Cosmological Structure Formation with Modified Gravity

A thesis submitted to the University of Manchester
for the degree of Doctor of Philosophy
in the Faculty of Engineering and Physical Sciences

2015

Samuel J. Cusworth
School of Physics and Astronomy
Simulations with Modified Gravity
Contents

Abstract .................................................. 10
Declarations .................................................. 11
Acknowledgements .......................................... 12
The Author ................................................ 14
Supporting Publications ..................................... 15

1 Introduction ................................................. 17
  1.1 Introduction to Modern Cosmology ....................... 17
    1.1.1 Cosmological Principle ............................ 17
    1.1.2 Introduction to General Relativity ................. 18
    1.1.3 Einstein’s Equations from an Action Principle .... 20
  1.2 Concordance Cosmology ................................ 21
    1.2.1 Background Cosmology ............................. 21
    1.2.2 The Perturbed $\Lambda$CDM universe ............... 23
    1.2.3 Non-linear Structure Formation ................... 27
  1.3 Observational Cosmology ................................ 30
    1.3.1 SNIa ............................................. 30
    1.3.2 CMB .............................................. 30
    1.3.3 Galaxy Clusters .................................. 33
  1.4 $f(R)$ as Dark Energy ................................ 34
    1.4.1 Gravitational Field Equations ..................... 35
    1.4.2 Einstein Frame .................................... 36
# Contents

1.4.3 Screening Mechanism ............................................. 37
1.4.4 Viable Models .......................................................... 39

2 Simulations of Structure Formation .................................... 43
  2.1 Initial Condition Generation ........................................ 44
  2.2 N-body Solvers ........................................................... 45
     2.2.1 Tree-Based Methods ............................................. 46
     2.2.2 Particle Mesh Methods ......................................... 47
     2.2.3 Adaptive Grid Methods ......................................... 49
  2.3 Hydrodynamics .......................................................... 50
     2.3.1 Smoothed Particle Hydrodynamics .............................. 51
  2.4 Measuring Large Scale Structure Statistics ......................... 54
     2.4.1 Matter Power Spectrum ........................................... 54
     2.4.2 Cluster Mass Function ............................................ 55
  2.5 Known Limitations ...................................................... 59
     2.5.1 Choice of Initial Conditions .................................... 59
     2.5.2 Boxsize Effects .................................................... 61

3 Influence of Baryons on the Cluster Mass Function ..................... 65
  3.1 Introduction ............................................................. 65
  3.2 Millennium Gas Simulations .......................................... 67
     3.2.1 First generation: GO and PC models ......................... 68
     3.2.2 Second generation: FO model .................................. 69
     3.2.3 Cluster sample .................................................... 70
     3.2.4 Baryon Fraction ................................................... 71
  3.3 Results ..................................................................... 74
     3.3.1 Cluster Mass Function ............................................ 74
     3.3.2 Impact of baryons on mass function ......................... 75
     3.3.3 Consequences for Cosmology ................................... 78
     3.3.4 Model Independent Correction ................................. 79

Simulations with Modified Gravity
4 Simulating $f(R)$ Gravity 87
4.1 Introduction 87
4.2 Background Expansion History 87
4.3 Equations of Motion 89
4.3.1 Quasi-Static Approximation 90
4.3.2 $f(R)$ Trace Equation 91
4.3.3 $f(R)$ Poisson Equation 92
4.4 Approximate Models 93
4.4.1 HS Model 94
4.4.2 Designer Model 95
4.5 Numerical Methodology 99
4.5.1 Solving for the Scalar Field 100
4.5.2 Modifications to GADGET-2 109
4.6 Static Examples 111
4.6.1 Analytic Examples 112
4.6.2 Computational Performance 119
4.7 Summary 122

5 Structure formation in the $f(R)$ Universe 123
5.1 Introduction 123
5.2 Validation of the MIRAGE Code 126
5.2.1 Winther et al. (2015) Code Comparison 126
5.2.2 Approximate Designer Models 131
5.3 $\Lambda$CDM Designer Model 134
5.3.1 Exact Form Results 134
5.3.2 Evaluating Approximate Models 136
5.4 Hu & Sawicki (2007) Model 137
5.4.1 Power-Law, $n = 1$ 137
## List of Figures

1.1 Linear matter power spectrum .............................................. 27  
1.2 Temperature power spectrum from the *Planck* 2015 results ........ 32  
1.3 Effective Potential for a Chameleon Model ............................... 38  

2.1 Barnes & Hut (1986) algorithm ............................................. 46  
2.2 Impact of initial condition choices ....................................... 61  
2.3 Finite boxsize corrections .................................................... 63  

3.1 Baryon fraction within clusters in the MGS ............................... 72  
3.2 Cluster mass functions from the MGS ..................................... 74  
3.3 Likelihood contours derived from the MGS mass functions .......... 77  
3.4 Distributions of mass ratios between clusters in the MGS and the DMO analogues .............................................................. 80  
3.5 Likelihood contours from the corrected MGS mass functions ...... 83  

4.1 Effective equation of state for $|f_{R0}| = 10^{-1}, 10^{-2}$ and $10^{-3}$ ............................................................... 88  
4.2 Power-law approximation in the HS model ......................... 94  
4.3 Approximate $f(R)$ designer models ...................................... 96  
4.4 Red-black iteration and V-cycle ........................................... 102  
4.5 Slab-based domain decomposition ........................................ 103  
4.6 Convergence rates of single grid and V-cycle methods .......... 105  
4.7 Schematic of cell-centred grids ............................................. 107  
4.8 Error in $P(k)$ due to finite PMO resolution ........................... 110

*Samuel Cusworth* 7
LIST OF FIGURES

4.9 Homogeneous $f_R$ field .................................................. 113
4.10 Point mass $f_R$ field .................................................. 114
4.11 Boxsize effects in the point mass test ............................ 115
4.12 Gaussian spike test .................................................... 117
4.13 Sine field test .......................................................... 118
4.14 Strong scaling of the FAS code ...................................... 120
4.15 Weak scaling of the FAS code ........................................ 121

5.1 Winther et al. (2015) Code Comparison: $z = 0$ ............... 127
5.2 Winther et al. (2015) Code Comparison: $z > 0$ ................ 128
5.3 Winther et al. (2015) Code Comparison: AMR Results, $z = 0$ . 130
5.4 Comparison to He et al. (2014) ......................................... 132
5.5 Comparison to He et al. (2015) ......................................... 133
5.6 Exact designer model .................................................... 135
5.7 Approximate Designer Models Relative to Exact ................. 137
5.8 Power-law $n = 1$ model with $f_{R0} = -10^{-2}$ .................... 139
5.9 Power-law $n = 1$ model at multiple redshifts ($f_{R0} = -10^{-5}$) . 140
5.10 Power-law $n = 1$ model with $f_{R0} = 10^{-5}$ .................... 141
5.11 Power-law $n = 1$ model at multiple redshifts ($f_{R0} = -10^{-5}$) . 142
5.12 Exact HS $n = 1$ model ................................................ 143
5.13 HS $n \neq 1$ model at $z = 0$ ........................................... 144
5.14 Ratio of HS $n \neq 1$ and HS $n = 1$ ................................. 145
List of Tables

1.1 Description of cosmological parameters . . . . . . . . . . . . . . . . 24
1.2 Cosmological parameter sets used in this thesis . . . . . . . . . . . . 42
4.1 Forms of $R(u)$ used in the literature . . . . . . . . . . . . . . . . . . 98
5.1 Simulations run with using the $\Lambda$CDM designer model . . . . . . 134
5.2 Simulations run using the $n = 1$ power-law model . . . . . . . . . . 138
ABSTRACT OF THESIS submitted by Samuel Cusworth
for the Degree of Doctor of Philosophy, PhD, and entitled

The large scale structure of the universe has been shown to be a powerful probe of cosmology and fundamental physics. In order for future surveys to continue to improve and constrain our model of the Universe we rely on predictions from $N$-body simulations regarding the cosmological matter density field. First, we examine the effect of baryons on the cluster mass function in an effort to ameliorate the apparent tension in cosmological parameters determined from the cosmic microwave background anisotropies and cluster number counts in the Planck survey. It is shown that ignoring baryonic depletion causes a decrement in the number of galaxy clusters of a fixed mass and an artificial shift in the inferred cosmological parameters. While this effect is not sufficient to completely resolve the tension in the Planck collaboration (2014) results, it will be an important factor in measurements from future cluster surveys.

In order to investigate the effects of modified gravity on the matter power spectrum we present an $f(R)$ gravity extension to the massively parallel $N$-body GADGET-2 code. After validating our multigrid enabled Newton-Raphson-Gauss-Seidel relaxation solver we investigate two different $f(R)$ models, namely the designer and [Hu & Sawicki (2007)] models. We find that the designer model power spectrum is well approximated by the models of [He et al. (2014)] and [He, Li & Hawken (2015)] to 0.2 per cent. Furthermore, the power spectrum found when using the exact functional form of the [Hu & Sawicki (2007)] model is in excellent agreement with the power-law approximation. Finally, we have performed simulations with the [Hu & Sawicki (2007)] model with $n > 1$. It is shown that increasing $n$ decreases the overall amplitude of the fractional power spectrum. Future measurements of large scale structure should be able to constrain both $n$ and $\bar{f}_{R0}$.
Declarations

No portion of the work referred to in this thesis has been submitted in support of an application for another degree or qualification of this or any other university or other institution of learning. The author of this thesis (including any appendices and/or schedules to this thesis) owns certain copyright or related rights in it (the “Copyright”) and she has given The University of Manchester certain rights to use such Copyright, including for administrative purposes. Copies of this thesis, either in full or in extracts and whether in hard or electronic copy, may be made only in accordance with the Copyright, Designs and Patents Act 1988 (as amended) and regulations issued under it or, where appropriate, in accordance with licensing agreements which the University has from time to time. This page must form part of any such copies made. The ownership of certain Copyright, patents, designs, trade marks and other intellectual property (the “Intellectual Property”) and any reproductions of copyright works in the thesis, for example graphs and tables (“Reproductions”), which may be described in this thesis, may not be owned by the author and may be owned by third parties. Such Intellectual Property and Reproductions cannot and must not be made available for use without the prior written permission of the owner(s) of the relevant Intellectual Property and/or Reproductions. Further information on the conditions under which disclosure, publication and commercialisation of this thesis, the Copyright and any Intellectual Property and/or Reproductions described in it may take place is available in the University IP Policy (see University website), in any relevant Thesis restriction declarations deposited in the University Library, The University Library’s regulations (see University website) and in The University’s policy on presentation of Theses.
Acknowledgements

I’d like to thank Richard Battye and Scott Kay for their support, insight, guidance and encouragement. They have both been my advisors in various capacities throughout the last five or so years. Before becoming my PhD supervisors Richard was my personal tutor and Scott was my summer project supervisor. They have been very patient with me. Thanks to them both for taking me under their respective wings and helping shape my career.

Thanks also to my co-author Peter Thomas for excellent feedback on drafts of my first paper, Frazer Pearce for providing the data from the DM1 simulation and Hans Winther for providing the set of initial conditions used in his code comparison project.

Much of this work used the DiRAC Data Centric system at Durham University, operated by the Institute for Computational Cosmology on behalf of the STFC DiRAC HPC Facility (www.dirac.ac.uk). In addition, work was undertaken on the COSMOS Shared Memory system at DAMTP, University of Cambridge operated on behalf of the STFC DiRAC HPC Facility. The first generation Millennium Gas Simulations were carried out at the University of Nottingham HPC Facility. I have been supported by an STFC quota studentship and the University of Manchester President’s Doctorial Scholar Award for the duration of my postgraduate studies. Thanks also to the State Library of Western Australia where much of this thesis was written up.

I’d like to thank everyone at the JBCA for making my time here memorable and enjoyable. Special mentions for Richard Newton, Simon Pike, Jonathan Pearson, David Barnes, Francesco Pace, Ian Harrison, Rafal Szepietowski, Christopher Wallis, Lee Whitaker, Monique Henson and Aaron Peters with whom I have enjoyed many en-
lightening conversations.

I would like to thank my parents and other family members for the love and moral support they have shown me during my studies. Finally, I would like to end by thanking my partner Hazel. Without her love and support this thesis would not have been possible. This thesis is dedicated to both her and my parents.
The Author

The author obtained a first class M. Phys. (Hons) degree in Physics with Astrophysics from the University of Manchester in June 2012, graduating second in his year. He then began his PhD studies in September 2012 at the Jodrell Bank Centre for Astrophysics, a part of the University of Manchester. The work presented in this thesis is the product of his time spent at the JBCA.
Supporting Publications

Impact of baryons on the cluster mass function and cosmological parameter determination

Sam J. Cusworth; Scott T. Kay; Richard A. Battye; Peter A. Thomas, 2014
MNRAS, 439, p.2485-2493 (This work forms the basis of Chapter 3).
Chapter 1

Introduction

In this chapter we start by stating the underlying principles of cosmology and outline the basics of General Relativity (GR), the best known mathematical description of our Universe. We will then describe the standard model of cosmology. In particular we will show how we can model the dynamics of the Universe on many scales by considering a uniform background and perturbing the solution. We describe a few of the key observational probes of cosmology in Section 1.3. Finally in this chapter we introduce \( f(R) \) gravity as an alternative to the concordance cosmology.

1.1 Introduction to Modern Cosmology

1.1.1 Cosmological Principle

Modern theories of cosmology are guided by two linked principles: the Copernican and cosmological principles.

The Copernican principle states that observers on Earth do not occupy a privileged position in the Universe. This means that we assume our observations of the Universe on large scales reflect a “typical” region of space. At its simplest, the cosmological principle generalises the Copernican principle to all observers in our Universe. Since we observe that the Universe is near isotropic (invariant under rotation) on large scales,
we can deduce that it appears isotropic in most regions of space. Thus, the Universe must be homogeneous (invariant under spatial translation) on large scales.

1.1.2 Introduction to General Relativity

In this section we review a number of important concepts in differential geometry and the general theory of relativity (GR). We refer to [Wald (1984) and Carroll (2004)] for substantial introductions to this topic. We use the convention of describing events occurring at coordinates \( x^\mu = (t, x) \) on a four dimensional manifold. This manifold is endowed with a metric tensor which relates coordinate distances to physical distances in space and time. The invariant line element is

\[
\mathrm{d}s^2 = g_{\mu\nu} \mathrm{d}x^\mu \mathrm{d}x^\nu \tag{1.1}
\]

where \( g_{\mu\nu} \) is the metric tensor and we have used the Einstein summation notation over indices \( \mu \) and \( \nu \). While the manifold as a whole may have a complicated topology, local regions of space-time are required to appear Euclidean in nature.

We aim to formulate physical laws which are invariant to the frame of reference of the observer. Therefore, it is vital that we are able to perform transformations between frames of reference, say from \( \mathcal{S} \) to \( \mathcal{S}' \). Since we use tensors in our description of gravity, we must define transformations

\[
A'^\mu = J^\mu_\alpha A^\alpha, \\
B'^{\mu}_{\nu} = J^{\mu}_{\alpha} J^{\beta}_{\nu} B^{\alpha}_\beta, \tag{1.2}
\]

where the primed frame could represent an observer in an accelerating frame or at a different point in a gravitational potential. In (1.2), the Jacobian and its inverse are the transformation matrices

\[
J^{\mu}_{\nu} = \frac{\partial x'^\mu}{\partial x^\nu}, \quad J^\nu_\mu = \frac{\partial x^\mu}{\partial x'^\nu}. \tag{1.3}
\]

We note that partial derivatives, \( \partial_\mu = \partial/\partial x^\mu \), are not tensors and so do not transform according to (1.2). The generalised derivative that includes the additional terms from
coordinate transformation is the covariant derivative,
\[ \nabla_
u A^\mu = \partial_\nu A^\mu + \Gamma^\mu_{\nu\alpha} A^\alpha \]  
(1.4)

where the affine connection is defined
\[ \Gamma^\gamma_{\beta\mu} = \frac{1}{2} g^{\gamma\alpha} \left( \partial_\mu g_{\alpha\beta} + \partial_\beta g_{\alpha\mu} - \delta_\alpha g_{\beta\mu} \right). \]  
(1.5)

In GR, spacetime is curved by the presence of gravitating mass or energy. The curvature of spacetime is encapsulated in the Riemann tensor
\[ R^\rho_{\sigma\mu\nu} = \partial_\mu \Gamma^\rho_{\nu\sigma} - \partial_\nu \Gamma^\rho_{\mu\sigma} + \Gamma^\rho_{\mu\lambda} \Gamma^\lambda_{\nu\sigma} - \Gamma^\rho_{\nu\lambda} \Gamma^\lambda_{\mu\sigma}. \]  
(1.6)

In four dimensions there are, in principle, 256 free components to the above (1,3) tensor. However, after symmetry considerations this number reduces to 20. The Ricci tensor, \( R_{\mu\nu} \), and Ricci scalar, \( R \), can be computed from the Riemann tensor via
\[ R_{\mu\nu} = R^{\lambda}_{\mu\lambda\nu}, \quad R = g^{\mu\nu} R_{\mu\nu}. \]  
(1.7)

Einstein’s field equations link the geometric curvature of spacetime to its energy density contents via
\[ R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = 8\pi G T_{\mu\nu} \]  
(1.8)

where the left-hand side of (1.8), the Einstein tensor, is often denoted as \( G_{\mu\nu} \) and \( T_{\mu\nu} \) is the energy-momentum tensor. Both the energy momentum tensor and the Einstein tensor satisfy the Bianchi identity
\[ \nabla_\mu G^\mu_{\nu} = \nabla_\mu T^\mu_{\nu} = 0. \]  
(1.9)

In this thesis we will use GR as our standard model of gravity. The classical tests of GR are the perihelion precession of the orbit of Mercury, the deflection of light by the Sun and the gravitational redshifting of light. GR continues to be tested through its applications on Earth, within the solar system and in binary pulsar systems (Will, 2001).
1: INTRODUCTION

1.1.3 Einstein’s Equations from an Action Principle

The field equations for GR (1.8) can be derived from the Einstein-Hilbert action. Since the vast majority of modified gravity theories, including $f(R)$ gravity, are extensions of GR it is instructive to carry out this derivation.

The Einstein-Hilbert action is the integral over spacetime of the Lagrangian density

$$S = \frac{1}{16\pi G} \int d^4x \sqrt{-g}R + \int d^4x \sqrt{-g}L_m[g_{\mu\nu}, \chi]$$

(1.10)

where $g = \det(g_{\mu\nu})$, $dx^4\sqrt{-g}$ is the invariant (four dimensional) volume element, $\chi$ represents the matter sector fields and as before $R$ is the Ricci scalar. The first term on the right-hand side of (1.10) contains our theory of gravity whereas the integrand $L_m$ represents the Lagrangian density of the matter, radiation and other fields present in our model Universe.

