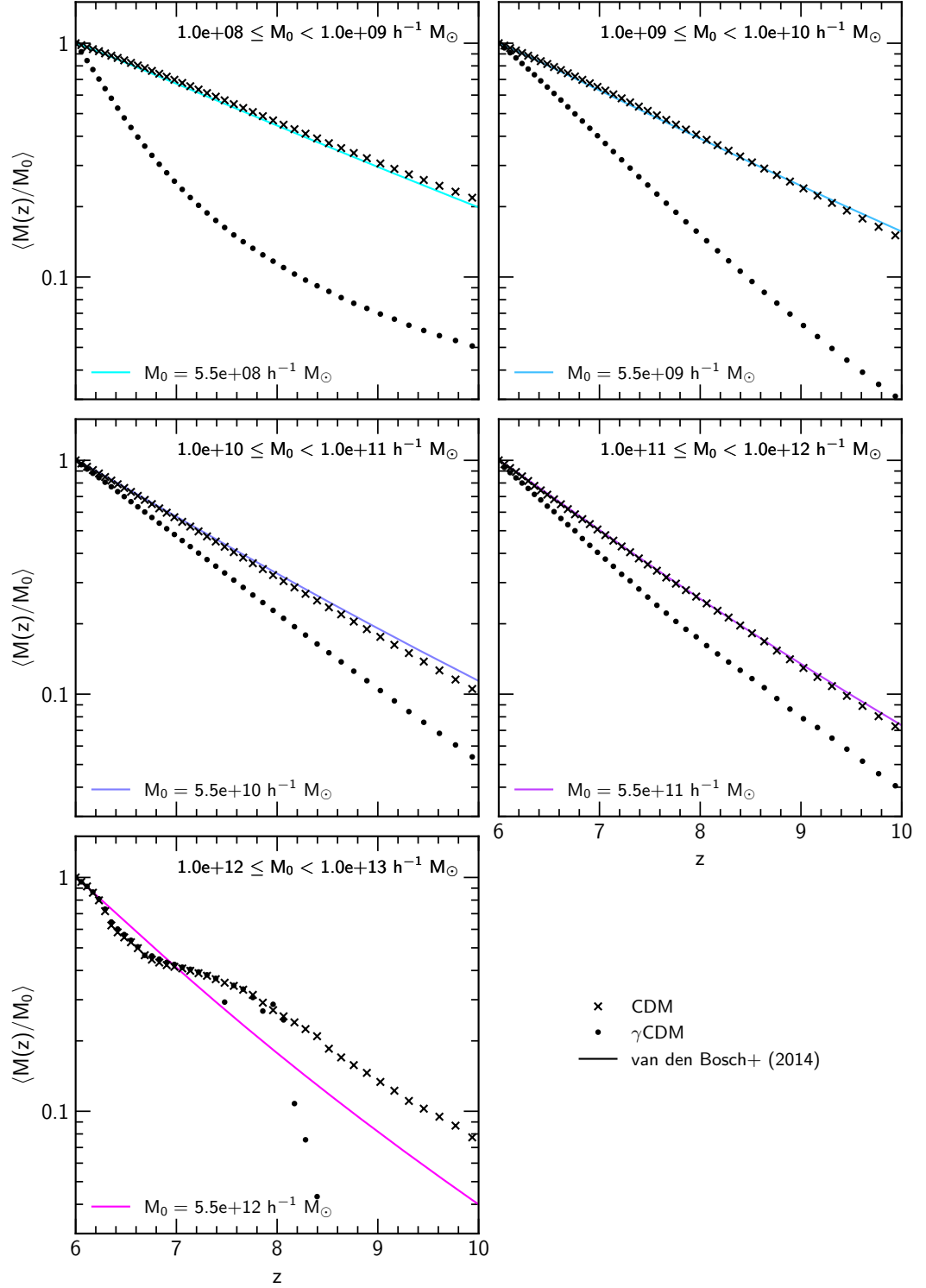


Figure 4.7: As in Figure 4.6, but over a smaller range of z . Note that z is now plotted on a linear scale.

4.4 Discussion

The matter power spectrum initially retains some memory of the initial suppression, but the amount of suppression decreases as the simulation progresses. This can be seen from Figure 4.2, which shows that at a given scale k the ratio of power spectra monotonically moves toward one as z decreases. Equivalently, from Figure 4.3 we can say that a given ratio shifts toward higher k as the simulation progresses. Hence, we can say that fluctuations in the γ CDM density field ‘catch up’ to those of the CDM, starting with the largest scales (i.e. least suppressed). This is not what you might expect from Figure 4.1, which is what you would observe if all the modes in your universe evolved linearly and independently down to $z = 0$. It is the fact that modes do not, in reality, always evolve linearly and independently that allows the small scales to catch up. Little et al. (1991) showed, using N -body simulations, that nonlinear mode coupling of large scales to small scales can erase a truncation in the initial small scale power spectrum. Further, this cascade of power is dominant in the direction of large to small scale modes, as opposed to small to large scales (Peebles, 1980; Bagla & Padmanabhan, 1997). Putting these together, we would naturally expect the two cases to begin catching up to each other since they are initialised with the same large scale modes and the suppressed small scales in the γ CDM case are not expected to have much of an impact on the larger scales. Boehm et al. (2005) found similar results for simulations of warm dark matter, which have an exponentially suppressed power spectrum above some cut-off scale.