Varying the action (1.10) gives

$$\delta S = \frac{1}{16\pi G} \int d^4x \sqrt{-g} \left( \delta R + \frac{R}{\sqrt{-g}} \delta(\sqrt{-g}) + \frac{16\pi G}{\sqrt{-g}} \delta(\sqrt{-g}L_m) \right),$$

(1.11)

where $\delta X$ represents the variation in a quantity $X$. Using the geometric identities

$$\frac{1}{\sqrt{-g}} \delta \left( \sqrt{-g} \right) = -\frac{1}{2} g_{\mu\nu} \delta g^{\mu\nu}, \quad \delta R = (R_{\mu\nu} + g_{\mu\nu} \Box - \nabla_\mu \nabla_\nu) \delta g^{\mu\nu},$$

(1.12)

we can rewrite (1.11) as

$$\delta S = \int d^4x \sqrt{-g} \left[ G_{\mu\nu} \delta g^{\mu\nu} + (g_{\mu\nu} \Box - \nabla_\mu \nabla_\nu) \delta g^{\mu\nu} + \frac{16\pi G}{\sqrt{-g}} \delta(\sqrt{-g}L_m) \right]$$

(1.13)

where the Einstein tensor has been identified. In (1.12) the d’Alembertian operator is defined as $\Box = \nabla^\mu \nabla_\mu$. It can be shown that the second term in the integrand can be written as a surface integral and neglected. Extremising the action with respect to the metric, $\delta S/\delta g^{\mu\nu} = 0$, gives

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = 8\pi G T_{\mu\nu}$$

(1.14)

as expected, where we identify the energy momentum tensor as

$$T_{\mu\nu} = -\frac{2}{\sqrt{-g}} \frac{\delta(\sqrt{-g}L_m)}{\delta g^{\mu\nu}}.$$

(1.15)
1.2 Concordance Cosmology

The \( \Lambda \)-Cold Dark Matter (\( \Lambda \)CDM) model outlined below is supported by a range of observational evidence (which is why it is commonly referred to as the concordance model) and is widely seen as the standard model of cosmology (Frieman, Turner & Huterer 2008; Weinberg et al. 2013). The model consists of dark energy (\( \Lambda \)), non-relativistic dark matter, baryonic matter and radiation components (Frenk & White 2012). It is possible to extend the model to include various other components. However we will not consider them here.

It is believed that the early universe underwent a period of rapid expansion known as inflation (Baumann 2009). After the epoch of inflation, radiation dominated the energy density. As will be discussed in Section 1.3.2, the baryonic matter and radiation field were strongly coupled at this time. We understand that the universe continued to expand and cool, through the matter dominated epoch, up until the present day. At present the expansion of the universe appears to be accelerating. In the \( \Lambda \)CDM universe we attribute this to the cosmological constant, otherwise known as the vacuum energy, becoming the dominant energy density.

1.2.1 Background Cosmology

Under the assumptions of isotropy and homogeneity, discussed in Section 1.1.1, there is only one form that the \( g_{\mu\nu} \) can take, the Friedmann-Robertson-Walker (FRW) metric. We note again that the cosmological principle only holds on large spatial scales. The form of the FRW metric, including a global curvature \( K \), is

\[
ds^2 = -dt^2 + a^2(t) \left[ \frac{dr^2}{1 - Kr^2} + r^2 (d\theta^2 + \sin^2 \theta d\phi^2) \right]
\]

(1.16)

and

\[
r = \begin{cases} 
\sin \chi & K = +1, \\
\chi & K = 0, \\
\sinh \chi & K = -1,
\end{cases}
\]

(1.17)
where $\chi, \theta$ and $\phi$ are spatial coordinates in the rest frame of the cosmic fluid, i.e. comoving coordinates. The scale factor of the metric, $a(t)$, represents the relative expansion of space as a function of cosmic time $t$. We set the scale factor to be unity at the present epoch\footnote{Throughout this thesis we denote the present day value of a variable with a subscript “0”.} $a(t_0) = 1$. The $K$ parameter represents global curvature of the Universe and can be positive (resulting in a “closed” universe), zero (Euclidean space) or negative (an “open” universe).

Assuming that the universe is filled with a uniform and isotropic fluid, the form of the energy momentum tensor is given by

$$T_{\mu\nu} = (\rho + P) u^\mu u_\nu + P \delta^\mu_\nu$$

(1.18)

where the energy density $\rho$ and pressure $P$ are both functions of time. In Eq. (1.18) $u^\mu = (1, 0, 0, 0)$ represents the four-velocity of the fluid in comoving coordinates and $\delta^\mu_\nu$ is the (1,1) Kronecker tensor. The above form of $T_{\mu\nu}$ is valid only for a fluid with no shear stresses, viscosity, or heat conduction. In this discussion the $\rho$ and $P$ terms represent the total energy density and pressure present in the universe respectively. In other words, $\rho = \sum_n \rho_n$ and $P = \sum_n P_n$ where we sum over $n$ components including the energy density from the cosmological constant $\rho_{\Lambda} = \Lambda/(8\pi G) = -P_{\Lambda}$.

In order to determine $a(t)$ and its derivatives for a universe with a given set of components we must solve the Einstein field equations (1.14). Using the metric in (1.16) the components of the Christoffel symbols, Ricci tensor and the value of Ricci scalar can be calculated. There are two independent equations of motion, known as the Friedmann equations. The time—time term gives

$$H^2 = \frac{8\pi G}{3} \rho - \frac{K}{a^2},$$

(1.19)

and the space—space term gives

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3} (\rho + 3P),$$

(1.20)

where the $H = \dot{a}/a$ is the Hubble parameter and overdots denote derivatives with

\textit{Simulations with Modified Gravity}
1.2: CONCORDANCE COSMOLOGY

respect to \( t \). In this thesis the Hubble parameter at the present epoch is denoted as
\[ H_0 = 100h \, \text{km s}^{-1} \text{Mpc}^{-1} \]
where \( h \) is a parameter to be determined experimentally.

One can see that the right-hand side of (1.19) represents the balance between energy density and global curvature. The critical density of the universe, so named as it is the energy density required to produce a globally flat topology, can be written as
\[ \rho_c(a) = \frac{3H^2}{8\pi G} \tag{1.21} \]
from (1.19). It is also common to express the Hubble parameter as
\[ \left( \frac{H}{H_0} \right)^2 = E(a)^2 = \Omega_r a^{-4} + \Omega_m a^{-3} + \Omega_K a^{-2} + \Omega_{\Lambda} \tag{1.22} \]
where we write \( \Omega_X = \rho_X / \rho_{c,0} \) for \( X = \{ r, m, \Lambda \} \) and \( \Omega_K = -K / H_0^2 \).

From (1.9) and assuming that the energy momentum tensor takes the form of (1.18), we can derive the fluid equation
\[ \dot{\rho} + 3H (\rho + P) = 0. \tag{1.23} \]
The above equation allows us to determine the dynamics of a toy universe composed of a single component fluid. Assuming an equation of state \( w = P / \rho \), one can show that \( \rho \propto a^{-3(1+w)} \).

While the possibility of global curvature has obvious theoretical importance, there is overwhelming evidence from experiments observing the Cosmic Microwave Background radiation indicating that \( \Omega_K = 0 \) (Planck Collaboration et al., 2015b). As such, from now on we will assume that \( K = 0 \). A summary of the \( \Lambda \)CDM cosmological parameters referenced in this thesis can be found in Table 1.1.

1.2.2 The Perturbed \( \Lambda \)CDM universe

In this section we account for small inhomogeneities in our model universe using linear perturbation theory (Mukhanov, Feldman & Brandenberger, 1992; Ma & Bertschinger, 1995). These perturbations are assumed to have been created during the epoch of inflation.
1: INTRODUCTION

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_0$</td>
<td>Hubble parameter at current epoch.</td>
</tr>
<tr>
<td>$\Omega_m$</td>
<td>Present day matter density relative to the critical density.</td>
</tr>
<tr>
<td>$\Omega_\Lambda$</td>
<td>Vacuum energy density relative to the critical density.</td>
</tr>
<tr>
<td>$\sigma_8$</td>
<td>R.M.S. matter density fluctuation (See Eq. 2.25 for definition).</td>
</tr>
<tr>
<td>$n_s$</td>
<td>Primordial power-law index of the matter power spectrum</td>
</tr>
</tbody>
</table>

Table 1.1: Description of cosmological parameters

The approach we take to perturbing the relativistic equations of motion is to write the metric as $g_{\mu\nu} = \bar{g}_{\mu\nu} + \delta g_{\mu\nu}$ where $\bar{g}_{\mu\nu}$ is the flat FRW metric (1.16) and the components of the perturbed metric $\delta g_{\mu\nu}$ are assumed to be small with respect to the zeroth order terms. Note that we will compute quantities using Cartesian spatial coordinates. We choose to parameterise scalar perturbations, i.e. density fluctuations, in the Newtonian gauge

$$ds^2 = -(1 + 2\Psi)\,dt^2 + a^2(1 + 2\Phi)\,dx$$

(1.24)

where $\Psi$ and $\Phi$ are small scalar quantities which are permitted to vary with space and time. The form of (1.24) has been made so to make physical interpretation of the equations of motion clear. It will be shown later that the metric perturbation $\Psi$ can be interpreted as the Newtonian gravitational potential in certain circumstances.

Computing the perturbed affine connection, Riemann and Ricci tensors is a straightforward if not time consuming task. As with the metric, we write each quantity as the sum of the background and first order terms,

$$\delta \Gamma^\beta_{\mu\nu} = \Gamma^\beta_{\mu\nu} - \bar{\Gamma}^\beta_{\mu\nu}, \quad \delta R_{\mu\nu} = R_{\mu\nu} - \bar{R}_{\mu\nu},$$

$$\delta R = R - \bar{R}, \quad \delta R^\beta_{\alpha\mu\nu} = R^\beta_{\alpha\mu\nu} - \bar{R}^\beta_{\alpha\mu\nu},$$

(1.25)

where again bars denote background level quantities.
Perturbing the energy momentum tensor to linear order gives

\[ T^0_0 = -(\bar{\rho} + \delta \rho), \]
\[ T^0_i = T^i_0 = (\bar{\rho} + \bar{P}) v_i, \]
\[ T^i_j = (\bar{P} + \delta P) \delta^i_j + \Sigma^i_j, \]

(1.26)

where \( v_i \) represents motion within the fluid, \( \delta^i_j \) is the Kronecker tensor, \( \hat{\theta}_k \) is the Fourier mode of the velocity divergence and \( \Sigma^i_j \) is a traceless tensor representing anisotropic stress in the fluid. Here we assume that the perturbed fluid remains a perfect fluid so \( \Sigma^i_j = 0 \).

It is useful to describe the density contrast field, \( \delta(x) \), as the sum of plane waves

\[ \delta(x) = \frac{\delta \rho(x)}{\bar{\rho}} = \sum_j \hat{\delta}_{k_j} \exp(i \mathbf{k}_j \cdot \mathbf{x}) \]

(1.27)

where \( \mathbf{k}_j \) is the comoving wavevector and the (potentially complex) Fourier modes can be written as

\[ \hat{\delta}_k = \int d^3 x \delta(x) \exp(i \mathbf{k} \cdot \mathbf{x}). \]

(1.28)

Under the assumptions of homogeneity and isotropy, we need only consider the magnitude of the wavevector, \( |\mathbf{k}| = k \).

After subtracting the background terms and transforming to Fourier space, the non-zero components Einstein equations are

\[ k^2 \ddot{\Phi}_k + 3H (\dot{\Phi}_k - H \Psi_k) = 4\pi G \bar{\rho} \hat{\delta}_k, \]

(1.29)

\[ k^2 (\dot{\Phi}_k - H \dot{\Psi}_k) = -4\pi G (1 + w) \bar{\rho} \hat{\theta}_k, \]

(1.30)

\[ \dot{\Psi}_k = -\dot{\Phi}_k, \]

(1.31)

\[ \ddot{\Phi}_k + 3H \dot{\Phi}_k - H \dot{\Psi}_k - \left( 3H^2 + 2\dot{H} \right) \dot{\Psi}_k = -4\pi G c_s^2 \bar{\rho} \hat{\delta}_k, \]

(1.32)

where the sound speed \( c_s^2 = \delta P/\delta \rho \) depends on the nature of the fluid. Note that each \( k \)-mode evolves independently in linear theory. Using the above results we can derive a vital equation, the gravitational Poisson equation

\[ -k^2 \ddot{\Psi}_k = 4\pi G \bar{\rho} \left( \hat{\delta}_k + \frac{3(1 + w)H}{k^2} \hat{\theta}_k \right). \]

(1.33)
1: INTRODUCTION

From (1.33) we can see that the Newtonian Poisson equation (in physical space)

\[ \nabla^2 \Psi = 4\pi G \bar{\rho} \delta \]  (1.34)

is valid on all but the largest scales since below the observable horizon, \( H/k \to 0 \).

Modes inside the horizon at a given epoch are known as subhorizon modes whereas modes on length scales larger than the horizon are called superhorizon modes.

Using the Bianchi identity we can derive two more equations of motion: from the time component,

\[ \dot{\delta}_k + 3H \left( c_s^2 - w \right) \delta_k = - (1 + w) \left( \theta_k + 3 \dot{\Phi}_k \right), \]  (1.35)

and from the position components,

\[ \dot{\theta}_k + \left( H (1 - 3w) + \frac{\dot{w}}{1 + w} \right) \theta_k = k^2 \left( \frac{c_s^2}{1 + w} \delta + \Psi_k \right) \]  (1.36)

where \( \dot{w} = 0 \) for a cosmological constant.

One of the most useful quantities that can be calculated from the above equations (1.29–1.36) is the matter power spectrum

\[ P(k) = |\delta_k|^2. \]  (1.37)

The power spectrum of perturbations in each species (radiation, neutrinos, etc.) is calculable. However, we will deal primarily with the matter power spectrum. Current models of inflation give rise to almost scale invariant Gaussian fluctuations, thereby imprinting a power law distribution

\[ P^{\text{inf}}(k) = A k^{n_s} \]  (1.38)

where \( n_s \) is near unity. The growth of structure relative to the primordial \( P(k) \) is suppressed by various processes encoded into the Einstein equations. These processes include the pressure support of baryonic matter and the washing out of small scale structure due to matter-radiation coupling. The modifications to the behaviour of \( \hat{\delta}_k(a) \) are encapsulated in the transfer function

\[ T(k) = \frac{\hat{\delta}_{k,0}}{\delta_k(a) D(a)}. \]  (1.39)
1.2: CONCORDANCE COSMOLOGY

Figure 1.1: Linear matter power spectrum for the PlanckI cosmology (Planck Collaboration et al., 2014b) computed using CAMB (Lewis, Challinor & Lasenby, 2000). In the superhorizon modes (smaller values of $k$) the primordial power spectrum (1.38) is evident whereas on subhorizon scales (larger $k$) $P(k)$ asymptotes to $k^{n_s-4}$. The peak of $P(k)$ is set by the horizon radius at matter-radiation equality, $k_{\text{eq}}$.

where the linear growth factor (Heath, 1977)

$$D(a) = \frac{5}{2} \Omega_m E(a) \int_0^a \frac{da'}{(a'E(a'))^{3/2}}$$

(1.40)

An example of a numerically computed power spectrum is shown in Fig. 1.1

1.2.3 Non-linear Structure Formation

We now consider structure formation in the non-linear regime, i.e. within collapsing perturbations where $\delta \rho/\rho \gg 1$. Here, we will address two analytic approaches: the Zel’dovich approximation and the spherical top-hat collapse model, before revisiting this subject using $N$–body simulations in Chapter 2.
1: INTRODUCTION

Zel’dovich Approximation

The approach of Zel’dovich (1970) is to compute the initial displacement field of fluid elements and assume that they continue to move according to the initial velocity field. In this model the position of a given particle at time \( t_2 \) is given by

\[
x(q, t_2) = q + \chi(q, t_2) \approx q - D(t_2) \nabla \Phi(q, t_1)
\]

where \( q \) is the initial position of the particle at time \( t_1 \), \( \chi(q, t) \) is the displacement field, \( \Phi(q, t_1) \) is the gravitational potential due to the particle distribution at \( t_1 \) and \( D(t) \) is the linear growth factor. The corresponding velocity of the particle is given by

\[
v = -DfH \nabla \Phi(q, t_1)
\]

where \( f = d \ln D / d \ln a \).

The approach outlined above is an efficient way to set initial conditions of \( N \)-body simulations. Unfortunately, this approximation allows particles to move through each other without consequence, leading to the prediction of caustics of infinite density in the low redshift density distribution.

In reality particles become gravitationally bound to each other and form structure beyond that predicted by this model. The Zeldovich approximation is first order Lagrangian perturbation theory: one can improve the accuracy of this approximation by including second order terms in the \( \chi(q, t) \) and velocity equations (Scoccimarro, 1998).

Spherical Top-hat Collapse Model

In this model we follow the formation of spherical overdensities with a top-hat density profile. In particular we consider a uniform density sphere of radius \( R \) (initially \( R_i \)) within a matter dominated universe (\( \Omega_m = 1 \)). The initial density field is

\[
\rho(t_i) = \frac{1}{6\pi G t_i^2} \begin{cases} 
1 & r > R_i \\
1 + \delta(t_i) & r < R_i
\end{cases}
\]

Simulations with Modified Gravity
We will consider spherical shells of matter within the overdensity. Newton’s shell theorem states that a spherically symmetric matter distribution outside a sphere exerts no force on that sphere. This means we can treat each shell independently. The equation determining the expansion of the shell is that of the Friedmann equation

\[
\dot{R}^2 = \alpha^2 R^{-1} - \epsilon^2
\]

(1.44)

where \( \alpha^2 = 8\pi G\bar{\rho}/3 \) and \( \epsilon^2 \) emphasises the positive curvature in the model. The Friedmann equation with positive curvature has known parametric solution

\[
R(\theta) = \frac{\alpha^2}{2\epsilon^2} (1 + \cos \theta), \quad t(\theta) = \frac{\alpha^2}{2\epsilon^3} (\theta - \sin \theta).
\]

(1.45)

Using this the overdensity within the sphere is given by

\[
1 + \delta = \frac{\rho}{\bar{\rho}} = \frac{9}{2} \left( \frac{\theta - \sin \theta}{1 - \cos \theta} \right)^2.
\]

(1.46)

It is instructive to compare the above to the overdensity expected from a linearly evolving density perturbation. In linear theory \( \delta_{\text{lin}} \propto D(a) \propto a \propto t^{2/3} \) therefore

\[
\delta_{\text{lin}} = \frac{3}{20} (6\pi)^{2/3} \left( \frac{t}{t_{\text{max}}} \right)^{2/3}.
\]

(1.47)

In this model each shell expands from \( r = 0 \) at \( \theta = 0 \) (\( t = 0 \)) and reaches a maximum at \( \theta = \pi \) (\( t = t_{\text{max}} \)). This maxima is known as turn around. After this point \( R(t) \) decreases and the structure collapses back to \( r = 0 \) at \( t = 2t_{\text{max}} \). Unfortunately, our model is no longer physical in this regime as proven by the prediction of an infinite overdensity at \( \theta = 2\pi \). The linearly extrapolated density field does not include the collapse fully and so does not suffer from the same singularity. We note that the linear prediction for the density contrast at collapse is \( \delta_{\text{lin}} = 1.686 \). In reality, at the point of collapse the individual oscillating shells of matter interact gravitationally and exchange energy. This process is called virialisation.