This phenomenon is reflected in other measures of fluctuations, for example by looking at the halo mass function. At early times, low-mass haloes are strongly suppressed in the γ CDM case and are even totally missing at $z = 20.1$, although it is worth noting that the CDM case is also below the Watson et al. (2013) prediction at these times. For the CDM case, the suppression compared to Watson et al. (2013) may be due in part to the finite box size, meaning we do not sample the rarer haloes that form first. Also, these first haloes, which are already close to the resolution limit, in principle form from smaller haloes, which are below our resolution limit and hence are missing from the simulation. Future work could involve running smaller simulation volumes, with better mass resolution, to probe the low-mass regime and assess convergence of the simulations. Looking now to the γ CDM simulation, we find that haloes are strongly suppressed below $\sim 10^{10} h^{-1} M_{\odot}$. As the smaller scale modes catch up to CDM, smaller mass haloes are able to form, though there persists some suppression. The formation of these smaller mass haloes will also boost the number and mass of higher mass haloes, through mergers and accretion.

This hierarchical nature of structure formation is also apparent in the MAHs, with the highest mass bin showing strong suppression at high z , since the small-scale structures from which haloes of this size will form do not exist in large numbers at early times. The very largest mass bin ($10^{12} < M/h^{-1} \text{ M}_{\odot} < 10^{13}$) contains only one halo and so the MAH appears much less smooth than in other mass bins, which show the average MAH over many halo lineages. It is in this mass bin that the impact of low-mass halo suppression on high-mass haloes is perhaps most plain—since the very low-mass progenitor haloes are suppressed, the high-redshift growth of this high-mass halo is then affected, forming later and from more massive progenitors.

4.5 Conclusions

We have presented preliminary results from a large-scale, cosmological simulation of non-linear structure formation in a universe where dark matter can interact with radiation in the early universe. To assess what impact the dark matter interaction had, a companion simulation, initialised with the standard CDM model, was also run. The γ CDM ICs show a damped oscillatory suppression on small scales ($k > 10 h \text{ Mpc}^{-1}$). Dark matter interactions are not included in the actual simulations, just the ICs, since the dark matter-radiation interaction rate is negligible from the start time of the simulations $z = 120$.

Nonlinear mode coupling allows the initially suppressed smaller scales in the γ CDM to begin catching up to the standard CDM case. Some suppression persists at the smallest scales of the matter power spectrum until the final snapshot ($z = 6$), with $k = 97.5 h \text{ Mpc}^{-1}$ in the γ CDM case having only half the power of the CDM case at $z = 6$. The reduction in power on the very smallest scales may remain to some extent, but the oscillatory nature of the suppression is largely washed out. Larger scales in γ CDM mostly catch up to the CDM case by $z = 6$, with the power at $k = 10 h \text{ Mpc}^{-1}$ going from a ratio of 0.69 at $z = 119.4$ to 0.91 at $z = 6$.

This suppression in small-scale power translates to a reduction in the number of low-mass haloes formed, with a significant reduction in the number of haloes with masses $< 10^{10} h^{-1} \text{ M}_{\odot}$.

We find good agreement between the mean MAH for the CDM simulation and the theoretical prediction of [van den Bosch et al. \(2014\)](#). Interestingly, despite the actual dynamics of the simulations being CDM, the scale-dependent suppression in the initial power spectrum changes the mean MAHs of haloes in the γ CDM case, quite significantly. The masses in the γ CDM case grow slowly at early redshifts, then grow more rapidly at

later redshifts. The difference in MAH between the γ CDM and CDM is less pronounced for larger final masses M_0 , which would be expected since larger scales are less affected, but, interestingly, even the largest haloes are affected in some way. This is because structure growth in CDM is hierarchical; large structures grow from small structures and thus even the most massive haloes are affected by the initial suppression in small-scale power.

Future work could look at trying to match haloes between the pairs of simulations, in order to quantify the effect on individual haloes, rather than looking at global quantities. The simulations begin from identical white noise fields, so it should be possible in principle to match haloes uniquely, although care must be taken since haloes that exist in the CDM simulation will not necessarily exist in the γ CDM simulation.

Chapter 5

Structure finding in the Cosmic Dawn III simulation

This work was carried out as part of the Cosmic Dawn collaboration, who are Pierre Ocvirk (PI), Kyungjin Ahn, Dominique Aubert, Jonathan Chardin, Luke Conaboy, Taha Dawoodbhoy, Nicolas Deparis, Yohan Dubois, Stefan Gottlöber, Max Gronke, Ilian T. Iliev, Joseph S. W. Lewis, Hyunbae Park, Yann Rasera, Jenny G. Sorce, Paul R. Shapiro, Romain Teyssier, Émilie Thélie and Gustavo Yepes. I ran the halo finder and performed the analysis of the resulting catalogues.

5.1 Introduction

The Cosmic Dawn (CoDa) simulations¹ are a series of large-scale, high-resolution simulations of galaxy formation in the EoR, which use the fully-coupled radiation-hydrodynamics code **RAMSES-CUDATON** to follow the evolution of dark matter, gas, stars and radiation in the cosmological context. **RAMSES-CUDATON** uses the **ATON** radiation-hydrodynamics module for **RAMSES**, ported to the GPU (hence ‘**CUDA**’). In **RAMSES-CUDATON**, the radiative transfer is performed on the GPU while the gas and dark matter dynamics are solved on the CPU. In this setup, information about the state of the gas is transferred from the CPU to the GPU at the end of a dynamics timestep and back again after a radiation timestep. The **CUDATON** part of the code can only deal with regular grids and so the AMR portion of **RAMSES** is turned off and the code is run in unigrid mode, meaning the gravity is solved using the PM solver (cf. Figures 1.5 and 1.6). When run in unigrid mode, **RAMSES** maintains a constant comoving resolution but the physical resolution decreases as the simulation

¹<https://coda-simulation.github.io/>

progresses. The speed increase resulting from doing performing the radiative transfer on the GPU means that the run can be carried out using the full speed of light without need to resort to the reduced speed of light approximation (see § 1.4.3 for a discussion on this approximation).