For the Einstein-de Sitter universe (\( \Omega_m = 1, \Omega_K = \Omega_\Lambda = 0 \)), the expected overdensity of virialised haloes is \( \Delta_{\text{vir}} = 18\pi^2 \). Bryan & Norman (1998) calculated a fitting...
function for $\Delta_{\text{vir}}$ at different redshifts and different cosmologies. For a universe with $\Omega_k = 0$

$$\Delta_{\text{vir}} = 18\pi^2 + 82x - 39x^2$$  \hspace{1cm} (1.48)

where $x = \Omega(z) - 1$, $\Omega(z) = \Omega_m \left(1 + z\right)^3 / E(z)^2$ and $E(z)$ is defined in (1.22).

### 1.3 Observational Cosmology

In this section we describe three of the many observational probes of cosmology (Weinberg et al., 2013). From a historical perspective, type 1a supernovae have been vital to our understanding of the Hubble flow. The cosmic microwave background on the other hand is arguably the cleanest measurement of linear perturbations. Finally in this section we describe constraints from galaxy clusters, our example of a non-linear probe.

#### 1.3.1 SN1a

Type 1a supernovae (SN1a) are extremely luminous bursts of radiation produced when the mass of a white dwarf star approaches the Chandrasekhar limit ($\sim 1.4M_\odot$). Since the explosion occurs at a set mass, SN1a have similar intrinsic luminosities. While there is a small spread in the absolute magnitude of a given explosion, Phillips (1993) showed that it is possible to correct the observed luminosity of a given SN1a using the width of its light curve. Applying this process to samples of SN1a allows them to be used as standard candles. Riess et al. (1998) and Perlmutter et al. (1999) independently showed that the observed dimming of high redshift sources is strong evidence of cosmic acceleration.

#### 1.3.2 CMB

The cosmic microwave background (CMB), photons that last scattered off electrons in the photon-baryon plasma present at high redshift ($z \approx 1100$), is one of the best
1.3: OBSERVATIONAL COSMOLOGY

probes of the physics of the early universe. While the temperature of the background is incredibly uniform, the anisotropies that do exist can be related to anisotropies in the primordial cosmic plasma.

A combination of the linear physics involved and the massive technological advances that have been made has allowed very precise measurements of cosmological parameters (Planck Collaboration et al., 2015b). Since the photons were in thermal equilibrium at the time of last scattering, the CMB also represents the best known example of a black-body spectrum.

The angular power spectrum of temperature fluctuations, $C_{\ell}^{TT}$, as a function of multipole moment, $\ell$, is a key observable in this field. Accurate measurements of $C_{\ell}^{TT}$ have been made using the WMAP (Spergel et al., 2003) and Planck (Planck Collaboration et al., 2015a) instruments (the latter is shown in Fig. 1.2). Under the assumption that the perturbations in the early universe are Gaussian, the angular power spectrum completely describes the anisotropies.

The complete calculation of $C_{\ell}^{TT}$ for a given set of cosmological parameters requires the coupled Einstein and Boltzmann equations to be solved, typically with a numerical solver such as CAMB (Lewis, Challinor & Lasenby, 2000) or CLASS (Blas, Lesgourgues & Tram, 2011). We now discuss a number of key features in Fig. 1.2 and how they relate to the physical conditions at the time of last scattering.

- Acoustic peaks ($\ell = 200, 500, 810, 1150, \ldots$): At very early times (before recombination) free electrons bound photons and baryons together into a hot plasma. Within the fluid, fluctuations in the gravitational potential lead to compressions which in turn lead to regions of hotter plasma. The resultant increase in radiation pressure would halt the collapse. Once the region had expanded and rarefied, gravitational collapse could once again begin to take place. When matter and radiation decoupled, the acoustic oscillations were frozen in the CMB.

- Silk damping tail: In the primordial photon-baryon fluid, photons diffuse from hot overdense matter perturbations into colder underdense regions. As the pho-
**1: INTRODUCTION**

![Temperature power spectrum graph]

Figure 1.2: Temperature power spectrum, $D_{TT}^l = l(l+1)C_{TT}^l/2\pi$, from the *Planck* 2015 results ([Planck Collaboration et al., 2015b](#)). The blue data points are the temperature power spectrum measurements from the full duration of the survey and best fit model is shown in red.

...tons diffuse, they pull baryonic matter along with them via the Coulomb force. This process acts to wash out small scale perturbations resulting in less power at large $l$.

- **Sachs-Wolfe plateau** ($10 < l < 30$): The Sachs-Wolfe (SW) effect is caused by perturbations in the gravitational potential at the time of last scattering. Photons within deep gravitational wells are redshifted as they lose energy climbing out. The perturbation also causes time dilation which reduces but does not cancel out the effect.

- **Integrated Sachs Wolf effect** ($2 > l > 10$): Photons passing through large overdense regions are blue-shifted as they enter a gravitational potential. In a matter dominated universe a given photon would then be equally redshifted as it left the gravitational potential of the region. However, because dark energy causes...
the expansion of the universe to accelerate, the potential of overdense region is not static. The net effect is that a given photon passing through a gravitational potential gains energy and is blueshifted.

As well as the temperature fluctuations, polarisation information can be used to probe both the epoch of reionisation and gravitational waves. In addition to being a cosmological probe, the CMB enables one to measure extragalactic sources and the properties of gas and dust within the Milky Way. The use of CMB experiments to detect galaxy clusters will be discussed further in the following section.

### 1.3.3 Galaxy Clusters

Galaxy clusters are the largest virialised structures in the known universe \cite{Voit2005, Allen2011}. They act as tracers of the matter density and can be used as powerful cosmological probes.

The mass content of a cluster is dominated by dark matter but it is typical to observe it via its baryonic components:

- **Galaxies**: Clusters typically contain $\mathcal{O}(10^3)$ individual galaxies. A typical cluster will also contain a non-star-forming elliptical galaxy, known as the Brightest Cluster Galaxy (BCG), at the centre of its gravitational potential.

- **Intracluster medium (ICM)**: Hot ($\mathcal{O}(10^7 \, \text{K})$) diffuse plasma not associated with a particular galaxy. The plasma is typically composed of ionised Hydrogen (free protons and electrons) and a small amount of heavier elements. This plasma radiates X-rays via thermal bremsstrahlung processes.

Given that clusters form in the regions of highest overdensity, their number density as a function of redshift and mass can be used as a powerful cosmological probe. They are also especially useful because, unlike the galaxies themselves, their dynamics are dominated by their dark matter content. In order to relate the observed number of clusters in a given survey to the underlying mass distribution it is vital to calibrate an
observable-mass relation. Since X-ray emission is proportional to the density of gas to the second power, cluster centres are readily observable in X-ray surveys. Clusters are also observable in the microwave regime via inverse Compton scattering of CMB photons in the ionised plasma. The spectral distortion left in the CMB is known as the Sunyaev-Zel’dovich effect. It is also possible to use weak gravitational lensing in order to measure the mass of a given cluster.

1.4 \( f(R) \) as Dark Energy

In Section 1.3 the case was made in support of the standard model of cosmology. In light of this one may ask “what is wrong with \( \Lambda \)CDM?”

One of the main problems with the concordance model is that the observed value of the cosmological constant is very small in comparison to the zero-point energy of the standard model of particle physics. In fact, the vacuum energy density is about 121 orders of magnitude larger than \( \rho_\Lambda \) inferred from cosmological observations. Supersymmetric particle physics theories can produce mechanisms to reduce the vacuum energy of space.

One alternative to \( \Lambda \)CDM is to replace the cosmological constant with a scalar field which minimally couples to matter, often known as Quintessence. In these theories the scalar field contributes to the total universal energy budget and its dynamics are determined by its potential. There exists a vast array of models which match this description, see Copeland, Sami & Tsujikawa (2006) or Clifton et al. (2012) for full reviews of the field.

On the other hand one may treat the observed dark energy as an extension to gravity. Schematically, one may see modified gravity theories as modification to \( G_{\mu\nu} \) on the left-hand side of (1.8) whereas scalar field theories are modifications to the energy momentum tensor, \( T_{\mu\nu} \).

The set of alternative models we test here are known as \( f(R) \) models because they...
are generalisations of the Einstein-Hilbert action,
\[
S = \frac{1}{16\pi G} \int d^4x \sqrt{-g} \left( R + f(R) \right) + \int d^4x \sqrt{-g} \mathcal{L}_m[g_{\mu\nu}, \chi]
\]  
(1.49)

where \( f(R) \) is a function of the Ricci scalar. Without identifying the mechanism or symmetry involved we will assume that the vacuum energy contribution in \( \mathcal{L}_m \) is exactly zero. Instead we treat \( \Omega_\Lambda \) as an effective energy density originating from our modification to GR. It is not realistic to think of \( f(R) \) theories as fundamental theories of gravity. However, the \( f(R) \) toy models can be considered as self-consistent classical extensions of GR.

In this section we derive the \( f(R) \) field equations and examine the behaviour of the background expansion. We also discuss the local tests of gravity that this model must adhere to before outlining the particular \( f(R) \) models that we will be testing in this thesis.

### 1.4.1 Gravitational Field Equations

The \( f(R) \) field equations are derived using the same methodology as the Einstein equations (1.8), i.e. by setting \( \delta S/\delta g^{\mu\nu} = 0 \). Extremising the action (1.49) and using the identities in (1.12) we obtain
\[
(1 + f_R) R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} (R + f(R)) + g_{\mu\nu} \Box f_R - \nabla_\mu \nabla_\nu f_R = 8\pi G T_{\mu\nu}
\]  
(1.50)

where \( f_R = df/dR \) and the energy momentum tensor contains the radiation and matter components. We note that the Bianchi identity (1.9) still holds: we have simply changed how the geometry of space-time reacts to energy sources. Taking the left-hand side of (1.50) as \( G_{\mu\nu} \) we know that \( \nabla_\mu G^\mu_\nu = 0 \).

The dimensionless \( f_R \) is an extra degree of freedom that does not exist in the concordance model. We will show later that this degree of freedom results in a “fifth force” in an \( f(R) \) universe. Taking the trace of the field equations (1.50) we obtain
\[
\Box f_R = \frac{1}{3} \left( R - f_R R + 2f - 8\pi G T \right)
\]  
(1.51)
where $T$ is the trace of the energy momentum tensor and we have identified (1.51) as the Klein-Gordon equation for the $f_R$ field.

Note that the first and second terms on the left-hand side of (1.50) resemble the $G_{\mu\nu}$ tensor while the third and fourth terms have no GR counterpart. To see this further if we set $f(R) = -2\Lambda$ (as we might in the $\Lambda$CDM case) we obtain

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R + \Lambda g_{\mu\nu} = 8\pi GT_{\mu\nu}. \quad (1.52)$$

where we identify the $\Lambda g_{\mu\nu}$ term as the vacuum energy previously incorporated in the energy momentum tensor.

The background expansion history of the $f(R)$ universe can be calculated in the same manner as the $\Lambda$CDM case (see Section 1.2.1). As before we assume a flat FRW metric (1.16) and that the energy momentum tensor can be described as a perfect fluid (1.18). Under these conditions the field equations (1.50) yield

$$H^2 + \frac{f}{6} - \frac{\ddot{a}}{a}f_R + H\frac{\dot{f}}{f_R} = \frac{8\pi G}{3}\bar{\rho}, \quad (1.53)$$

and

$$\frac{\ddot{a}}{a} + \frac{f}{6} - f_RH^2 + \frac{1}{2}\left( H\frac{\dot{f}}{f_R} + \frac{\ddot{f}}{f_R} \right) = -\frac{4}{3}\pi G(\bar{\rho} + 3P) \quad (1.54)$$

These are the $f(R)$ equivalent of the Friedmann equations.

### 1.4.2 Einstein Frame

In the action (1.49) and in all of the above calculations the matter term, $\mathcal{L}_m$, is universally coupled to the gravitational metric $g_{\mu\nu}$. This is known as the Jordan frame. One can transform to a frame known as the Einstein frame in which our modifications to the Einstein-Hilbert action are manifest as a scalar field which couples non-minimally to the matter Lagrangian density. This frame is mathematically equivalent to the Jordan frame but some physical interpretations are different. In the Einstein frame the $f(R)$
action is
\[ S_E = \frac{M_{pl}^2}{2} \int d^4x \sqrt{-\tilde{g}} \tilde{R} + \int d^4x \sqrt{-\tilde{g}} \left[ \frac{1}{2} \tilde{g}^{\mu \nu} \tilde{\nabla}_{\mu} \phi \tilde{\nabla}_{\nu} \phi - V(\phi) \right] + \mathcal{L}_m [e^{-\beta \phi/M_{pl}} \tilde{g}_{\mu \nu}; \chi] \] (1.55)

where \( M_{pl} = (8\pi G)^{-1/2} \), \( \beta = \sqrt{2/3} \) and tilde denotes the Einstein frame quantities. In (1.55), we have performed the conformal transformation
\[ \tilde{g}_{\mu \nu} = e^{\beta \phi/M_{pl}} g_{\mu \nu} \] (1.56)
and defined the field via
\[ 1 + f_R = e^{2\beta \phi/M_{pl}}. \] (1.57)

The potential, \( V(\phi) \) can be linked to Jordan frame quantities via
\[ V(\phi) = \frac{1}{2} R f_R - f \left( 1 + f_R \right)^2. \] (1.58)

There is a debate over which of these viewpoints is the most physically relevant. We will remain in the Jordan frame, where our modifications to the gravitational action are explicit, and transform to the Einstein frame when it is useful.

### 1.4.3 Screening Mechanism

In viable theories of modified gravity, the gravitational force law is modified on large scales so to produce late time acceleration. In order to ensure that the theory reverts to GR within the solar system, these theories usually have a screening mechanism to suppress the fifth force in certain regions of space. With a screening mechanism, modified gravity theories can replicate experimental results from lunar laser ranging and measurements from the Cassini probe.

In \( f(R) \) gravity, the chameleon mechanism suppresses the fifth force in regions of high density (Khoury & Weltman, 2004a,b). To see this we move to the Einstein frame. From the action (1.55) we can derive
\[ \tilde{\nabla}^2 \phi = \frac{dV}{d\phi} + \frac{\beta}{M_{pl}} e^{\beta \phi/M_{pl}} \] (1.59)
by varying with respect to $\phi$ (see [Waterhouse 2006] for a line by line derivation). In the above we have assumed the usual form of $T_{\mu \nu}$ appropriate for non-relativistic matter where we note that $\tilde{\rho} = \rho e^{3\beta \phi/M_{pl}}$. We can simplify the chameleon equation of motion to

$$\tilde{\nabla}^2 \phi = \frac{dV_{\text{eff}}}{d\phi}$$

(1.60)

where the effective potential,

$$V_{\text{eff}}(\phi) = V(\phi) + \rho e^{\beta \phi/M_{pl}},$$

(1.61)

is an explicit function of matter density. In Fig [1.3], we show the effective potential of a chameleon model for a power-law potential.

Broadly, there are three regimes of interest here. In the limit of high density the effective mass of the scalar field,

$$m^2 = \frac{d^2V}{d\phi^2} + \frac{\beta^2}{M_{pl}^2} \tilde{\rho} e^{\beta \phi/M_{pl}},$$

(1.62)

becomes large. When the scalar field acquires a large effective mass it becomes indistinguishable from a background (vacuum) energy density. This is the limit in which

Figure 1.3: The effective potential for a chameleon model with a power-law potential. **Left:** the effective potential is dominated by the large matter density term. **Right:** the bare potential term dominates in regions of low matter density. From [Khoury & Weltman 2004a]
local gravity tests are conducted. In the opposite limit, i.e. a region of low matter density, the scalar field does not possess such a large effective mass and so is free to act as a fifth force. The low density limit also ensures that the scalar field can act as the source of cosmological acceleration. The third regime of interest is the case where the matter density is not the dominant term in the effective potential but it is not negligible. In the intermediate case the scalar field equation can be solved analytically for idealised spherical matter overdensities (Khoury & Weltman [2004a]). In general it is necessary to solve for the scalar field numerically, either in the Einstein or Jordan frame. It is important to emphasise that although we have described the dynamics in the Einstein frame the chameleon mechanism is also present in the Jordan frame.

1.4.4 Viable Models

Theories of \( f(R) \) gravity have been used to model both periods of rapid cosmological expansion: the inflation and the dark energy epochs ([Sotiriou & Faraoni, 2010; de Felice & Tsujikawa, 2010]). Here we choose to study \( f(R) \) models designed to replicate the late time expansion with \( w \approx -1 \). We also note that it is possible to modify these models in order to produce both early time inflation and late time acceleration ([Appley, Battye & Starobinsky, 2010]).

In order to be considered a viable \( f(R) \) theory, a model must address classical and quantum stability constraints ([Starobinsky, 1980]):

- \( 1 + f_R > 0 \),
- \( f_{RR} > 0 \).

The constraint on the first derivative prevents ghost degrees of freedom as well as ensuring that gravity remains attractive. Ensuring that the second derivative is positive ensures that Dolgov-Kawasaki instabilities do not occur ([Dolgov & Kawasaki, 2003]).