Each of the CoDa simulations uses constrained realisations of the Local Universe from the CLUES collaboration, thereby offering an insight into how reionisation progressed in the local neighbourhood. The combination of large-scale and high-resolution means that CoDa is able to accurately model ionising sources both internal (e.g. MW and M31) and external (e.g. Virgo) to the Local Group. The original CoDa I simulation (Ocvirk et al., 2016) was performed in a $64 h^{-1}$ Mpc box using 4096^3 dark matter particles and (radiation-)hydrodynamic cells. In this simulation, reionisation ends very late, finishing at $z = 4.6$. CoDa II (Ocvirk et al., 2020) was performed in the same size box, with the same number of resolution elements, but improved upon the original in several aspects, most notably recalibrating star formation to produce a more realistic reionisation history, where reionisation ends at $z = 6.2$.

Next in line, and the focus of this chapter, is the CoDa III simulation. Again, this was run in a $64 h^{-1}$ Mpc box, but this time using 8192^3 particles and cells, making CoDa III the largest fully-coupled radiation-hydrodynamics simulation ever performed, as well as giving it twice better spatial resolution and eight times better mass resolution than CoDa II. The magnitude of the simulation required vast amounts of compute resources to run, using 131072 CPUs and 24576 GPUs across 4096 nodes on the Summit supercomputer at Oak Ridge² over 10 days of wallclock time.

The improvements in CoDa III relate not only to its size, but also to the physics included in the run. CoDa III includes a dust model which tracks the creation and destruction of dust on-the-fly in each computational cell, using the model of Dubois et al. (in prep., see Trebitsch et al. (2021) for a similar implementation). Preliminary results from CoDa III show that we are able to reproduce the short mean free path of ionising photons at $z = 6$, as recently reported by Becker et al. (2021) (Lewis et al., 2022).

This extreme resolution also generates extreme volumes of data. All 118 of the outputs together occupy 20 PB of disk space, with each snapshot consisting of ~ 170 TB of data. This huge volume of data is vastly reduced when considering only what is essential for the halo finding, and in the end we were able to reduce the amount of data to be processed down to ~ 6.5 TB per snapshot.

²<https://www.olcf.ornl.gov/summit/>

In addition to the main **RAMSES-CUDATON** run, a companion dark matter-only **GADGET-2** simulation was also run, starting from the same ICs and using 4096^3 dark matter particles. Since this companion simulation (called ‘ESMD’) was run with **GADGET-2**, the gravitational interactions between particles were computed using a TreePM solver which means that, despite having eight times worse mass resolution, ESMD has superior force resolution (see § 1.4.1). The force resolution in **RAMSES** is approximately 1.5 times the cell width (see Figure 1 in Teyssier, 2002) which for CoDa III gives a force resolution of $11.7 h^{-1}$ kpc. The comoving³ gravitational softening in **GADGET-2** was set to $\epsilon = 1.0 h^{-1}$ kpc and, for Plummer softening, the force is exact above 2.8ϵ so the force resolution in the **GADGET-2** run is $2.8 h^{-1}$ kpc, roughly four times better than in CoDa III. Having higher force resolution means that ESMD is able to better resolve low-mass haloes (Figure 1.6 shows this effect, though in that case the difference is between AMR and PM), though it is unable to push down to as low masses as CoDa III due to the poorer mass resolution.

On account of the extreme mass resolution of CoDa III and broad range of included physics, it is able to accurately model the growth and evolution of the high- z , low-mass galaxies that drive the process of reionisation. It is therefore an excellent simulation for making theoretical predictions about these galaxies, which are especially topical given the recent flurry of discoveries by JWST (e.g. Castellano et al., 2022; Naidu et al., 2022; Adams et al., 2022).

In order to make accurate predictions about these galaxies, it is essential to robustly identify the dark matter haloes and their associated gas and stellar content. There are many algorithms available for finding haloes in simulations (see § 1.5.2) and the choice of algorithm is often driven by striking a balance between performance and accuracy. Whatever the choice of algorithm, it is essential to verify that the identified structures faithfully represent the actual underlying density distribution.

In this chapter we will focus on assessing the halo finding for CoDa III. We will discuss and motivate our choice of halo finder; present halo mass function results from this analysis; discuss shortcomings of the chosen algorithm; and, finally, offer some suggestions for future work which could improve the halo catalogues. CoDa III assumes a flat Λ CDM cosmology consistent with the Planck Collaboration et al. (2014) results, with parameters: $\Omega_m = 0.307$, $\Omega_\Lambda = 0.693$, $\Omega_b = 0.0482$, $n_s = 0.963$, $\sigma_8 = 0.829$ and $h = 0.6777$.

³At much later redshifts, $z = 1.5$, **GADGET-2** switches to using a fixed *physical* gravitational softening of $0.4 h^{-1}$ kpc, but at all the redshifts considered in this chapter the comoving softening is constant, as is the case in CoDa III.

5.2 Results and discussion

5.2.1 Halo mass function

As described in § 5.1, processing the enormous CoDa III dataset presents a significant technical challenge and motivates the choice of halo finder to one that can efficiently work with vast amounts of RAMSES data. To this end, we opted to use the pFoF halo finder (Roy et al., 2014) which natively works with RAMSES outputs and was used to analyse CoDa I and II, as well as the Dark Energy Universe Simulation (DEUS) (Alimi et al., 2012), which used 8192^3 particles in a $21 h^{-1}$ Gpc box⁴. We perform FoF on the dark matter particles only, rescaling the simulation particle mass m_p as

$$m'_p = \frac{\Omega_m}{\Omega_m - \Omega_b} m_p \quad (5.2.1)$$

which is equivalent to assuming that each particle has the cosmic mean fraction of baryons (i.e. that baryons trace dark matter exactly). Assuming that all of the simulation mass is in dark matter is a necessary approximation to aid the processing, however it is important to note that the inclusion of baryons has been shown to suppress the low-mass end of the halo mass function (e.g. Sawala et al., 2013) and reionisation preferentially impacts the baryon content of low-mass galaxies, so a more accurate treatment would involve analysing the baryons too. We use the standard linking length of $b = 0.2$, and keep haloes containing at least 50 particles, where the rescaled particle mass for CoDa III is $m'_p = 4.02 \times 10^5 h^{-1} M_\odot$. FoF catalogues for the ESMD simulation were produced using a slightly different FoF implementation (due to Gottlöber & Turchaninov, see Section 2.7 in Knebe et al. (2011) for a discussion of the algorithm). The ESMD simulation contains only dark matter, so no rescaling of the particle mass is necessary.

In Figure 5.1 we show the halo multiplicity function for the CoDa III simulation at $z = 15.0$ and $z = 5.0$, along with the closest snapshot from the ESMD run and the FoF fitting function of Watson et al. (2013). At $z = 15.0$ the shape of the CoDa III mass function is radically different to both the ESMD and Watson et al. (2013) curves—CoDa III exhibits a paucity of low-mass haloes and an excess of high-mass haloes. In contrast, the shape of the ESMD curve function agrees well with the Watson et al. (2013) curve, but has fewer haloes at lower masses. The missing low-mass haloes in CoDa III are likely caused, at least in part, by the limited force resolution of CoDa III, which is too coarse to properly resolve these small haloes. The high-mass excess could also be due

⁴Though DEUS used the same number of particles as CoDa III, the box size was vastly larger and so CoDa III resolves many more small-scale structures, which dominate the processing time.

to the force resolution, working in tandem with a deficiency in the FoF algorithm: the limited force resolution makes haloes less centrally concentrated and thus it is easier for the FoF algorithm to ‘overlink’ (spuriously connect two unrelated FoF groups through some bridging particle), as the particles are more loosely associated to a halo. In the ESMD case, the slight underestimation of the mass function could just be a resolution issue, as there has not been enough time for haloes near the resolution limit to accrete mass.

At the latest redshift analysed, $z = 5.0$, the two mass functions show remarkable agreement above $\sim 10^9 h^{-1} M_{\odot}$, both with each other and the [Watson et al. \(2013\)](#) curve. Below $10^9 h^{-1} M_{\odot}$ there is significant suppression of the CoDa III mass function with respect to both ESMD and [Watson et al. \(2013\)](#), while ESMD exhibits good agreement with [Watson et al. \(2013\)](#) down to the resolution limit. In CoDa III, there is possibly some overlinking, as evidenced by a slight excess in the abundance of the highest-mass haloes. The suppression of the low-mass CoDa III haloes could be due, again, to the poor resolution of the PM gravity solver. There is also likely some impact from reionisation, which affects the baryon content of haloes. Though we do not explicitly treat the baryons here, they will still have an (albeit minor) impact on the dark matter distribution, and consequently on the dark matter halo masses.