The models we study in this thesis are designed to produce a \( \Lambda \)CDM-like expansion history (\( \lim_{R \to \infty} f(R) \to -2\Lambda \)). Therefore, we enforce \( f_R < 0 \) at all redshifts and
$f_R \rightarrow 0$ as $R \rightarrow \infty$. In terms of cosmology, models must reproduce viable radiation, matter and acceleration epochs. To produce a spacetime that behaves exactly as a de Sitter space (with constant curvature) the model must satisfy

$$R (1 + f_R) - 2 (R + f(R)) = 0,$$

(1.63)

where we have assumed negligible matter content. The spacetime is stable if

$$\frac{1 + f_R(R_1)}{f_R(R_1)} > R_1.$$

(1.64)

One can apply strong constraints to the value of $f_R$ measured in the local solar system. These conditions can be evaded globally in $f(R)$ because of the chameleon mechanism.

**Power-law Models**

The models of [Hu & Sawicki (2007)](#) and [Starobinsky (2007)](#) are effectively power-law like models. They both have no true cosmological constant ($\lim_{R \rightarrow 0} f(R) \rightarrow 0$) and have both been shown to pass the necessary validity tests presented earlier in this section. In our work we will use the [Hu & Sawicki (2007)](#) formalism:

$$f_{\text{HS}}(R) = -m^2 \frac{c_1 (R/m^2)^n}{1 + c_2 (R/m^2)^n},$$

(1.65)

where $n$, $c_1$ and $c_2$ are free parameters and $m^2 = H_0^2 \Omega_m$. One can show that $f_R$ for this model can be approximated as

$$f_R = -n \frac{c_1 (R/m^2)^{n-1}}{(1 + c_2 (R/m^2)^n)^2} \approx -n \frac{c_1}{c_2} \left( \frac{m^2}{R} \right)^{n+1}.$$

(1.66)

in the limit of high curvature.

**Exponential Model**

The model of [Appleby & Battye (2007)](#) introduces exponential corrections to GR,

$$f_{\text{AB}}(R) = -\frac{R}{2} + \frac{\epsilon_{\text{AB}}}{2} \log \left[ \frac{\cosh (R/\epsilon_{\text{AB}} - b)}{\cosh (b)} \right]$$

$$= -\frac{b \epsilon}{2} + \frac{\epsilon}{2} \log \left( \frac{1 + \exp \left( \frac{2R}{\epsilon_{\text{AB}} - 2b} \right)}{1 + \exp (2b)} \right),$$

(1.67)
where \( b \) and \( c \) are dimensionless constants, \( \epsilon_{AB} = R_{\text{vac}}/(b + \log(2 \cosh(b))) \). One can see the explicit exponential term by taking the first derivative with respect to the Ricci scalar

\[
f_R = \frac{1}{2} \left( \tanh \left( \frac{R}{\epsilon_{AB}} - b \right) - 1 \right) = \left[ 1 + \exp \left( \frac{2R}{\epsilon_{AB}} - 2b \right) \right]^{-1}.
\] (1.68)

### Designer/Minimal Model

The designer or minimal model (Song, Hu & Sawicki, 2007; Pogosian & Silvestri, 2008) is distinct from the power-law and exponential models in that the functional form of \( f(R) \) is specified by the expansion history.

In He & Wang (2013) the authors derived the analytic form of \( f(R) \) which reproduces a \( \Lambda \)CDM expansion history. Here, we write it as

\[
f(R) = -6 (1 - \Omega_m) H_0^2 - \frac{3D \Omega_m H_0^2}{p_+ - 1} \left( \frac{3 \Omega_m H_0^2}{R - 12 (1 - \Omega_m) H_0^2} \right)^{p_+} \\
\times {}_2 F_1 \left[ q_+, p_+ - 1; r_+; - \frac{3 \Omega_m H_0^2}{R - 12 (1 - \Omega_m) H_0^2} \right]
\] (1.69)

where

\[
q_+ = \frac{1 + \sqrt{73}}{12}, \quad r_+ = 1 + \frac{\sqrt{73}}{6}, \quad p_+ = \frac{5 + \sqrt{73}}{12}
\] (1.70)

and \( D \) is a parameter used to calibrate the deviation from GR behaviour. We can link \( D \) to the value of \( \bar{f} R_0 \) via

\[
\bar{f} R_0 = D \times {}_2 F_1 \left[ q_+, p_+; r_+; - \frac{1 - \Omega_m}{\Omega_m} \right].
\] (1.71)
### Table 1.2: Cosmological parameter sets used in this thesis. Each parameter is defined in the text. All of the models we consider are flat ($\Omega_\Lambda = 1 - \Omega_m$).

<table>
<thead>
<tr>
<th>Name</th>
<th>$\Omega_m$</th>
<th>$\Omega_b$</th>
<th>$h$</th>
<th>$\sigma_8$</th>
<th>$n_s$</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>WMAP1</td>
<td>0.25</td>
<td>0.045</td>
<td>0.7</td>
<td>0.9</td>
<td>1.0</td>
<td>Consistent with the first year <em>Wilkinson Microwave Anisotropy Probe</em> results (Spergel et al., 2003). Used in the first generation MGS (Section 3.2.1).</td>
</tr>
<tr>
<td>WMAP7</td>
<td>0.272</td>
<td>0.0455</td>
<td>0.704</td>
<td>0.81</td>
<td>0.961</td>
<td>Consistent with the WMAP 7 year results (Komatsu et al., 2011). Used in the second generation MGS (Section 3.2.2).</td>
</tr>
<tr>
<td>Winther</td>
<td>0.2708</td>
<td>0.045</td>
<td>0.704</td>
<td>0.8</td>
<td>0.966</td>
<td>Used by the Winther et al. (2015) code comparison project</td>
</tr>
<tr>
<td>Planck1</td>
<td>0.316</td>
<td>0.049</td>
<td>0.671</td>
<td>0.834</td>
<td>0.962</td>
<td>Based on the results from Planck Collaboration et al. (2014b). Used by He et al. (2014) and He, Li &amp; Hawken (2015).</td>
</tr>
<tr>
<td>EAGLE</td>
<td>0.307</td>
<td>0.04825</td>
<td>0.6777</td>
<td>0.8288</td>
<td>0.9611</td>
<td>Used by Eagle simulations (Schaye et al., 2015) and adopted for the work in Chapter 2.</td>
</tr>
<tr>
<td>PL</td>
<td>0.3</td>
<td>0.0455</td>
<td>0.67</td>
<td>0.8</td>
<td>0.9603</td>
<td>Adopted for the work in Chapter 5.</td>
</tr>
</tbody>
</table>
Chapter 2

Simulations of Structure Formation

In our simulations we follow both dark matter and baryonic matter using massive tracer particles. On galactic and cosmological scales dark matter can be described as a collisionless fluid. On the other hand, the description of regular matter must include pressure as well as other baryonic processes. The aim of an $N$–body solver is to obtain the acceleration of each particle due to the gravitational forces to which it is subjected.

While we aim to simulate a semi-infinite universe we are obviously limited by computational resources. To this end we will always assume periodic boundary conditions in the spatial domain. This means that, in principle, it is possible for a particle to leave a structure and pass over the periodic boundary and rejoin the structure on the other side of the box. This scenario is permitted if the simulated volume is large enough that we can apply the cosmological principle. However, there are effects that are known to be caused by the boundary conditions and they will be discussed later in this chapter.

In this chapter we summarise the methods used in simulations of large scale structure formation. Firstly, in Section 2.1 we review the process of generating initial conditions for simulations of cosmological volumes. In Section 2.2 the various methods that can be used to calculate gravitational forces on particles are outlined. Hydrodynamical forces and the methods used to compute them are addressed in Section 2.3. In Section 2.4 we cover how to convert the raw particle data into useful structure statistics. Finally, in Section 2.5 we quantify two of the current limitations of $N$-body simulations.

Throughout this chapter we refer to the comprehensive reviews of [Bertschinger].
2: SIMULATIONS OF STRUCTURE FORMATION

(1998) and Dolag et al. (2008) in addition to the individual works that are noted.

2.1 Initial Condition Generation

The initial conditions of any of our simulations must statistically resemble the conditions of the universe at the starting redshift. At high redshift the matter density of universe is known to have been near-homogeneous with small Gaussian perturbations.

Taking a uniformly random distribution of particle positions within the computational volume would satisfy our desire for a homogeneous field, however it is rarely ever used. This is because randomly generated positions would lead to very small displacements between some particles which in turn lead to unphysically large accelerations. Instead, there are two common starting points for producing acceptable particle distributions, a grid or a glass. A regular grid distribution is commonly adopted as it is a simple and efficient way to achieve a homogeneous density field. There are known issues with this approach, namely the fact that forces on grided particles will be anisotropic on the scale of the interparticle separation. On the other hand, a glass distribution maintains isotropy. A glass distribution is constructed by taking an initially random particle distribution and evolving it for many timesteps with an $N$-body code with the sign of gravity reversed ($G \rightarrow -G$). The small random displacements are quickly removed and the distribution becomes homogeneous and isotropic.

Perturbations are usually added to the particle distribution by a process known as $k$-space sampling\footnote{It has been shown by Hahn & Abel (2011) that since this method enforces periodicity of $\delta$ in real space, it can lead to errors on the scale of the box.}. In this process the Fourier pair of the density contrast field is computed on a regular grid,

$$\hat{\delta}(k) = \sqrt{P(|k|)}\hat{\mu}(k),$$

(2.1)

where $P(k)$ is the power spectrum previously discussed in Section 1.2.2 and $\hat{\mu}$ is the Fourier transform of a Gaussian field (see Jenkins 2013 for details regarding the generation of white noise fields). Throughout this chapter, Fourier transform operations

Simulations with Modified Gravity
are invoked because Fast Fourier Transform (FFT) algorithms, such as FFTW (Frigo & Johnson, 2005), make these operations quick, efficient and readily parallelisable. In this calculation it is common to use a factor of $2^3$ more cells in the grid than particles so to ensure a smooth interpolation. From the Poisson equation, (1.34), one can compute the potential field

$$
\Psi(q) = -4\pi G \bar{\rho} \sum_k \frac{\hat{\delta}_{|k|} e^{ik\cdot q}}{|k|^2} (2.2)
$$

where, as before, $q$ is the initial position of the particle and we have transformed from $k$-space via a Fourier transform. This potential can now be plugged into the equations for the position and velocity displacement fields (1.41 & 1.42). We note that this procedure can be extended to use second order perturbation theory (Scoccimarro, 1998).

## 2.2 N-body Solvers

The $N$-body simulations we describe here evolve the initial particle distribution over a number of timesteps according to Newtonian gravity in an expanding spacetime. The gravitational potential on the $i$th particle can, in principle, be calculated directly via

$$
\Psi(r_i) = -G \sum_{j \neq i} \frac{m_j}{\sqrt{|r_i - r_j|^2 + \epsilon^2}} (2.3)
$$

where the mass of the $j$th particle is $m_j$. A small softening length $\epsilon$ is required in order to suppress unphysical two-body interactions when $|r_i - r_j| \to 0$. A direct calculation of the gravitational force on each particle from every other particle is not often implemented as this involves $\mathcal{O}(N^2)$ operations. In the following sections we outline numerical methods that aim to balance the accuracy of the calculation and the computational expense required.
2: SIMULATIONS OF STRUCTURE FORMATION

Figure 2.1: A two dimensional version of the Barnes & Hut (1986) tree algorithm described in the text. Each layer from left to right represents a level in the tree structure. One can see that each cell can be split into 4 (8) daughter cells in 2 (3) dimensions if it contains more than a single particle. This figure is from Springel, Yoshida & White (2001).

2.2.1 Tree-Based Methods

Tree-based methods approximate the gravitational force on a particle as a multipole expansion. The approximate force on each particle is obtained by grouping distant particles into cells and calculating a single force multipole from each cell (Appel, 1985). The Barnes & Hut (1986) algorithm consists of two parts, the tree construction and the tree walk.

During the construction of the tree, the simulated volume is split into 8 cubical cells each with length $l = L/2$, where $L$ is the length scale of the cube. The cells are then recursively split into 8 subcells until each contains either one or zero particles (see Fig. 2.1 for a two dimensional example of this). The hierarchy of cells is analogous to a tree with the smallest daughter cells representing leaves on branches.

Calculating the gravitational force on the $i$th particle is known as walking the tree. In this routine the total mass and the centre of mass, $\mathbf{x}_{\text{CoM}}$, are calculated for each of the original 8 cells. The angle

$$\theta = \frac{l}{|\mathbf{x}_i - \mathbf{x}_{\text{CoM}}|}$$

(2.4)
is calculated in each cell. In (2.4), \( l \) is the side length of the cell and the denominator is the distance between the particle and the cell centre of mass. If the angle criterion is not satisfied in a cell (\( \theta < \theta_{\text{crit}} \), where \( \theta_{\text{crit}} \) is a constant) then the cell is “opened” and each of the 8 daughter cells are considered. This process is applied recursively until all open branches satisfy the angle criterion. The gravitational force is then calculated treating each of the open daughter cells as a “macro” particle.

Computing the gravitational force using a tree instead of the direct calculation, (2.3), reduces the number of operations from \( \mathcal{O}(N^2) \) to \( \mathcal{O}(N \log(N)) \). The level of the approximation in the calculation can be easily controlled by the \( \theta_{\text{crit}} \) parameter. It is common to set \( \theta_{\text{crit}} = 0.5 \) radians and we note that the case \( \theta_{\text{crit}} = 0 \) is the same as the direct force calculation. PKDGRAV (Stadel, 2001) and GADGET (Springel, Yoshida & White, 2001) are both examples of tree-based cosmological codes.

### 2.2.2 Particle Mesh Methods

Particle Mesh (PM; Hockney & Eastwood, 1981; Klypin & Shandarin, 1983; Efstathiou et al., 1985) methods involve smoothing the particle distribution onto a grid and solving for the potential in Fourier space. The PM methods we describe here consist of three main routines.

Firstly, the mass of each particle is assigned to cells on a grid. In the simplest imaginable scheme, called Nearest Grid Point (NGP) assignment, the mass of each particle is assigned wholly to the cell point that is closest. For reasons that will be outlined later in this chapter, NGP is rarely used in practice. More commonly used is the Cloud In Cell (CIC) algorithm where the mass of each particle is distributed over the 8 nearest cells. In this charge assignment scheme the particle is approximated as a cube of uniform density with extent equal to a single grid cell. The mass that is assigned to each cell is weighted by the overlapping volume of the cubical particle. While this algorithm is obviously an approximation, it does ensure that the computed forces are continuous. Higher order schemes, such as the Triangular Shaped Cloud
2: SIMULATIONS OF STRUCTURE FORMATION

(TSC), are possible but more computationally expensive: for example TSC involves distributing each particle mass across 27 cells. One can write the assignment procedure as

$$\rho(x_{\text{cell}}) = \frac{1}{h^3} \sum_i m_i W(|x_i - x_{\text{cell}}|)$$  \hspace{1cm} (2.5)

where $x_{\text{cell}}$ is the position of the cell, $x_i$ is the position of the $i$th particle, $h$ is the grid spacing and $W(x)$ is the appropriate weighting function (Hockney & Eastwood [1981]).

The second routine involves solving Poisson’s equation in Fourier space. The solution to Poisson’s equation on the real space grid can be written as

$$\Psi(x_i) = \sum_j G(x_i - x_j)\rho(x_j)$$  \hspace{1cm} (2.6)

where $N_{\text{cell}}$ is the total number of grid cells and $G$ is the Green’s function. In Fourier space (2.6) becomes a simple multiplication

$$\hat{\Psi}(k) = \hat{G}(k)\hat{\rho}(k)$$  \hspace{1cm} (2.7)

by the convolution theorem. The real space potential on the grid can be obtained via an inverse Fourier transform. In the final routine of this algorithm, the potential is interpolated onto the particles. The weighting function, $W(x)$, must be deconvolved out of the gridded potential before being applied to the particle distribution.

PM methods are generally quick compared to tree based methods (Section 2.2.1) and can be written in an efficient way (they scale $O(N + N_{\text{cell}} \log(N_{\text{cell}}))$. However, the spatial resolution of a PM method is limited by $N_{\text{cell}}$. To this end it is common to combine a small scale solver and a PM solver, for example the hybrid TreePM method (Xu [1995] Springel [2005]). In this approach the potential is split into short-range and long-range terms, $\hat{\Psi}_k = \hat{\Psi}^\text{short}_k + \hat{\Psi}^\text{long}_k$, where

$$\hat{\Psi}^\text{long}_k = \hat{\Psi}_k \exp(-k^2 r_s^2)$$  \hspace{1cm} (2.8)

and

$$\Psi^\text{short}(r_i) = -G \sum_{j \neq i} \frac{m_j}{x_j^2} \text{erfc} \left( \frac{x_j}{2r_s} \right)$$  \hspace{1cm} (2.9)
where $x_j$ is the distance from particle $i$ to particle $j$. The GADGET code utilises the TreePM method.

An alternative to the TreePM algorithm is the Particle-Particle - Particle-Mesh (P³M) method where small-scale forces are computed directly [Hockney & Eastwood, 1981; Efstathiou et al., 1985]. While being more memory efficient, the two-body calculations in this approach are known to be very CPU-intensive compared to the tree in the TreePM algorithm (Xu, 1995). In order to improve performance it is possible to use multiple grids (Merz, Pen & Trac, 2005). CUBEP³M (Harnois-Déraps et al., 2013) is a modern example of a cosmological code utilising the P³M algorithm.

### 2.2.3 Adaptive Grid Methods

It is possible to solve the Poisson equation using Adaptive Mesh Refinement (AMR) techniques. In these methods the cells of a base grid are subdivided in regions of high density. The process of refinement creation is usually carried out recursively until the number of particles per cell reaches a small number (usually 3 or 4). Once the density field has been stored on the grid hierarchy, the gravitational potential can be solved for.

An early implementation of these methods was presented by Couchman (1991) where the P³M algorithm was generalised to be used on a base grid as well as on refined regions. This technique is known as AP³M and has been combined with a hydrodynamical solver in the cosmological simulation code HYDRA (Couchman, Thomas & Pearce, 1995).

Modern AMR codes use iterative relaxation techniques [Hockney & Eastwood, 1981; Press et al., 1992] to solve for the gravitational potential. In these techniques the Poisson equation is rewritten as

$$\frac{d\Psi}{d\tau} = \nabla^2 \Psi - 4\pi G \bar{\rho} \delta$$  \hspace{1cm} (2.10)

where $\tau$ is a fictitious time parameter representing the iterative update procedure. Adopting a valid update rule [Kravtsov, Klypin & Khokhlov, 1997; Knebe, Green...
& Binney, 2001) ensures that as the number of iterations increases, \( \frac{d\Psi}{d\tau} \rightarrow 0 \). The optimal update rule for a given PDE is often hard to determine a priori. For the Poisson equation, a good balance between accuracy and efficiency can be derived from using Newton’s method (see Chapter 4 for more details). It is typical to utilise multigrid methods (Brandt, 1977; Wesseling, 1992; Brandt & Livne, 2011) in order to accelerate the rate of convergence.