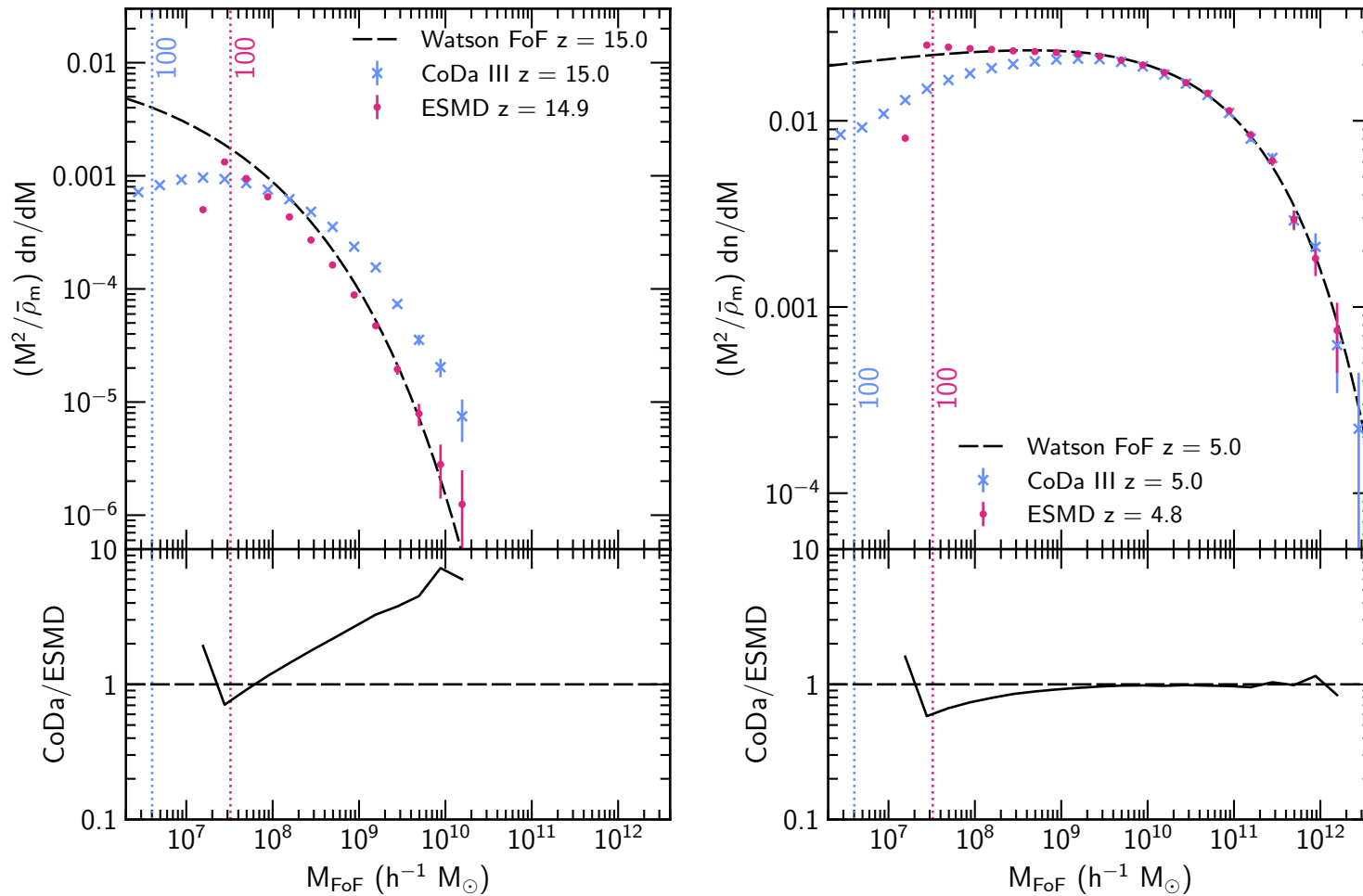


Figure 5.1: Top: the halo multiplicity function at $z = 15.0$ (left) and $z = 5.0$ (right) for the CoDa III simulation (blue crosses). Also shown is the companion ESMD run (pink points) at $z = 14.9$ (left) and $z = 4.8$ (right), as well the [Watson et al. \(2013\)](#) FoF fitting function at each CoDa III redshift (black dashed). Coloured dotted lines indicate the 100 particle limit for each simulation. Bottom: the ratio of the CoDa III mass function to that of ESMD.

Figure 5.2 shows the ratio of the CoDa III to ESMD mass functions as a function of redshift, showing that as time increases the high-mass ends of the ESMD and CoDa III mass functions generally become more alike. Interestingly, the low-mass ends of the mass functions actually move apart. Reionisation could be the culprit here, as the largest drop of $\sim 10\%$ occurs between $z = 9.0$ and $z = 5.0$, i.e. as the universe reionised. It could also be the case that the low-mass haloes in ESMD grow more quickly than the same haloes in CoDa III. It is unlikely the fixed comoving force resolution (i.e. worsening physical resolution) of CoDa III is to blame here since, at these redshifts, the comoving force resolution in ESMD is also fixed.

5.2.2 Overlinking

We have discussed at length a key deficiency in the FoF algorithm, namely that nearby haloes can become spuriously linked by an intermediate particle bridge. In Figure 5.3 we show such an example, where the algorithm has overlinked a large halo residing in a filament. Overlaid on the top panel of Figure 5.3 are all the haloes with $M > 10^9 h^{-1} M_\odot$ found by **rockstar** when it is run on the region surrounding the overlinked halo. In the bottom panel of Figure 5.3 we show the projected dark matter density for this region, where the smaller structures found by **rockstar** are clearly visible.

The question now is, is it possible to avoid overlinking when using FoF? One avenue to explore is changing the choice of linking length. The top panel of Figure 5.4 shows the same region, this time analysed with a linking length of $b = 0.15$, instead of $b = 0.2$, where for clarity we only show haloes with $M > 10^{10} h^{-1} M_\odot$. This linking length does a much better job at separating haloes and does not overlink the filamentary structure. However, this is not the end of the story, as moving to $b = 0.15$ does not totally remove all overlinking. Looking now at all haloes with $M > 10^9 h^{-1} M_\odot$, bottom panel of Figure 5.4, we can see that overlinked haloes do exist in this catalogue, they have just been shifted down to lower masses. It is also not possible to keep pushing down to arbitrarily small linking lengths since, as the linking length decreases, the corresponding halo overdensity increases. Decreasing the linking length has the effect of removing low-mass haloes which may never reach such high overdensities.

5.3 Conclusions

In this chapter we discussed the analysis of structures within the CoDa III simulation, a newly-completed simulation of the EoR using 8192^3 dark matter particles and grid cells.