There are two types of modern AMR methods used to solve the Poisson equation: structured refinement schemes and unstructured refinement schemes. Unstructured AMR schemes subdivide individual cells which contain more than a certain number of particles. On the other hand, the structured AMR schemes use a hierarchy of grid patches. While refinements are usually irregular in shape, it is possible to carry out the multigrid relaxation on them using the parent cells as boundary conditions. The data structures in both schemes typically resemble the data structures used in tree-based methods.

We will return to multigrid methods in Chapter 4. Two popular AMR enabled cosmological codes are RAMSES (Teyssier, 2002) and ENZO (Bryan et al., 2014).

### 2.3 Hydrodynamics

In the previous section we described the calculation of gravitational forces in the absence of hydrodynamics. In this section we describe how one can include the dynamics of baryonic gas in \( N \)-body simulations. Throughout our discussion we will treat baryonic gas as inviscid.

The acceleration of the fluid is given by

\[
\frac{dv}{dt} = -\frac{\nabla P}{\rho} - \nabla \Psi \tag{2.11}
\]

where \( v \) is the fluid velocity, \( P \) is the pressure of the gas and \( \rho \) is the density. This is known as the Euler equation. In collision-less dynamics the Euler equation links the acceleration of a test particle with the gradient of the gravitational potential. Here, the
acceleration is determined both by the gravitational dynamics and the pressure-density term. The gas is also subject to the continuity equation,

$$\frac{d\rho}{dt} + \rho \nabla \cdot \mathbf{v} = 0,$$

(2.12)

which ensures conservation of mass. In addition, the fluid is subject to the first law of thermodynamics,

$$\frac{du}{dt} = -\frac{P}{\rho} \nabla \cdot \mathbf{v} - \Lambda(u, \rho),$$

(2.13)

where $u$ is the internal energy per unit mass and $\Lambda(u, \rho)$ is the cooling function that describes radiative losses. In the so called non-radiative case the cooling function is set to zero for all $u$ and $\rho$. For an ideal monoatomic fluid the above set of equations (2.11-2.13) are closed by the equation of state

$$P = (\gamma - 1) \rho u$$

(2.14)

where $\gamma = 5/3$.

### 2.3.1 Smoothed Particle Hydrodynamics

Smoothed Particle Hydrodynamics (SPH) is a common technique used to describe the dynamics of a fluid using particles (Monaghan, 1992; Dolag et al., 2008; Springel, 2010b). Since the first formulation by Lucy (1977) and Gingold & Monaghan (1977), the technique has been subsequently improved over the years by multiple authors. SPH is a particularly appealing technique because describing the fluid using particles enables one to make the scheme adaptive in spatial resolution. As such, it is the technique of choice in the GADGET-2 code (Springel, 2005).

The density of a fluid in SPH is the kernel summation

$$\rho(r) = \sum_{j} N_{\text{neigh}} m_j W(r - r_j, h)$$

(2.15)

where $W(x, h)$ is the smoothing kernel, $x$ is the separation between particles and $h$ is the scale parameter describing the kernel width (known as the SPH smoothing length).
The summation in (2.15) is not performed over all particles. Instead, the density is taken to be the weighted sum of \( N_{\text{neigh}} \) nearby particles.

There are multiple properties required of the smoothing kernel. Firstly, it is required that \( W(x, h) \) is normalised to unity via \( \int_V W(x', r, h) dV' = 1 \). This ensures that the total mass is a conserved quantity. The weighting must be positive and decrease monotonically with \( x \). It is necessary for \( W(x, h) \) to have smooth derivatives and to be symmetric with respect to \( x \). In the limit of \( h \to 0 \), the kernel should reduce to a Dirac delta function. It is also desirable for \( W(x) \) to remain approximately constant for small values of \( x \). This final condition ensures that the density estimate is not strongly affected by a small change in position of a near neighbour.

While the first formulations of SPH used a Gaussian kernel, it is now rarely used because of the fact that it is infinite in extent. Instead, it is common to use the \( B_2 \) spline defined as

\[
W(x, h) = \frac{\sigma}{h^\nu} \begin{cases} 
1 - 6 \left( \frac{x}{h} \right)^2 + \left( \frac{x}{h} \right)^3 & 0 \leq \frac{x}{h} < 0.5, \\
2 \left( 1 - \frac{x}{h} \right)^3 & 0.5 \leq \frac{x}{h} < 1, \\
0 & 1 \leq \frac{x}{h},
\end{cases}
\]  

(2.16)

where \( \nu \) is the number of dimensions and \( \sigma \) is the normalisation (\( \sigma = 8/\pi \) for \( \nu = 3 \)). The \( B_2 \) spline is a good approximation to the Gaussian function and is computationally cheap to evaluate. Note that this spline has finite extent, a property known as compact support.

The smoothing length, \( h_i \), of particle \( i \) is sometimes set to vary with the number of nearby particles, other formulations fix \( N_{\text{neigh}} \) in order to determine \( h_i \). In the former case we require that the kernel volume contains a constant mass

\[
M = \frac{4\pi}{3} h_i^3 \rho_i = N_{\text{neigh}} \bar{m}
\]  

(2.17)

where \( \rho_i \) is the density calculated using (2.15) and \( \bar{m} \) is the average gas particle mass.

Using the SPH formalism we can write the value of any continuous fluid quantity \( Y(r) \) as

\[
Y(r) = \int Y(r') W(r - r', h) dr'.
\]  

(2.18)
The above integral is discretised as

\[ Y(\mathbf{r}) = \sum_j \frac{m_j}{\rho_j} Y_j W(\mathbf{r} - \mathbf{r}_j, h). \]  
\[ (2.19) \]

where, as before, the summation is over \( N_{\text{neigh}} \) nearby particles and \( Y_j \) is the value of field quantity \( Y(\mathbf{r}) \) at the position of the \( j \)th particle. Since the kernel is known, one can compute the spatial derivative of \( Y(\mathbf{r}) \) via

\[ \nabla Y(\mathbf{r}) = \sum_j \frac{m_j}{\rho_j} Y_j \nabla W(\mathbf{r} - \mathbf{r}_j, h). \]  
\[ (2.20) \]

The \textbf{GADGET-2} code uses the SPH formulation of \cite{Springel2002} which conserves both entropy and energy if adaptive smoothing lengths are used. In this scheme the thermodynamic state of each particle is measured in terms of \( A = P/\rho^\gamma \) where \( \gamma \) is the specific heat (\( \gamma = 5/3 \) for an ideal monatomic gas). This variable has been chosen because \( A \) is conserved in an adiabatic flow. After computing \( A_i \), one can infer the internal energy per unit mass via

\[ u_i = \frac{A_i}{\gamma - 1} \rho_i^{\gamma - 1}. \]  
\[ (2.21) \]

Physical shocks are near impossible to track in SPH because of the smoothing of thermodynamic quantities. In order to correct this, one introduces an artificial viscosity, \( \Pi_{ij} \), which transforms kinetic energy into heat. The artificial viscosity acts to change the entropy of the gas at a rate

\[ \frac{dA_i}{dt} = \frac{1}{2} \frac{\gamma - 1}{\rho_i^{\gamma - 1}} \sum_j m_j \Pi_{ij} (v_j - v_i) \cdot \nabla_i \bar{W}_{ij} \]  
\[ (2.22) \]

where \( \bar{W}_{ij} = \frac{1}{2} \left( W(|\mathbf{r}_i - \mathbf{r}_j|, h_i) + W(|\mathbf{r}_i - \mathbf{r}_j|, h_j) \right) \).

In the scheme of \cite{Springel2002}, the hydrodynamic part of the Euler equation is

\[ \frac{dv_i}{dt} = - \sum_j m_j \left[ f_i \frac{P_i}{\rho_i^2} \nabla_i W(|\mathbf{r}_i - \mathbf{r}_j|, h_i) + f_j \frac{P_j}{\rho_j^2} \nabla_i W(|\mathbf{r}_i - \mathbf{r}_j|, h_j) \right] \]  
\[ (2.23) \]

where

\[ f_i = \left[ 1 + \frac{h_i}{3\rho_i} \frac{\partial \rho_i}{\partial h_i} \right]^{-1}. \]  
\[ (2.24) \]
2: SIMULATIONS OF STRUCTURE FORMATION

While we will focus on SPH, there are a wide variety of other methods that are used to compute hydrodynamical forces in N-body simulations including AMR (e.g. Fryxell et al., 2000; Bryan et al., 2014) and moving-mesh techniques (e.g. Springel, 2010a).

2.4 Measuring Large Scale Structure Statistics

In this section we outline how we compute the matter power spectrum and the halo mass function from a snapshot of particle positions and velocities.

2.4.1 Matter Power Spectrum

In Section 2.1 we described how to use the linear power spectrum to set up the initial conditions of cosmological simulations. On large scales, the modes should evolve according to linear theory. However, as the simulation proceeds structures on small scales enter the nonlinear regime \( \delta \gg 1 \) and the clustering of matter on small scales deviates from the linear theory prediction. In other words, evolving the particle distribution to redshift \( z \) modifies the matter power spectrum at large \( k \). Measuring the power spectrum of a simulated volume allows us to verify that low \( k \) modes evolve as \( \delta \propto D(a) \) as well as predicting the nonlinear growth of structure on smaller scales.

The standard method for calculating the power spectrum from a simulated matter distribution is to smooth the particles onto a grid and compute the Fourier transform of the \( \delta \) field. This procedure is identical to that of the PM calculation described in Section 2.2.2. Since \( P(k) = |\hat{\delta}(k)|^2 \), this calculation is relatively simple and computationally cheap. The power spectrum calculated in this manner is subject to aliasing due to the finite spatial resolution of the grid, discreteness effects due to the finite number of particles in a simulation and damping of small scale modes due to the deconvolution (Colombi et al., 2009).

The finite resolution of a single grid can be surpassed by using an AMR scheme (Teyssier).
2.4: MEASURING LARGE SCALE STRUCTURE STATISTICS

It is also possible to use a Delaunay tessellation estimator (Schaap & van de Weygaert, 2000; Cautun & van de Weygaert, 2011) to compute the density field, however one must then interpolate onto a regular grid in order to obtain the Fourier transform (Li et al., 2013). Assuming that \( P(k) \) behaves as a power-law at large \( k \), one can correct the power spectrum for the fact that we are sampling the density field from a set of discrete particles (Jing, 2005; Cui et al., 2008). Colombi et al. (2009) demonstrated that a Fourier-Taylor transform can be used to avoid the aforementioned errors and compute an unbiased estimate of \( P(k) \) from a distribution of particles.

We will use the POWMES\(^2\) implementation (Colombi et al., 2009) of the Fourier-Taylor method throughout this thesis. POWMES calculates the power spectrum using a regular fixed grid mesh and supplements this crude \( P(k) \) with higher order terms. These Taylor expansion terms are calculated using the particle distribution within each cell.

2.4.2 Cluster Mass Function

In both \( N \)-body and hydrodynamic simulations, structures can be identified from the particle distribution. In this section we will describe the algorithms used to identify haloes, the formalism that we use when describing a mass function and limitations we must consider when analysing simulated mass functions.

Halo Identification

There are a number of different algorithms which can be used to identify halo structures (see Knebe et al., 2011 for a complete review). These algorithms are commonly used in combination so we only outline the processes and will not cover all of the computational details.

\(^2\)The POWMES code is publicly available at [www.projet-horizon.fr](http://www.projet-horizon.fr)
Friends-of-Friends  The Friends-of-Friends (FOF; Davis et al. 1985) algorithm links particles that are nearby in space. In particular, FOF links particles that are within $b$ times the mean interparticle separation (so within $b LN^{-1/3}$ where $L$ is the length of the simulated cubic volume and $N$ is the total number of particles). The FOF linking parameter is commonly, although not exclusively, set to $b = 0.2$. In an Einstein-de Sitter universe this choice of linking parameter should yield haloes with $\Delta \approx 180$ (Lacey & Cole 1994), although this is disputed (Warren et al. 2006). The algorithm is geometric in that it only considers particle positions and does not include velocity information.

FOF is the standard halo finding algorithm in computational cosmology as it can be carried out at relatively low computational expense compared to other halo finding techniques. Unfortunately, there is no condition within the algorithm for the structures that it forms to be gravitationally bound. As such, it suffers from the “over-bridging” problem where two spatially close haloes can be linked by FOF if a bridge of unbound particles intersects them.

Spherical-Overdensity  The Spherical-Overdensity (SO; Press & Schechter 1974; Lacey & Cole 1994) algorithm assumes that haloes are spherically symmetric overdensities of matter which have monotonically decreasing density profiles. The radius of a given halo is determined by where the overdensity, $\Delta = \rho(< r)/\rho_{ref}$, falls to a predetermined overdensity threshold, $\Delta_{\text{thresh}}$. SO implementations usually require the pre-identification of halo centres. This selection procedure is often made using peaks in the density field. Starting from a central point within a halo structure the matter density within a fixed radius $r$ is calculated. If the overdensity is above $\Delta_{\text{thresh}}$ then the radius is increased and the density is recalculated. If the overdensity is below $\Delta_{\text{thresh}}$ then the algorithm stops and records the present radius as the $R_{\Delta_{\text{thresh}}}$.

The reference density, $\rho_{ref}$, is usually taken to be either the critical density of the universe or the mean matter density and common values of $\Delta_{\text{thresh}}$ are 200, 500 & 2500. Higher values of $\Delta_{\text{thresh}}$ correspond to measurements of the central regions of clusters while lower values include the outer edges.
SUBFIND  The SUBFIND (Springel et al., 2001) algorithm aims to identify gravitationally bound substructures within FOF haloes. There are two stages in the routine, a geometric part (not dissimilar to FOF) and a phase-space part. The geometric part aims to identify many subhalo candidates from within a FOF halo. On the other hand, the phase-space part aims to remove particles that are spuriously identified as part of the structure which are in fact not gravitationally bound to the central halo.

The geometric part of this algorithm proceeds by estimating the density at each particle position. Starting from the particle in the densest region, the nearest neighbours of each particle are considered. If there are no nearby particles which have higher estimated densities, the particle is marked as a local density maxima and a subgroup is to be grown around it. If the nearby particles are both of lower density then the neighbours are attached to the subgroup. If the particles are already attached to different subgroups then the particle is labeled as a saddle-point in the isodensity contours. In this case the two subgroups are merged to form one single subgroup. The phase-space (or “unbinding”) routine aims to identify whether the subhalo candidates are true substructures. It does this by iteratively removing particles with positive total energy until only the bound particles are left in the subgroup.

Applying SUBFIND to a typical cosmological density field usually yields multiple subhaloes within each FOF group.

Mass Function Formalism

We follow Press & Schechter (1974); Bond et al. (1991); Jenkins et al. (2001) and use $\ln \sigma^{-1}(M, z)$ as our mass variable of choice. $\sigma(M, z)$ is the rms of the linear overdensity field extrapolated to redshift $z$ after smoothing with a spherical top-hat filter with radius $R = (3M/4\pi \rho_{m, 0})^{1/3}$. The variance of the smoothed field can be computed via

$$\sigma^2(R, z) = \frac{D(z)^2}{2\pi^2} \int_0^\infty k^2 P(k) W^2(kR) \, dk$$

(2.25)
where $D(z)$ is the linear growth factor normalised so that $D(0) = 1$, $P(k)$ is the linear matter power spectrum and

$$W(x) = \frac{3}{x^3} (\sin (x) - x \cos (x))$$

(2.26)

is the Fourier transform of the top-hat window function. Alternatively one can view $\sigma^2(M, z)$ as the mass variance within spheres of radius $R$ that contain mass $M$. For a given cosmology there is a one to one relationship between $\sigma$ and halo mass $M$.

We take $n(M)$ to be the number of haloes with mass greater than $M$ and we describe the halo mass function as the differential number density of haloes in logarithmic mass bins,

$$\frac{dn}{d \ln M} = f(\sigma, z) \frac{\rho_m}{M} \left| \frac{d \ln \sigma}{d \ln M} \right|$$

(2.27)

where $\rho_m(z) = \rho_m(0)(1 + z)^3$ is the mean matter density of the universe and $f(\sigma)$ is the multiplicity function. While $f(\sigma, z)$ can be treated as a free function that can be fitted to, it physically represents the fraction of mass that has collapsed to form haloes per unit interval in $\ln \sigma^{-1}$. While (semi)-analytic approaches to the calculation of $f(\sigma)$ were relatively successful, these have largely been surpassed by fits from $N$-body simulations (Murray, Power & Robotham, 2013a).

We will first consider the mass function produced by running the FOF halo finder on the particle positions at a fixed redshift from a simulation with Gaussian initial conditions. This is the case that $M = M_{\text{FOF}}$ and $\Delta \approx \Delta_c$. It has been shown that a single $f(\sigma)$ can be used to fit the mass function of many simulated volumes with a wide variety of cosmologies and over a range of redshift snapshots. This is known as the universality of the mass function (Jenkins et al., 2001; Tinker et al., 2008).

While universality is impressive, it does not always hold. For example, Bhat-tacharya et al. (2011) found that mass functions taken from cosmological volumes of non-standard dark energy models did not display this characteristic. In particular, they found deviation from universality for some cases where $w \neq -1$.

The universality of the mass function is also not observed when using the SO algorithm with larger values of $\Delta$ on $\Lambda$CDM simulated volumes. In fact it has been shown
that the free parameters in \( f(\sigma) \) depend explicitly on \( \Delta \) and \( z \) \cite{Tinker2008}. \cite{Watson2013} also note that the mass function can have a dependence on the algorithm used to identify haloes, i.e. how subhaloes are identified and whether they are included in the analysis.

Throughout this thesis \( \sigma(M) \) is computed using (2.25) where the linear matter power spectrum \( P(k) \) is calculated using the publicly available CAMB code \cite{Lewis2000}.

\section*{2.5 Known Limitations}

\subsection*{2.5.1 Choice of Initial Conditions}

As previously outlined in this chapter, the initial conditions of a cosmological simulation is generated as a realisation of a Gaussian density field. Throughout the literature authors have run simulations with and without second order terms included in the initial conditions. These simulations have also been run with different starting redshifts. In this section we run a suite of simulations to examine the impact of these choices on the power spectrum.

The choice of starting redshift, \( z_{\text{init}} \), is crucial to reducing numerical error in the calculations. Given that the primordial perturbations are assumed to evolve linearly until \( z_{\text{init}} \), choosing a low initial redshift will result in a simulation that fails to properly capture the non-linear evolution. On the other hand, starting a simulation at a very high redshift could result in the initial matter perturbations being dominated by discretisation error (since the density field is discretised into particles). It is not clear a priori how to choose \( z_{\text{init}} \).