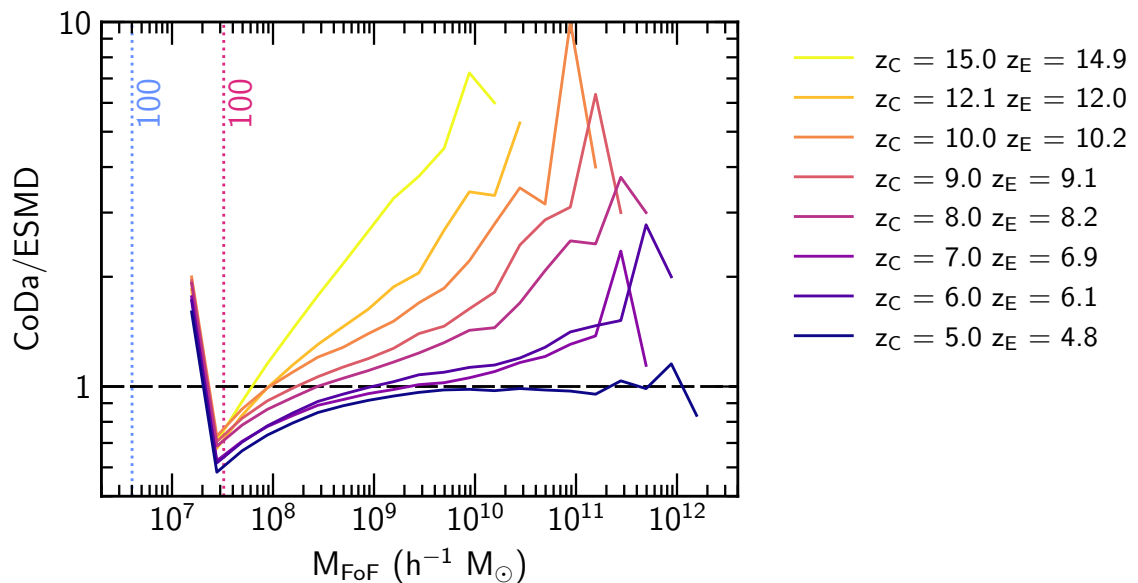


Figure 5.2: The ratio of the CoDa III to ESMD mass functions as a function of FoF mass at selected redshifts. Note that CoDa III and ESMD have outputs at slightly different times, hence the two redshifts listed in the legend.

Analysing this simulation presented a difficult technical challenge, which motivated the choice of a lightweight halo finder, pFoF, which uses the 3D spatial FoF algorithm. Using pFoF, we were able to produce halo catalogues at a range of redshifts.

As discussed previously, it is important to verify that the halo analysis accurately reflects the structures present in the simulation. In this chapter, we focused on that verification by comparing to a companion 4096³ dark matter-only simulation run with GADGET-2. We found that the high-mass end of halo mass function shows good agreement to the companion simulation and the [Watson et al. \(2013\)](#) FoF fitting function at $z = 5.0$, but exhibits significant differences at $z = 15.0$. We attribute this discrepancy to two effects working in tandem: overlinking and poor force resolution. Overlinking is a natural deficiency of the FoF algorithm, whereby particles close in space (but not bound) can become spuriously linked together through a particle bridge. This effect cannot be the entire cause of the discrepancy between the two simulations, since the companion simulation was also analysed using a (different) FoF implementation. However, the poorer force resolution in CoDa III means that haloes are less centrally concentrated and it is thus easier to form these spurious particle bridges in the first place. In addition to the discrepancy at the high-mass end, we also found that the low-mass end of the CoDa mass function moves further away from ESMD with time, which could be due to reionisation impacting the masses of low-mass galaxies, or could be an artefact of low-mass haloes growing at different rates