It has previously been shown that using second order Lagrangian perturbation theory (2LPT; \cite{Scoccimarro1998} as opposed to the first order Zel’dovich approximation (ZA) allows one to use a lower starting redshift \cite{Reed2013}. This reduces the
number of timesteps needed by the \( N \)-body solver and therefore reduces the computational cost of the simulation. An additional advantage of using a lower \( z_{\text{init}} \) is that the amplitude of initial matter perturbations is larger and therefore more distinctive from the discretisation noise.

We chose to simulate 4 versions of a 1600\(^3\) Mpc\(^3\) volume in the \textit{Eagle} cosmology described in Table 1.2 using \textsc{gadget-3}. The initial conditions were generated using the 2LPT package\(^4\) of Scoccimarro (1998). The same random seed was used in each version so the structures that form in each volume should be the same.

The first case we consider is that used in the \textit{Eagle} (Schaye et al., 2015) simulations where 2LPT has been applied and the starting redshift is relatively high (\( z_{\text{init}} = 127 \)). We also consider the case of the Millennium XXL simulation (Angulo et al., 2012) for which ZA was used and the simulation was started at \( z_{\text{init}} = 63 \). The other two cases are those of 2LPT applied at low redshift and the ZA applied at high redshift (as used in the Millennium simulation of Springel et al. 2005).

The fractional difference between the power spectra are shown in Fig. 2.2. In agreement with Schneider et al. (2015) we find that the 2LPT results agree to within 1 per cent for this range of \( k \). The large scale modes are consistent across the 4 simulations. Since low \( k \) modes evolve linearly the discrepancies are on smaller scales.

The ZA simulations produce power spectra that are 1 and 1.5 per cent discrepant from the 2LPT \( z_{\text{init}} = 127 \) result at \( k = 1 h \text{Mpc}^{-1} \). Since the ZA is a first order procedure, is it more correct at higher redshift. The fact that the ZA \( z_{\text{init}} = 63 \) power spectrum is more discrepant than the ZA \( z_{\text{init}} = 127 \) power spectrum is expected because of the lower starting redshift.

Overall, we can see that common choices made in the initial conditions generation can lead to a \( \sim 2 \) per cent uncertainty in the \( k \sim 1 h \text{Mpc}^{-1} \) modes of the \( z = 0 \) power spectrum. This uncertainty can be reduced to \( \sim 0.5 \) per cent by using 2LPT initial conditions.

\(^4\)http://cosmo.nyu.edu/roman/2LPT
2.5: KNOWN LIMITATIONS

Figure 2.2: Fractional difference in the power spectra (relative to 2LPT $z_{\text{init}} = 127$) at $z = 0$ induced by choices made regarding the initial conditions. The results for the runs using ZA $z_{\text{init}} = 127$, 2LPT $z_{\text{init}} = 63$ and ZA $z_{\text{init}} = 63$ are shown in red, blue and purple respectively.

2.5.2 Boxsize Effects

Our simulations are obviously limited by the finite computational domain we consider. This presents two problems. Firstly, our simulations are cosmic variance limited, that is we are only measuring one realisation of the underlying matter distribution. Secondly, the boxsize limits the maximum scale of initial perturbation that can influence the collapse of structure. In other words, the power spectrum of any simulation we run is truncated at low $k$.

In an effort to estimate the impact of the second problem we have made use of two different finite box correction methods. Both methods truncate the theoretical $\sigma(M)$. [Watson et al. (2013)] based their method on the extended Press-Schechter formalism.
Their correction is

\[
\sigma_{\text{cor}}^2 = \sigma^2 - \sigma_L^2
\]  

(2.28)

where \(\sigma_L\) is the mass variance smoothed on the scale of the box. On the other hand, Yoshida et al. (2003) proposed using a modified mass variance

\[
\sigma_{\text{box}}^2(M, z) = \frac{D^2(z)}{2\pi^2} \int_{2\pi/L}^{\infty} k^2 P(k) W(k; M) dk.
\]  

(2.29)

It has been noted that correcting the mass function using this method assumes that the mass function is accurately known at high redshift.

In Fig. 2.3 we plot the predicted fractional error on the fitting function \(f(\sigma)\) caused by the finite extent of a simulated volume. The boxsizes in the top panel are roughly 64, 128 and 256 \(h^{-1}\) Mpc respectively and are shown in reference to simulations described in Chapter 5. The results in the lower panel of Fig. 2.3 are pertinent to the simulations discussed in the previous section and those in Chapter 3. As a general trend one can see that finite volume corrections affect the most massive and rarest (since the mass function steeply declines as a function of mass) haloes in a simulation. The maximum finite volume correction in \(f(\sigma)\) for a 1600\(^3\) Mpc\(^3\) volume is approximately 5 per cent at \(10^{16} h^{-1} M_\odot\) and approaches the 1 per cent level at \(10^{15} h^{-1} M_\odot\). We trivially conclude that large computational volumes are required in order to accurately compute the mass function at large masses.
Figure 2.3: Each of the color coded lines represent the fractional error on the multiplicity function expected due to the finite extent of the simulated volume. The full lines are the predictions using the method of Yoshida et al. (2003), (2.29), while dashed lines use the method of Watson et al. (2013). In these plots we assume the form of $f(\sigma)$ reported by Angulo et al. (2012) and the cosmology of Planck Collaboration et al. (2014b) (although the conclusions we draw from this plot are not strongly dependent on either).
Chapter 3

Influence of Baryons on the Cluster Mass Function

3.1 Introduction

Clusters of galaxies map peaks in the cosmic density field and as such can be used to determine information about the Universe on the largest scales (Voit 2005; Allen, Evrard & Mantz 2011; Kravtsov & Borgani 2012). In particular, the abundance of clusters as a function of mass and redshift has been shown to be a particularly sensitive probe of cosmological parameters $\Omega_m$ and $\sigma_8$, the matter density parameter and the linear rms matter fluctuation within a spherical top-hat of $8 \, h^{-1} \, \text{Mpc}$ radius respectively (Vikhlinin et al., 2009; Rozo et al., 2010; Reichardt et al., 2012; Hasselfield et al., 2013; Planck Collaboration et al., 2014c). In order to link the observed mass function of clusters to an underlying cosmology one must appeal to an analytic description of cluster abundance (Press & Schechter, 1974; Bond et al., 1991; Sheth & Tormen, 2002) or to one of many numerical studies investigating dark matter halo formation, e.g. Jenkins et al. (2001); Tinker et al. (2008); Watson et al. (2013). One of the most commonly adopted descriptions of cluster halo abundance is the Tinker et al.

$^1$Throughout we express the Hubble parameter today as $H_0 = 100h \, \text{km s}^{-1} \text{Mpc}^{-1}$.

$^2$See Murray, Power & Robotham (2013b) for a recent comparison of mass functions in the literature.
The implicit assumption made in linking simulated dark matter halo masses with galaxy cluster masses is that the ratio of baryons to dark matter within clusters does not differ significantly from the cosmic value. This assumption, however, has been challenged by multiwavelength observations (Lin, Mohr & Stanford, 2003; Giodini et al., 2009; Laganá et al., 2011). It has also been shown in $N$-body simulations that the pressure forces within baryonic gas are capable of segregating the distribution of collisional gas relative to pressure-less dark matter (Navarro & White, 1993), thereby changing the baryon fraction within clusters (Crain et al., 2007). Numerical studies have also shown that galaxy formation processes and non-gravitational heating can modify the baryon fraction (McCarthy et al., 2011; Planelles et al., 2013) and thereby the total mass within clusters (Stanek, Rudd & Evrard, 2009).

The measurement of the cluster mass function from observations requires the calibration of an observable-mass ($X - M$) relation, where common observables, $X$, are X-ray luminosity, galaxy richness and Sunyaev–Zel’dovich (SZ) flux. Multiple ongoing observational surveys including the Planck mission (Planck Collaboration et al., 2014c), the South Pole Telescope survey (SPT; Reichardt et al., 2012), Dark Energy Survey (DES; The Dark Energy Survey Collaboration, 2005) and the XMM Cluster Survey (XCS; Romer et al., 2001; Sahlén et al., 2009) have made the cosmological analysis of the galaxy cluster mass function one of their key scientific goals. In order to parameterise the systematic uncertainties in the measurement of a given scaling relation, e.g. of incorrectly assuming hydrostatic equilibrium in clusters, the mass bias parameter $b_{\text{hyd}} = 1 - M_{\text{true}}/M_X$ is commonly employed, where $M_X$ is the mass inferred from observable $X$.

In the near future, large-volume observational surveys such as eROSITA (Pillepich, Porciani & Reiprich, 2012), Euclid (Laureijs et al., 2011), the Large Synoptic Survey Telescope (LSST; LSST Science Collaboration et al., 2009) and the proposed PRISM mission[1] will detect a greater number of galaxy clusters than ever before. It is there-
fore of great importance that the cluster mass function is accurately calibrated against theoretical predictions (Reed et al., 2013).

Recent results from the Planck cluster survey (Planck Collaboration et al., 2014c) have been found to be in tension with cosmological parameter determinations made using anisotropies in the cosmic microwave background (CMB; Planck Collaboration et al., 2014b). It has been argued that the discrepancy between the two measured values of $\sigma_8$ and $\Omega_m$ could be due, in part, to cluster biases and selection effects. Alternatively, it has been proposed that the influence of additional physical processes, such as the influence of massive neutrinos on the power spectrum, could lead to an underestimation in the mass function.

In this chapter, we use large cosmological simulations with baryonic physics to investigate whether such tension can at least in part be explained by the effects of baryonic depletion in clusters. Such an effect, due to gas being expelled by feedback processes, produces a shift in the cluster mass function to lower abundance at fixed mass which if not accounted for in the cosmological analysis, leads to derived values for cosmological parameters (\(\Omega_m\) and \(\sigma_8\)) that are systematically underestimated.

The remainder of this chapter can be summarised as follows. In Section 3.2 we outline details of the simulations used and how the cluster samples were defined. In Section 3.3 our main results are presented, quantifying the effect of the baryon depletion on the mass function and its subsequent effect on the cosmological parameters $\Omega_m$ and $\sigma_8$, before suggesting a simple corrective procedure. Finally, in Section 3.4 we discuss our results in the context of other work in the literature and draw conclusions.

3.2 Millennium Gas Simulations

We use results from three cosmological Millennium Gas simulations (MGS; Hartley et al., 2008; Stanek, Rudd & Evrard, 2009; Stanek et al., 2010; Short et al., 2010; Young et al., 2011; Kay et al., 2012) and two dark matter-only versions of the same volumes. The MGS are designed to include the dynamics of gas that were not present in the
dark matter-only Millennium simulations. Each simulation in the suite is run with a different treatment of large scale baryonic physics. We group these simulations into two “generations”, determined by the underlying cosmological model employed.

3.2.1 First generation: GO and PC models

In the Gravitation Only (GO) simulation, first described in Crain et al. (2007), baryonic gas is only permitted to change in entropy through shock heating. As a counterpoint to the adiabatic GO simulation, in the Pre-heating & Cooling (PC) simulation, described in Hartley et al. (2008), radiative cooling of gas was implemented (assuming a metallicity $Z = 0.3 Z_\odot$). Furthermore, in order to emulate the effects of high redshift galaxy formation and reproduce the observed X-ray luminosity-temperature relation at $z \simeq 0$, the gas within the volume was uniformly heated to 200 keV cm$^2$ at $z = 4$.

The GO and PC simulations were run using the GADGET-2 code (Springel, 2005) with the same cosmological model as the Millennium simulation (Springel et al., 2005). The parameters used were $\Omega_m = 0.25$, $\Omega_b = 0.045$, $h = 0.73$ and $\sigma_8 = 0.9$; consistent with the first year Wilkinson Microwave Anisotropy Probe results (WMAP1; Spergel et al., 2003). Because of computational constraints, the simulations were run with a slightly decreased mass resolution compared to the original Millennium run. A downgraded version of the Millennium initial conditions was used in the GO and PC simulations. At early times ($z > 3$) the gravitational softening length was fixed in comoving coordinates to $\epsilon = 100 h^{-1}$kpc, whereas at late times ($z < 3$) the softening was fixed in physical coordinates to $\epsilon = 25 h^{-1}$kpc. The particle masses were set to $m_{dm} = 1.4 \times 10^{10} h^{-1} M_\odot$ and $m_{gas} = 3.1 \times 10^{9} h^{-1} M_\odot$ for the dark matter and gas respectively. In both simulations the dark matter was evolved self-consistently with the gas. As such the baryons influence the formation and growth rate of dark matter structures.

We compare the first generation MGS to a version of the original Millennium simulation (Springel et al., 2005) with the same initial conditions, mass resolution and
gravitational softening lengths as the GO and PC models. We will refer to this simulation as DM1.

### 3.2.2 Second generation: FO model

In the *Feedback Only* (FO) simulation, the effects of stochastic active galactic nuclei (AGN) and supernovae feedback on the gas dynamics were inferred using the semi-analytic model of Guo et al. (2011). At each timestep the hydrodynamics was supplemented using the properties of the galaxies from the semi-analytic model. For example, the star formation rate in a model galaxy was linked to a level of energy input to the gas. For full details regarding the treatment of the gas dynamics in FO see Short, Thomas & Young (2013). The principal improvement of the FO simulation over the PC is that the baryonic feedback is better physically motivated, although radiative cooling is not included. One caveat of note is that in the FO model the baryonic contribution to the gravitational potential is ignored. In other words, the gas is evolved with zero gravitational mass and so there is no baryon-dark matter back-reaction.

The FO simulation was run using an updated version of the Gadget code, GADGET-3 at the resolution of the original Millennium simulation. Smaller softening lengths than the first generation simulations (\(\epsilon = 37h^{-1}\text{kpc}\) in comoving coordinates before \(z \simeq 3\) and \(\epsilon = 9.3h^{-1}\text{kpc}\) in physical coordinates thereafter) were set. The gravitational softening lengths in the second generation MGS are significantly smaller than those in the first generation. This is because of the increased particle number in the second generation. The masses of dark matter and gas particles were set to \(7.8 \times 10^8h^{-1}\text{M}_\odot\) and \(3.1 \times 10^8h^{-1}\text{M}_\odot\) respectively.

We will compare FO to an updated version of the dark matter-only Millennium simulation (DM2; Springel et al. 2005). Both simulations in the second generation used the same set of initial conditions, generated using second order Lagrangian perturbation theory (2LPT; Scoccimarro 1998). In addition, the FO and DM2 simulations

---

*The MGS2-FO simulation described in Hilton et al. (2012) implemented the same physical model, albeit with a smaller simulated volume.*
were carried out using cosmological parameters consistent with the 7 yr WMAP results (WMAP7; Komatsu et al. 2011): $\Omega_m = 0.272$, $\Omega_b = 0.0455$, $h = 0.704$ and $\sigma_8 = 0.81$.

### 3.2.3 Cluster sample

Clusters were identified from the simulated density field using combinations of the friends of friends (FOF; Davis et al. 1985), SUBFIND (Springel et al. 2001) and spherical overdensity (Press & Schechter 1974; Lacey & Cole 1994) algorithms (see Knebe et al. (2011) for a review of halo-finding techniques). In all of the analysis presented here we consider clusters with mass $\mathcal{O}(10^{14}h^{-1}M_\odot)$. These clusters correspond to groups containing $> 10^4$ particles.

In the first generation MGS (GO, PC) and DM1 simulation, clusters were identified using the procedure outlined in Kay et al. (2012). Briefly, the dark matter particles were initially grouped using a FOF algorithm, with dimensionless linking length $b = 0.1$. The linking length parameter was chosen to be smaller than the canonical $b = 0.2$ in order to avoid the so called “over-bridging” problem whereby distinct, neighbouring haloes are linked together (Knebe et al. 2011). Next, the centre of each cluster was identified as the dark matter particle with the most negative gravitational potential energy. Finally the bulk properties of the clusters (mass, radii, etc.) were calculated using the properties of all particles within spherical regions of overdensity $\Delta = \rho(< R_\Delta)/\rho_c(z)$ where $\rho_c(z) = (3H_0^2/8\pi G)E(z)^2$ is the cosmic critical density at redshift $z$ and $E(z)^2 = \Omega_m(1 + z)^3 + \Omega_\Lambda$. Throughout we take $\Delta = 500$, therefore cluster masses are defined

$$M_{500} = 500\frac{4\pi}{3} R_{500}^3 \rho_c(z),$$

where $R_{500}$ is the proper radius of the spherical overdensity. For reasons described in Section 3.3.1 we will consider clusters with $M_{500} = 10^{14} - 10^{14.5}h^{-1}M_\odot$. In the GO, PC and DM1 simulations there are 1016, 800 and 965 clusters respectively, at $z = 0$.

In the second generation MGS (FO) and dark matter-only DM2 simulation, a similar procedure was implemented. First, a FOF algorithm was run with $b = 0.2$. In
order to avoid the over-bridging problem, SUBFIND was used to identify gravitationally bound structures within each FOF group. We then took the centre of the most massive substructure within the FOF groups to be the cluster centre. Finally, the bulk properties were calculated using the spherical overdensity algorithm. At $z = 0$ there are 707 and 830 clusters with $M_{500}$ within the range of interest, for the FO and DM2 models, respectively. The different number of clusters found in DM1 and DM2 is mainly due to the fact that they utilise different cosmological models. While we had access to these particular halo catalogues, the raw particle data of the first generation MGS was not available. As such, we were unable to run the same group finder on all sets of simulations.

It should be noted that since the peak of the density field within a FOF group is considered to be the centre of a cluster in the analysis of both generations, the procedures used here are largely equivalent. The selection criteria in both generations exclude low mass clusters whose centres lie within the $R_{500}$ of more massive clusters, in line with other studies [Tinker et al. 2008].

### 3.2.4 Baryon Fraction

In the simulated clusters we define the baryon fraction

$$f_b = \frac{M_\ast (< R_{500}) + M_{\text{gas}} (< R_{500})}{M_{500}},$$

where $M_\ast$ and $M_{\text{gas}}$ are the masses of stars and gas respectively within $R_{500}$.