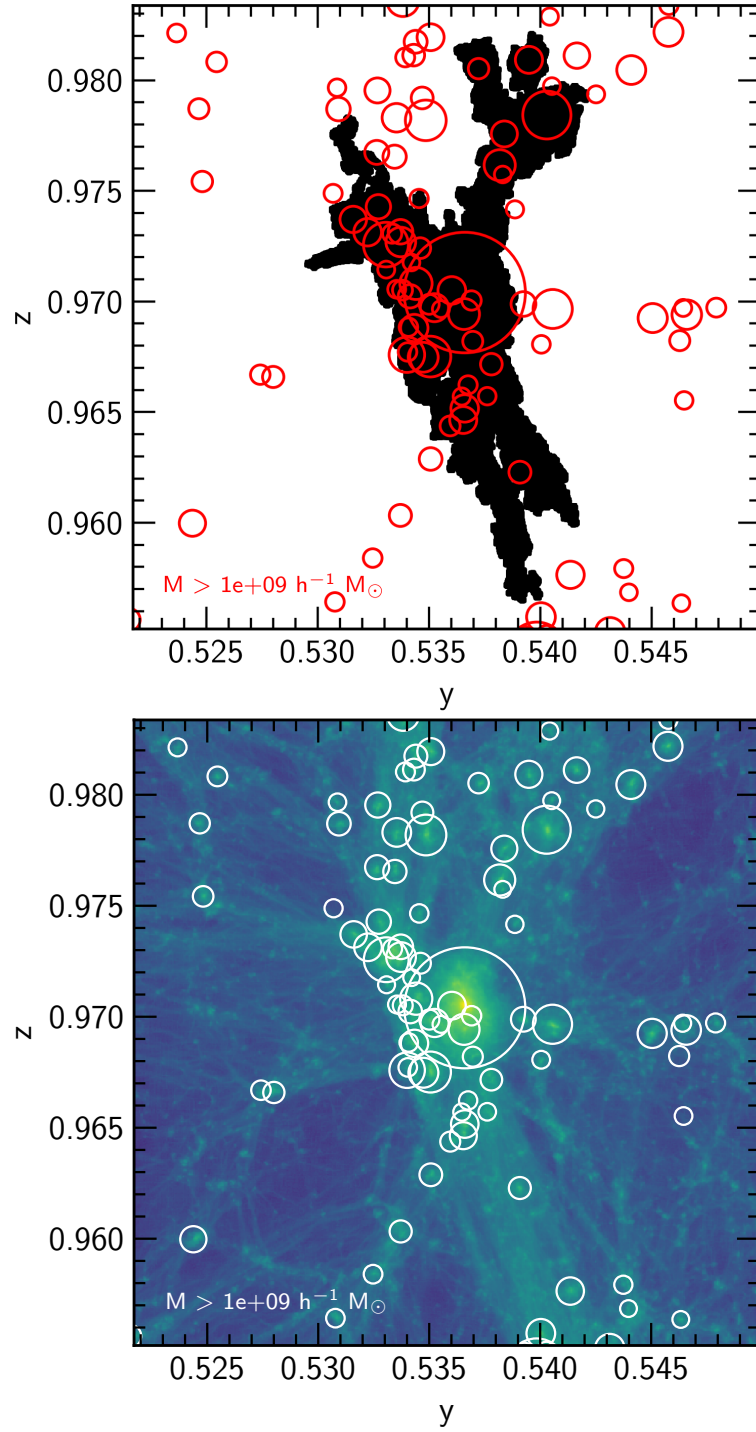


Figure 5.3: Top: a large overlinked halo found at $z = 7.0$, where the black points are the $b = 0.2$ FoF group and red circles are all the haloes found by **rockstar** in that region with $M > 10^9 h^{-1} M_{\odot}$. Bottom: same region as top panel, but this time showing the projected dark matter density, overlaid in white are the same **rockstar** haloes.

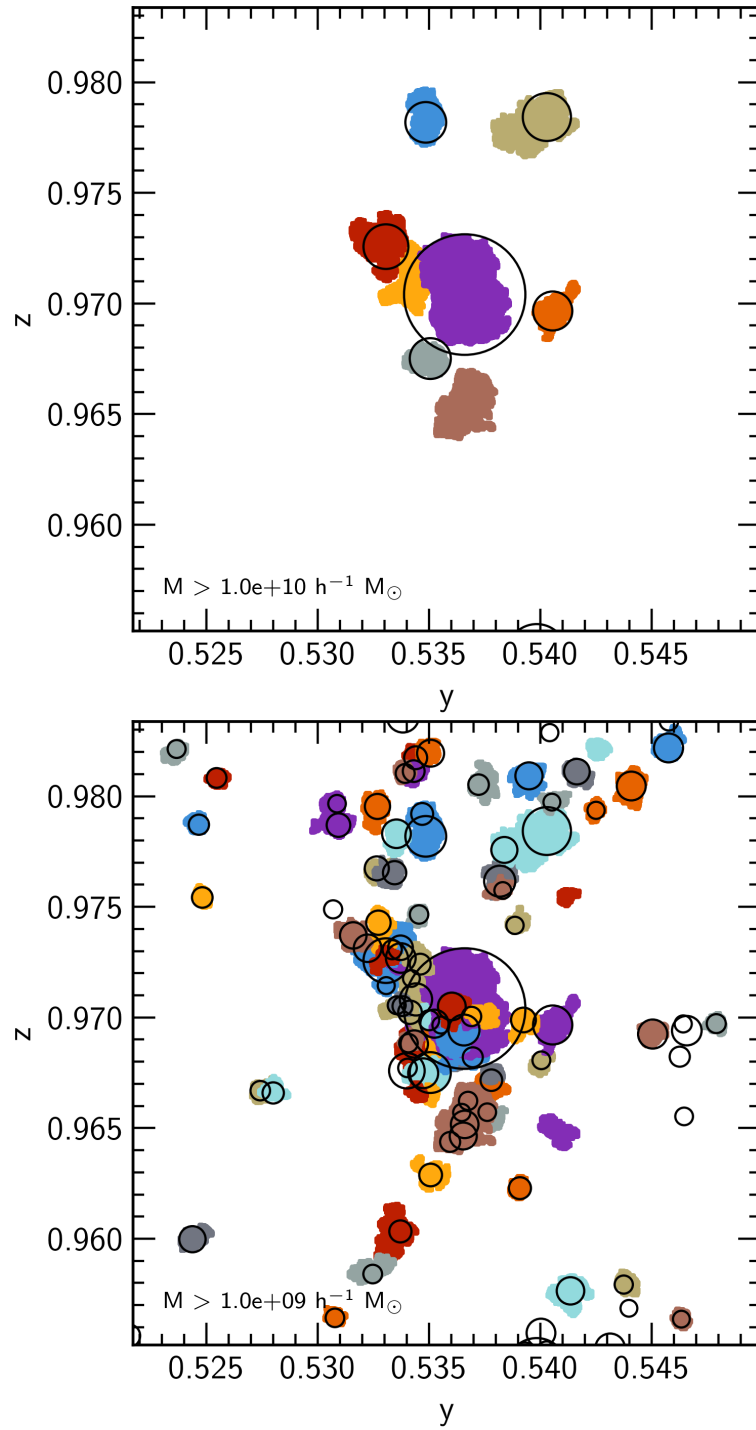


Figure 5.4: Top: the same region as in Figure 5.3, this time analysed with $b = 0.15$ and only showing FoF haloes with $M > 10^{10} h^{-1} M_{\odot}$. The different colours indicate separate structures. The black circles are now haloes found by **rockstar** with $M > 10^{10} h^{-1} M_{\odot}$. Bottom: same as top panel, except that now all haloes with $M > 10^9 h^{-1} M_{\odot}$ are shown for both FoF and **rockstar**.

between the two simulations (given the different mass resolutions).