The baryon fractions calculated from the clusters in the two generations of MGS are plotted in Fig. 3.1 as a function of cluster mass $M_{500}$. The baryon fraction for the GO and PC clusters, presented in [Young et al. 2011], is also shown in the left-hand panel of Fig. 3.1 (cyan and green curves respectively). We follow [Young et al. 2011] and fit the FO baryon fraction scaling relation to the function

$$\log_{10} f_b = \log_{10} f_0 + s \left[ \mu - \frac{1}{4} \ln (1 + \exp(4\mu)) \right]$$

(3.3)
3: INFLUENCE OF BARYONS ON THE CLUSTER MASS FUNCTION

Figure 3.1: The baryon fraction as a function of $M_{500}$ is shown for both generations of MGS. Results from GO and PC are shown in the left-hand panel (cyan and green, respectively) while results from FO are shown in red in the right-hand panel. The simulated data derived from simulation outputs at $z = 0$ are plotted, where bars indicate the 16th and 84th percentiles of the distribution and the coloured points show the median value within each mass bin. In the left-hand panel, we plot the fits to the simulated data (GO and PC) from Young et al. (2011) and in the right-hand panel we plot the fit computed for the FO simulation. We also plot the low redshift observational bounds of Lin, Mohr & Stanford (2003), Giodini et al. (2009) and Laganá et al. (2011) in the orange, purple and blue regions respectively. In each panel, the cosmic mean, $\Omega_b/\Omega_m$, calculated using the corresponding WMAP1/7 parameters is also shown in black.

where $\mu = \log_{10} (M/M_{\text{piv}})$ is the mass variable scaled by a pivot mass $M_{\text{piv}}$ and $f_0$ and $s$ are two free parameters. The best fitting parameters, for $\log_{10} (M_{\text{piv}} [h^{-1} M_\odot]) = 14.47$, were $f_0 = 0.146 \pm 0.001$ and $s = 0.204 \pm 0.008$. Errors quoted here were calculated using bootstrap resampling, keeping $M_{\text{piv}}$ fixed.

In both panels of Fig. 3.1, we also plot the best fits to the observational data of Lin, Mohr & Stanford (2003), Giodini et al. (2009) and Laganá et al. (2011) along with the associated uncertainties. Estimations of $f_b$ within clusters require knowledge of bulk properties, such as mass and radius, measurements of the intra-cluster gas and observations of the stellar mass distribution. These observations are often made difficult by
the contributions of intra-cluster light and fainter dwarf galaxies.

In non-radiative simulations, such as GO, the baryonic gas distribution within a cluster becomes more extended than the dark matter because it is able to gain energy in halo merger events (Crain et al., 2007). The resulting baryon fraction within $R_{500}$ is therefore slightly reduced relative to the cosmic mean in a manner that is independent of halo mass. As a counterpoint, the baryon fraction in the PC and FO simulations is scale dependent. In the PC case, gas heated within a small halo is more likely to be ejected than gas in a halo with a deeper gravitational potential well. Similarly, the net effect of AGN and supernovae feedback is to eject more baryonic gas from lower mass clusters.

It is clear from Fig. 3.1 that the baryon fraction in $z \simeq 0$ galaxy clusters, both observed and simulated, is less than the cosmic mean $\Omega_m/\Omega_b$ for the mass range plotted. There is excellent agreement between the simulated baryon fraction and the observational bounds plotted in both the PC and FO models. While the baryon fraction within clusters can itself be used as a cosmological probe (Allen, Evrard & Mantz, 2011), here we use it as a test of the validity of the gas physics model employed in our simulations.

The baryonic depletion in the hydrodynamically simulated clusters leads directly to lower values of $M_{500}$ relative to the dark matter-only counterparts. The effect of the depletion on the cluster mass function and subsequent cosmological parameter estimations is the subject of the following section.
Figure 3.2: Top: Differential mass functions plotted from the two generations of MGS. In the left panel the GO and PC results are shown as cyan squares and green diamonds respectively. In the right hand panel the FO and DM2 mass functions are plotted as red circles and black triangles respectively. Also plotted are fits to each cluster population computed by allowing the parameters in equation (3.6) to vary. In each panel the TMF is also shown in solid blue. Lower: Ratio of each mass function best fit with the TMF. Over the range plotted here the mean fit/Tinker values are $\approx 0.82, 0.86$ for the PC and FO mass functions respectively. For a similar comparison of GO and PC (using $\Delta = 200$) see Fig. 4 of Stanek, Rudd & Evrard (2009).

3.3 Results

3.3.1 Cluster Mass Function

As before, we express the halo mass function as the logarithmic derivative of the number density, $n(M_{500})$, with respect to mass

$$\frac{dn}{d \ln M_{500}} = f(\sigma)\bar{\rho}_m(z)\frac{d \ln \sigma^{-1}}{dM_{500}}$$

5We note that the baryon fraction in low mass simulated clusters ($M_{500} \lesssim 10^{14} h^{-1} M_\odot$; not shown) was found to be significantly lower than the cosmic mean ($f_b \approx 0.1$) in agreement with Lin, Mohr & Stanford (2003) and simulations which include AGN feedback (e.g. McCarthy et al. 2011; Planelles et al. 2013).
where the variance of the density field within spheres of radius $R \ [h^{-1} \text{ Mpc}]$,

$$\sigma^2(R, z) = \frac{D^2(z)}{2\pi^2} \int P(k)W^2(kR)k^2\,dk, \quad (3.5)$$

$P(k)$ is the linear matter power spectrum, $D(z)$ is the linear growth factor and $W(x) = 3(\sin x - x \cos x) / x^3$ is the Fourier transform of the real-space top-hat filter. The function $f(\sigma)$ is independent of cosmological parameters by design. Recent studies, (Tinker et al., 2008; Watson et al., 2013), have taken the parameterisation

$$f(\sigma) = A \left[ \left( \frac{\beta \sigma}{\sigma} \right)^\alpha + 1 \right] \exp \left( -\frac{c}{\sigma^2} \right), \quad (3.6)$$

and computing the constants $A, \alpha, \beta, c$ from their respective dark matter-only cosmological simulations for a range of $z$ and $\Delta$.

Fig. 3.2 shows mass functions computed from the cluster distributions in the MGS at $z = 0$, where the mass bins were spaced with $\Delta \ln M_{500} = 0.16$ and the position of each bin was taken to be the mid-point $^6$ We also plot the appropriate TMF in both panels, where $P(k)$ was calculated using the publicly available code CAMB $^7$ (Lewis, Challinor & Lasenby, 2000). It is evident from the right hand panel that the TMF is broadly consistent with the dark matter-only simulation for $14 < \log_{10} (M_{500} [h^{-1} \text{ M}_\odot]) < 14.5$. Above this mass, Poisson noise due to rare objects starts to become significant.

The agreement between the DM1 and DM2 mass functions and the TMF is within the 5 per cent statistical errors of the TMF fitting at the low mass end of the mass function. For confirmation of the agreement between DM1/DM2 and the TMF, see Fig. 3.3.

### 3.3.2 Impact of baryons on mass function

As discussed in Stanek, Rudd & Evrard (2009), the clusters in the PC simulation showed a systematic suppression relative to both the GO clusters and the TMF. We demonstrate this effect again in the left hand panel of Fig. 3.2 for $\Delta = 500$. One can

---

$^6$We have confirmed that the conclusions of this chapter are not sensitive to either taking the bin mid-point, rather than the mean or median, nor the logarithmic width of the bins.

$^7$http://camb.info
also see from the right hand panel of Fig. 3.2 that the mass function computed from FO is also offset from both the data of DM2 and the TMF.

We note that there is agreement between the GO mass function and the TMF. In this model the mass independent baryonic depletion, detailed in Section 3.2.4, is sufficiently mild that the expected underlying dark matter-only (DM1) mass function is recovered. In both the PC and FO mass functions, the larger relative offset is a consequence of the lower, mass dependent, cluster baryon fraction resulting from gas ejection processes.

One can parameterise the deviation from the TMF by generalising the mass bias parameter described in Section 3.1 to include the effects of baryon depletion. Since we know the true masses of our simulated clusters, we will ignore the complexities of hydrostatic bias in cluster observations. Instead, we define the baryonic depletion bias
\[ b_{\text{dep}} = 1 - \frac{M_{\text{DM}}}{M_{\text{hyd}}}, \]
where \( M_{\text{DM}} \) and \( M_{\text{hyd}} \) are the masses of a cluster in dark matter-only and hydrodynamic simulations, respectively. We found that rescaling the mass variable, \( M_{500} \), in the DM2 mass function at \( z = 0 \) (\( z = 0.17 \)) by \( 1 - b_{\text{dep}} = 0.9 \) (0.93) brought the FO and DM2 curves into closer agreement. We note however, a noticeable difference in shape between the FO and adjusted DM2 mass functions was evident. While the zeroth-order effect of the baryons on the mass function is to shift it relative to the dark matter-only mass function by 10 per cent (7 per cent), we argue that it is insufficient for precision cosmology. Further, arguments of this type do not account for changes in \( R_{500} \) in a consistent manner.

We will return to the problem of baryonic influence on the mass function in Section 3.3.4 and discuss the effect of back-reaction of baryons on the dark matter. It will be shown that the primary reason for the change in mass is ejection of baryons from clusters.
Figure 3.3: Likelihood contours computed from the simulated cluster mass functions at $z = 0$ (top) and $z = 0.17$ (lower) assuming the TMF (see Fig. 3.2). In the top-left panel, cyan contours were computed using the GO mass function and the green contours were calculated using the results of the PC simulation. Similarly in the top-right and lower panels, the DM2 and FO likelihood contours are shown in black and red respectively. Also shown are the lines of best fit describing the degeneracy between $\Omega_m$ and $\sigma_8$ for each generation. In order to directly evaluate the shift in the degeneracy we enforce the PC and GO power-law indices to be that of the DM1 and the FO power-law index to be that of the DM2. The points of maximum likelihood are shown as coloured dots. The discrepancy between the PC and FO distributions and the fiducial values of $\Omega_m$ and $\sigma_8$ (indicated by the blue dashed lines) is the key result of our investigations.
3: INFLUENCE OF BARYONS ON THE CLUSTER MASS FUNCTION

3.3.3 Consequences for Cosmology

As outlined in the introductory section, the primary function of the TMF is to link measurements of the halo mass function to the \( \Omega_m \) and \( \sigma_8 \) parameters of the underlying cosmology. By using the TMF to constrain cosmology from galaxy cluster measurements it is assumed that the gas content of clusters traces the dark matter component. Given that we have demonstrated that simulating the baryonic content within clusters suppresses cluster abundance at fixed mass relative to the dark matter-only result (particularly in the PC and FO cases), we now investigate the impact of this result on estimations of cosmological parameters.

We use the simulated cluster mass functions described in the previous sections (see Fig 3.2) as our mock data. Taking the TMF as our assumed model, we computed likelihood distributions for each of the simulated populations on a regular grid.

At each point in \( \Omega_m, \sigma_8 \) space the Cash statistic (Cash, 1979)

\[
C = -2 \sum_{k=1}^{N_{\text{tot}}} \ln \mathcal{P}(N_k|n_k)
\]

\[
= -2 \sum_{k=1}^{N_{\text{tot}}} \left( N_k \ln(n_k) - n_k - \ln(N_k!) \right),
\]

was calculated, where \( \mathcal{P}(N_k|n_k) \) is the probability of finding \( N_k \) clusters in a bin given a number \( n_k \) predicted by the model. We then used the fact that \( \Delta C \) is distributed as \( \Delta \chi^2 \) with two degrees of freedom (Press et al., 1992).

As in Section 3.3.1, we used CAMB to calculate \( P(k) \) and hence the model \( dn/d \ln M_{500} \) through equation (3.4). Throughout we assumed the values of other cosmological parameters were known since they do not contribute significantly to the variance in the mass function measurement (Murray, Power & Robotham, 2013b).

The likelihood contours calculated using the MGS clusters are shown in Fig. 3.3. As before, in this analysis we conservatively used clusters with \( 14 < \log_{10} (M_{500}[h^{-1}M_\odot]) < 14.5 \). We show the earlier epoch since it is the median \( z \) of the 2013 Planck SZ high S/N catalogue (Planck Collaboration et al., 2014a). The lines of degeneracy between \( \sigma_8 \) and \( \Omega_m \) are also shown in Fig. 3.3.

Simulations with Modified Gravity
In the upper panel of Fig. 3.3 the offset between the GO and PC likelihood contours is clear. While the peak of the $z = 0$ PC distribution is offset along the degeneracy, the movement of the degeneracy itself is the crucial characteristic.

The likelihood distribution contours resulting from the FO and DM2 mass functions are shown in right hand panel of Fig. 3.3. The change in the FO/DM2 power-law indices of the degeneracy between the top-right and bottom panels is due to the redshift dependence of the mass function. As the mass function evolves with redshift, it enables one, in principle, to break the $\Omega_m - \sigma_8$ degeneracy with multi-redshift observations. The FO contours are clearly shifted relative to the dark matter-only simulation at both epochs. We quantify this shift as $\Delta [\sigma_8 (\Omega_m/0.27)^{\gamma_z}] = \Delta B_z$, where $\gamma_z$ and $\Delta B_z$ are constants, by fitting a power-law relation to the likelihood contours. Over the redshifts of interest ($z = 0 \rightarrow 0.17$) $\gamma_z$ varies from 0.52 to 0.38 whereas $\Delta B_z$ remains $\simeq -0.03$. The discrepancy between the Planck CMB and cluster count measurements can be described as $\Delta [\sigma_8 (\Omega_m/0.27)^{0.3}] \simeq -0.08$. It should be noted that the widths of the error contours (but crucially not the offset $\Delta B_z$) in Fig. 3.3 reflect the size of the simulation volume (and hence the number of clusters) rather than any particular observational survey. Though we urge caution when comparing simulated snapshots and observations, our calculations demonstrate that the effects of baryonic depletion in clusters is non-negligible in this context.

### 3.3.4 Model Independent Correction

As we have demonstrated in the previous sections, the mass of a given cluster in a hydrodynamic simulation is not equal to the mass of the same object in a dark matter-only simulation. In the previous section we attributed this to baryonic depletion in clusters. Since dark matter-only simulations do not capture this behaviour there is an implicit assumption that $f_b = \Omega_b/omm$. We now outline and test a method for “correcting” a baryon influenced cluster mass function in order to enable one to use the TMF (or similar) for cosmological parameter determinations.
Figure 3.4: Distributions of mass ratios, $y = M_{500}/M_{DM1/2}$, where $M_{500}$ is the total mass of a cluster (dark matter and baryonic matter within $R_{500}$) in the hydrodynamical simulation (GO, PC and FO are shown in cyan, green and red respectively) and $M_{DM1/2}$ is the mass of the same cluster in the appropriate dark matter-only simulation. We also plot the ratio of the cluster masses after correcting the hydrodynamical mass as outlined in Section 3.3.4. In the FO model, the correction is near exact by construction; the ±0.006 scatter about $y = 1.001$ is due to numerical error in recomputing $R_{500}$ from the $M_{\text{est}}(< r)$ profile rather than the particle distribution. In the GO and PC models, where baryons can influence the dark matter density profile, the corrected halo masses do not exactly match the cluster masses in DM1.
Our proposed three-step methodology is as follows:

- Calculate the dark matter mass profile of each cluster, $M(<r)$, using knowledge of the total density profile and removing the stellar and gas components;

- Supplement the dark matter mass with baryons such that the baryon fraction is equal to the cosmic value everywhere in the cluster, i.e. estimate the mass profile $M_{\text{est}}(<r) = M_{\text{DM}}(<r)/(1 - \Omega_b/\Omega_m)$;

- Recalculate $R_{500}$ and $M_{\text{est,500}}$ using the new mass profile.

Observationally, it is too expensive to calculate the dark matter mass profile of every cluster in a survey. This would require, for example, high quality X-ray data allowing the estimation of total density and temperature profiles, or weak lensing data with sufficiently high density of background sources. Additionally, the mass distribution of gas (using X-ray data) and stars (including any additional diffuse component) would also be required. In practice, a mass-observable relation (ideally with minimal scatter) is calibrated for a smaller number of clusters and the observable used as a mass proxy for the full sample (e.g. Arnaud, Pointecouteau & Pratt [2007]). The practice of mass proxy calibration is common to all cluster surveys including the Planck analysis (Planck Collaboration et al., 2014c). In this case, the simple procedure outlined above could be applied to re-calibrate the mass-observable relation for cosmological purposes (we leave feasibility of such a procedure to future study).

The advantage of this procedure (rather than attempting to correct the theoretical mass function) is that it is empirical, relying on only the observational data and not assuming any theoretical model for how the baryons affect the total cluster mass. However, it does assume that the baryonic processes do not significantly influence the underlying dark matter mass profile of clusters.

We test our methodology using the clusters in the GO, PC and FO simulations. In Fig. 3.4 we plot the ratio of the mass of individual clusters in the hydrodynamical simulations and the dark matter-only simulations. We also plot the same mass ratio
after the correction procedure was applied to the hydrodynamic cluster masses. The halo structures in PC were matched with their DM1 counterparts by considering the dark matter-only haloes within $0.5R_{500}$ of the cluster centre. A match was found for around 98 per cent of the PC clusters. In the FO case, each cluster was mapped directly to the equivalent DM2 halo using the data from the SUBFIND analysis of the dark matter distribution. In the absence of baryon-dark matter back-reaction, we expect the corrected distributions to be centred at unity.

In the FO simulation, the dark matter particles are not gravitationally influenced by the baryons and so no back-reaction is possible (Short, Thomas & Young, 2013). This fact is demonstrated by the purple distribution in the right hand panel of Fig. 3.4 being centred around unity. The small amount of scatter is due to the error in calculating $M_{500}$ from cluster profiles rather than the actual particles themselves. As a further test of our method, we confirm in the right hand panel of Fig. 3.5 that the corrected FO mass function reproduces the DM2 mass function.

The GO and PC implementations, on the other hand, do evolve the dark matter and gas consistently. As shown in the upper-left and upper-right panels of Fig. 3.4, the median mass ratios for the GO and PC clusters are $1.046 (\sigma_{GO} = +0.039_{-0.052})$ and $0.949 (\sigma_{PC} = +0.048_{-0.045})$ respectively; whereas after correction procedure the median values are $1.020$ and $1.053$ with scatter $\sigma_{GO} = +0.033_{-0.048}$ and $\sigma_{PC} = +0.047_{-0.054}$. The quoted values of scatter were calculated from the 16th and 84th percentiles of the distributions. The fact that the corrected distributions are not centred on unity with minimal scatter is a reflection of the baryon-dark matter back-reaction. This irreducible effect is the central limitation of our method. Without a greater understanding of the effects of baryons on the gravitational potential, the procedure may be unable to recover the abundance of clusters to within around 5 per cent.

In Fig. 3.5, we compute likelihood contours from the GO, PC and FO mass functions before and after applying the above correction procedure. Note that because of

---

8 We also checked that at lower overdensity ($\Delta = 200$), the difference between DM1 and GO masses was smaller than at $\Delta = 500$. 