That some of the haloes in the CoDa III catalogues are compromised is an important result, since it means that any results dependent on the halo finding must be checked thoroughly. One option to remedy the impact of compromised haloes is to try and manually remove the most egregiously overlinked structures (e.g. the filamentary overlinking in Figure 5.3), though this would be time-consuming and may preferentially remove haloes in certain environments (e.g. filaments), introducing bias. Another option is to use a shorter linking length (cf. Figure 5.4) though this is also not totally satisfactory since shorter linking lengths correspond to higher halo overdensities, thus preferentially removing low-mass haloes, and the effect of overlinking persists (albeit to a more minor extent).

A further remedy, and the avenue of future work, is to reanalyse a subset of the snapshots using a more advanced halo finder, such as **rockstar** and augment the catalogues with the results of this more accurate method. It will only be possible to analyse a subset of the snapshots, since the more advanced method is also more computationally demanding.

Chapter 6

Conclusions

In this thesis, we have presented studies on the formation of structure in the high-redshift universe, with a particular focus on small scales. Low-mass galaxies are posited to initially drive cosmic reionisation, so any process that can affect their formation is important to study.

In Chapter 2 we presented our methodology for incorporating the effects of post-recombination supersonic relative-baryon dark matter velocities self-consistently into cosmological simulations. Simulations are often initialised using linear transfer functions which either include the effect of the relative velocity from the start time of the simulation (if the transfer functions have separate amplitudes for baryon and dark matter velocities), or miss out on the effect altogether. Our methodology accounts for the effect of the relative velocity on the baryons all the way from recombination to the start time of the simulation. The novelty of this work lies in the use of zoom simulations, where a small, high-resolution region is nested inside a large, low-resolution parent box. Large boxes are required to properly sample the full range of scales associated with the relative velocity, so we selected a $100 h^{-1}$ Mpc subbox from a $400 h^{-1}$ Mpc parent, centred on a $\sim 3.3\sigma_{v_{bc}}$ value of the relative velocity. We ran a set of simulations with a $543 h^{-1}$ kpc zoom region placed at the centre of this subbox, and found that the relative velocity significantly impacts baryon fraction of haloes and delays the onset of star formation by roughly the lifetime of a $9 M_{\odot}$ Pop III star. These results are in qualitative agreement with previous studies. Since this new methodology is the first, to our knowledge, to self-consistently sample the relative velocity from a large box, it will be useful for exploring the effect of the spatial fluctuations of the relative velocity on, e.g., inhomogeneous chemical enrichment by Pop III star formation. An avenue for further work is simulating more regions, with varying magnitudes of the relative velocity, and different densities, to improve the statistics and

better sample the real universe. In addition to sampling more and more varied regions, future work could look at running simulations which include important high- z physics, such as: Lyman-Werner radiation; molecular hydrogen cooling; and radiative transfer (photo-heating and ionisation). The simulations in this work were computationally expensive, so developing a subgrid prescription for incorporating this effect into larger simulations could also be fruitful.

Chapter 3 details preliminary results from our work on modelling the HESTIA suite of constrained simulations through the EoR. The original HESTIA suite was run using a completely different code, so producing and validating the ICs for this work has been time-intensive. We produced a working set of zoom ICs and ran an extremely high-resolution (16384^3 effective particles in the zoom region) dark matter-only simulation down to $z = 0$, demonstrating excellent agreement with the original HESTIA run, both on final halo properties and their evolution in time. This 16384^3 simulation is the highest resolution HESTIA run produced to date, and so is already useful for studying the dynamics of dwarf and satellite galaxies in the LG. Work stemming from this chapter is ongoing, and currently involves calibrating star formation and feedback parameters in order to produce a realistic ionisation history. Once the parameters are calibrated, we will be able to produce the highest-resolution fully-coupled radiation-hydrodynamical simulation of the LG, which will be used to study the impact of reionisation on the star formation histories of the LG’s low-mass galaxy population.

For Chapter 4, we looked at the impact of an alternative dark matter model on the growth of high-redshift structure. This model considers the case where dark matter can have a non-negligible cross-section for interaction with photons in the very early universe. This interaction leads to a damped, oscillatory suppression in the small-scale ($k \gtrsim 10 \, h \, \text{Mpc}^{-1}$) matter power spectrum. We found that the initial suppression decreases with time, as power cascades down from the unaffected large scales to the suppressed small scales. The suppression in small-scale power is reflected in a reduction of the number of low-mass ($M \lesssim 10^{10} \, h^{-1} \, \text{M}_\odot$) haloes formed and, as with the power, the suppression in halo abundance also decreases with time. We also look at the growth of haloes, through their mass accretion history, finding that haloes in the interacting dark matter case accrete their mass later than in the standard dark matter case. As a next step, we will explore the change in mass accretion more closely, looking at the rate of accretion and halo formation times, with the aim of using these to inform radiative transfer simulations which account for the merger history of haloes.

Finally, in Chapter 5 we present the FoF halo catalogues for the new CoDa III simulation, comparing them to a companion dark matter-only **GADGET-2** run, and the fitting function of [Watson et al. \(2013\)](#). At high redshifts ($z \gtrsim 7$), we find strong deviation between the CoDa III halo mass function and the comparison mass functions, which agree well with each other. This deviation is likely due to the poorer force resolution compared to the companion run, working in tandem with a drawback of the FoF algorithm, that leads to overlinking groups of particles. At low redshifts and high masses we find better agreement between CoDa III, ESMD and [Watson et al. \(2013\)](#). This is an important result for the CoDa III simulation, as it identifies an area where care must be taken when conducting analysis, e.g. when exploring the effect of reionisation on low-mass galaxies. Future work will look at producing supplementary halo catalogues using a different halo finding method, to try and alleviate the overlinking problem; and at why the low-mass end of the CoDa III mass function appears to diverge from the ESMD mass function at high redshifts.

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