Simulations with Modified Gravity
3.3: RESULTS

Figure 3.5: Likelihood contours calculated from $z = 0$ mass functions in the same manner as those in Fig. 3.3. “Corrected” distributions were derived from the cluster mass function after applying the procedure to each cluster. As before, the results from the GO, PC and FO simulations are shown in cyan, green and red respectively. The likelihood distributions calculated using the corrected mass functions are shown in purple. Additionally, the distributions obtained using the DM1/ DM2 simulations are shown in black. The power-law index of the fitting is fixed to the value of the dark matter-only degeneracy

the mass limit made on the PC cluster catalogue and the fact that the correction invariably increased the mass of clusters, we only consider clusters with $\log_{10} \left( \frac{M_{500}}{h^{-1}M_{\odot}} \right) > 14.1$. This additional condition decreases the number of clusters in the mass function and therefore increases the width of the contours shown in the left hand panel of Fig. 3.5 as well as moving the contours along the $\sigma_8 - \Omega_m$ degeneracy. In the lower
panel of Fig. [3.5] the corrected FO contours map almost directly on to the DM2 contours. This excellent agreement is due to the fact that, in the FO model, baryons do not influence the dark matter mass profile: scaling the dark matter mass profile by \((1 - \Omega_b/\Omega_m)^{-1}\) recovers the DM2 mass distribution by design.

As expected from the offset in the GO/DM1 and PC/DM1 cluster mass ratio distributions shown in Fig. [3.4] the contours from the corrected mass functions do not match the DM1 contours. In fact, the correction procedure does not appear to improve agreement between the GO/PC contours and the DM1. The fact that the input cosmology is not recovered by this correction procedure is a demonstration that the baryons do have a significant influence on the shape of the dark matter mass profile in these models.

### 3.4 Discussion and Conclusions

In this chapter, we have discussed the impact that baryonic physics can have on the observed cluster mass function. Although further study is required in order to fully model the gas physics in clusters, we have shown that the baryon fraction measured in MGS is broadly consistent with observations. We argue that since the baryon fraction is similar to that observed in other simulated clusters (Sembolini et al., 2013; Planelles et al., 2013), the suppression in the mass function shown in Fig. [3.2] is generic to realistic baryonic treatments.

In contrast to our findings, a \(\sim 7\) per cent overabundance of clusters relative to dark matter only haloes was reported by Cui et al. (2012). In their simulations efficient radiative cooling of gas ensures that the hydrodynamically simulated clusters are more concentrated than their dark matter-only counterparts and therefore have larger values of \(M_{500}\). We reason that the lack of AGN feedback or early heating in their simulations allowed clusters to retain their baryon content and thereby allowed the mass of a given cluster to increase relative to its dark matter-only counterpart. Due to the functional form of the halo mass function, a shift in mass of this nature would result in an increase in the number of clusters of a fixed mass.
3.4: DISCUSSION AND CONCLUSIONS

We have shown that assuming the TMF leads to an incorrect measurement of the \(\sigma_8 - \Omega_m\) degeneracy by \(\Delta [\sigma_8 (\Omega_m/0.27)^{0.38}] \simeq -0.03\) at \(z = 0.17\) when considering realistic clusters with \(14 < \log_{10} (M_{500} [h^{-1} M_\odot]) < 14.5\). The discrepancy we describe here is not specific to the TMF. We confirmed that using the Watson et al. (2013) fit as the assumed model, instead of the TMF, produced a similar offset between the derived dark matter-only and hydrodynamic likelihood distributions.

The analysis of Balaguera-Antolínez & Porciani (2013) came to similar conclusions as presented in this work, though through different means. In that study, predictions regarding the observed mass function were made using the TMF and assuming the form of \(f_b(M_{500})\) from Laganá et al. (2011). By creating mock catalogues, the above authors showed a systematic shift of the similar order and sense as that shown in Fig 3.3. Recently however, Martizzi et al. (2014) extended the Balaguera-Antolínez & Porciani methodology using the \(f_b - M_{500}\) relation derived from their set of high resolution cluster resimulations. They concluded that the mass function should be boosted by the effects of baryonic physics because, in contrast with the observational data shown in Fig. 3.1, the baryon fraction they use is higher than the cosmic mean over the mass range. Our investigations differ from the above methodology in that we make no assumption regarding the functional form of the cosmic mass function or the \(f_b - M_{500}\) relation at the run-time of our simulations. Further, we have shown the \(\Omega_m - \sigma_8\) degeneracy offset is present in two very physically distinct scenarios (PC and FO).

In future Planck analyses, where lower mass clusters are studied, the influence of baryonic physics on cluster masses will have to be considered and accounted for. Further, our calculations are applicable to any cosmological survey with clusters of mass \(\lesssim 10^{14.5} h^{-1} M_\odot\) (particularly XCS) and provide qualitative information on what might happen at larger masses, although we leave this for future investigations.

In our final section, we proposed and tested a model-independent procedure designed to recover the results of dark matter-only simulations from measurements of clusters with baryonic effects. The correction procedure was demonstrated to work...
well in the case where baryon-dark matter gravitational interaction was neglected (FO model). However in simulations in which baryons significantly contribute to the gravitational potential (GO/PC), the procedure was deemed to be insufficient. We conclude that further modelling of baryonic physics in clusters is required in order to ensure that future cluster surveys are able to make unbiased constraints on cosmological parameters.

Subsequent to the publication of this work there have been multiple studies (Cui, Borgani & Murante, 2014; Velliscig et al., 2014; Bocquet et al., 2015) which have drawn, broadly, the same conclusions using their own hydrodynamical simulations.
Chapter 4

Simulating $f(R)$ Gravity

4.1 Introduction

In this chapter we outline the methodology used to solve the equations of motion in $f(R)$ gravity. Firstly, in Section 4.2 we calculate the background expansion history of the HS model. We derive the equations of motion for $f(R)$ gravity under the quasi-static approximation in Section 4.3. We will then describe the approximations that are often made to the models in Section 4.4. In Section 4.5 we describe in detail the multigrid methods we use to solve the $f(R)$ equations in our $N$-body simulations. Finally, in Section 4.6 we show a number of tests of our implementation.

4.2 Background Expansion History

We calculate the background expansion history of $f(R)$ gravity models using the method of Hu & Sawicki (2007). In this calculation, the modified Friedmann equation (1.53),

$$H^2 - f_R (H H' + H^2) + \frac{1}{6} f + H^2 f_{RR} R' = \frac{8\pi G}{3} \bar{\rho}_{m,0} e^{-3N},$$

(4.1)

and the background Ricci scalar,

$$R = 12H^2 + 6HH',$$

(4.2)
Figure 4.1: Effective equation of state for \( |\bar{f}_{R0}| = 10^{-1}, 10^{-2} \) and \( 10^{-3} \) is shown in red, blue and green respectively. As expected, as \( |\bar{f}_{R0}| \) increases the deviations from \( w = -1 \) increase also.

are solved for \( H(a) \) and \( R(a) \). In (4.1) and (4.2) the primes denote derivatives with respect to \( N = \ln(a) \). We recast the above equations using the variables

\[
y_H = \frac{H^2}{\Omega_m H_0^2} - a^{-3} \tag{4.3}
\]

and

\[
y_R = \frac{R}{\Omega_m H_0^2} - 3a^{-3}. \tag{4.4}
\]

These new variables are chosen so that they both tend to zero at high redshift. After this change of variables, the dynamical equations are

\[
y_H' = \frac{1}{3} - 4y_H \tag{4.5}
\]

and

\[
y_R' = 9a^{-3} - \frac{1}{y_H + a^{-3}} \frac{1}{f_{RR}\Omega_m H_0^2} \left[ y_H - f_R \left( \frac{1}{6} y_R - y_H - \frac{1}{2} a^{-3} \right) + \frac{1}{6} \Omega_m H_0^2 \right]. \tag{4.6}
\]
Note that these are coupled first order ODEs with variable coefficients. In these variables, the effective equation of state for the model is given by

\[ 1 + w_{\text{eff}} = -\frac{1}{3} \frac{y_H'}{y_H}. \]  

(4.7)

We solve (4.5) and (4.6) numerically using the VODE package (Brown, Byrne & Hindmarsh 1989). This library was chosen as it is able to correctly calculate the solution of numerically stiff ODEs. The calculations were started with \( z_{\text{init}} = 99 \) and \( y_H = y_R = 0 \). The results for \( |\bar{f}_{R0}| = 0.1, 0.01 \) and \( 10^{-3} \) are shown in Fig. 4.1.

We note that the results of \( |\bar{f}_{R0}| = 10^{-1} \) and \( 10^{-2} \) match those published in Hu & Sawicki (2007). In addition, we further validated our implementation by reproducing the \( w_{\text{eff}}(a) \) for the Appleby & Battye (2007) model as shown in Appleby, Battye & Starobinsky (2010).

From Fig. 4.1 we can see that decreasing the value of \( |\bar{f}_{R0}| \) from 0.1 to \( 10^{-3} \) reduces the amplitude of the deviations from \( w = -1 \). This is expected since models with larger \( |\bar{f}_{R0}| \) correspond to “stronger” modified gravity models. In the \( |\bar{f}_{R0}| = 10^{-3} \) case the maximum deviations from \( w = -1 \) are \( w_{\text{eff}} = -0.997 \) at \( z \approx 0.3 \) and \( w_{\text{eff}} = -1.001 \) at \( z \approx 4 \). For the HS model with \( |\bar{f}_{R0}| = 10^{-4} \) and \( n = 1 \), the deviations from \( w = -1 \) are within 0.03 per cent. Decreasing the value of \( |\bar{f}_{R0}| \) or increasing the value of \( n \) reduces the discrepancies further. We conclude that the background expansion history is practically indistinguishable from the \( \Lambda \)CDM result for \( |f_{R0}| \leq 10^{-4} \). For the remainder of this thesis we will assume a \( \Lambda \)CDM background expansion history when using the HS model with \( |f_{R0}| \leq 10^{-4} \).

### 4.3 Equations of Motion

In this section we will derive the equations of motion for \( f(R) \) gravity (Hu & Sawicki 2007; although see Arnold, Puchwein & Springel 2014; Bose, Hellwing & Li 2015 for more in depth derivations) under the quasi-static approximation (Noller, von Braun-Bates & Ferreira 2014). We will do this, as we did for \( \Lambda \)CDM, via linear perturbation
Simulating $F(R)$ Gravity

theory (Bean et al., 2007; Pogosian & Silvestri, 2008). We will use the same conventions when writing the metric perturbations and other geometric quantities as we did previously in Chapter 1.

### 4.3.1 Quasi-Static Approximation

In the literature, the quasi-static approximation is the term used to describe two separate assumptions regarding perturbed quantities $X = \{\Phi, \Psi, f_R, f'_R, \delta f_R, \delta f'_R\}$. These assumptions are often made when studying scalar-tensor theories of modified gravity such as $f(R)$ gravity. In particular:

1. We only consider sub-horizon modes ($k \gg H$). In the spatial domain this means that $|\nabla^2 X| \gg H^2 |X|$

2. Spatial derivatives of metric perturbations dominate over temporal derivatives: $|\dot{X}| \leq H |X|$.

Note that we previously assumed the first condition in the derivation of the GR Poisson equation (1.34).

We will see that adopting the above assumptions simplifies the solution of the equations of motion. The quasi-static approximation also removes high frequency oscillatory features in the perturbed quantities. It has been estimated (Brax et al., 2013) that running a simulation with small enough time steps to capture the oscillations would require a factor of $O(10^7)$ longer runtime. The oscillations are also highly constrained since these are generally associated with particle production.

It is obviously important that we ensure that by making the quasi-static approximation we are not removing important features from the dynamics of the model. There has been recent work attempting to establish if excluding explicit time derivatives from the evolution equations changes any of the structures formed. Llinares & Mota (2013) found that in a time varying symmetron model they were able to identify domain wall structures in the scalar field. Later work on the same model (Llinares & Mota, 2014)
found that the effect of including explicitly time varying terms on the matter power spectrum was about 0.2 per cent for \( k < 10 \, h^{-1} \text{Mpc} \) (although the authors note that domain walls can cause changes in the locally measured power spectrum). For \( f(R) \) models [Bose, Hellwing & Li (2015)] showed that including explicit time derivatives made no significant change to the matter power spectrum (after accounting for resolution issues).

### 4.3.2 \( f(R) \) Trace Equation

The \( f(R) \) trace equation

\[
\Box f_R = \frac{1}{3} \left( R + 2f - f_R R - 8\pi G \rho_m \right)
\]  

(4.8)

derived pervously in Section 1.4.1 describes the dynamics of the scalar field \( f_R \). Taking the lefthand side term, one can show that

\[
\Box f_R = g^{\mu\nu} \nabla_\mu \nabla_\nu f_R
\]

\[
= (-1 + 2\Psi) \ddot{f}_R + \frac{1}{a^2} (1 - 2\Phi) \partial_i \partial_i f_R
\]

\[
+ \left( 3H (-1 + 2\Psi + \dot{\Psi} - 3\Phi) \dot{f}_R + \frac{1}{a^2} \partial_i f_R \partial_i \Phi \right)
\]  

(4.9)

where we only retain zeroth and first order terms in \( \Phi \) and \( \Psi \). At the background level the \( \bar{f}_R \) field follows

\[
\ddot{\bar{f}}_R + 3H \dot{\bar{f}}_R = \frac{1}{3} \left( 8\pi G \bar{\rho}_m + \bar{f}_R \bar{R} - \bar{R} - 2f(\bar{R}) \right).
\]  

(4.10)

In principle it is possible to follow the dynamics of (4.10). Given that we will be assuming the quasi-static approximation throughout this thesis, we will neglect the time varying terms and assume that \( \Box \bar{f}_R = 0 \).

At the perturbative level the dynamics of the scalar field are more interesting. Taking the variation of the trace equation gives

\[
\delta (\Box f_R) = \frac{1}{3} \left( \delta R + 2\delta f - \delta f_R R - f_R \delta R - 8\pi G \delta \rho \right)
\]

\[
= \frac{1}{3} \left( \delta R (1 + f_R) - \delta f_R R - 8\pi G \delta \rho \right)
\]  

(4.11)
where we have approximated $\delta f \approx f_R \delta R$. There are two terms in (4.11) that can be neglected in the case where $f_R$ is small. Firstly, $1 + f_R \approx 1$ for all the models we consider. Secondly, perturbations in the scalar field are small therefore the $\delta f_R R$ term is negligible compared to the $\delta R$ and matter terms.

Ignoring explicitly time varying terms in (4.9), one can see that $\delta (\Box f_R) = \nabla^2 f_R$ where $\nabla^2$ is the Laplacian operator in physical space. Combining this with (4.11) gives the truncated trace equation
\[
\nabla^2 f_R = \frac{1}{3c^2} (\delta R - 8\pi G \delta \rho)
\] (4.12)
where we have restored factors of the speed of light. The process of solving (4.12) will be outlined in Section 4.5.

### 4.3.3 $f(R)$ Poisson Equation

We can derive the $f(R)$ Poisson equation from the time-time component of the $f(R)$ field equations
\[
(1 + f_R) R_{00} + \frac{1}{2} (R + f) (1 + 2\Psi) - (1 + 2\Psi) \nabla^2 f_R = 8\pi G \rho.
\] (4.13)
where the explicitly time varying terms have been dropped. In the weak field limit ($|\Psi| \ll 1$ and $|f_R| \ll 1$) this becomes
\[
R_{00} + \frac{1}{2} (R + f) - \nabla^2 f_R = 8\pi G \rho.
\] (4.14)
After subtracting the background we have
\[
\delta R_{00} = \nabla^2 f_R - \delta R + 8\pi G \delta \rho
\] (4.15)
where we again assume that $\nabla^2 f_R = 0$ and $|\delta f| \approx |f_R \delta R| \ll |\delta R|$. In the Newtonian gauge
\[
\delta R_{00} = \frac{1}{a^2} \partial^i \partial_i \Psi + 3H (\dot{\Psi} - 2\dot{\Phi}) - 3\ddot{\Phi}
\approx \nabla^2 \Psi
\] (4.16)
where the quasi-static approximation has been made in the second line. Equating (4.15) and (4.16) one can show that

$$\nabla^2 \Psi = \frac{16\pi G}{3} \delta \rho - \frac{1}{6} \delta R(f_R).$$  \hspace{1cm} (4.17)

Before moving on it is worth examining the limiting cases of (4.17). In the limit of small curvature perturbation, usually a region of low matter density, the Poisson equation gives

$$\nabla^2 \Psi = \frac{4}{3} (4\pi G) \delta \rho$$

or to express it another way

$$\nabla^2 \Psi = 4\pi G_{\text{eff}} \delta \rho$$  \hspace{1cm} (4.18)

where $G_{\text{eff}} = \frac{4}{3} G$.

In the limit of high curvature perturbation, such as a region of high matter density, the chameleon mechanism ensures that the equations of motion become indistinguishable from GR. In this case the Ricci scalar perturbation returns to the GR limit

$$\delta R_{\text{GR}} = 8\pi G \delta \rho$$  \hspace{1cm} (4.19)

and $G_{\text{eff}}/G = 1$.

### 4.4 Approximate Models

In the literature it is common practice to approximate the form of $f(R)$. Doing so makes the $f_R(R)$ function invertible, enabling one to compute $R(f_R)$.

Before discussing particular models it is worth examining the range of $R$ over which the model must be well defined. We first consider a hypothetical void-like region with low matter density ($\rho \sim 0$ so $\delta \rho \sim -\bar{\rho}$). In the extreme case where the void is large enough that the field is near homogeneous in the centre then $\nabla^2 f_R \sim 0$. In this case we can show from (4.12) that $R \sim 12 (1 - \Omega_m) H_0^2$ if the background expansion history is approximately that of $\Lambda$CDM. Strictly speaking there is no limit on the maximum curvature in an $f(R)$ universe. We conclude that we must define our $f_R(R)$ function over the range

$$4\Lambda \leq R < \infty.$$  \hspace{1cm} (4.20)
4.4.1 HS Model

The Hu & Sawicki (2007) model is the most commonly simulated form of \( f(R) \). There are two separate assumptions that are made with this model, the first regarding the functional form and the second regarding the background expansion history.

In the high \( R \) limit the model can be written as

\[
  f_R(R) = \tilde{f}_{R0} \left( \frac{\bar{R}_0}{R} \right)^{n+1}
\]

(4.21)

where \( \tilde{f}_{R0} \) is the background value of \( \tilde{f}_R \) at the current time, i.e. \( \tilde{f}_{R0} = \tilde{f}_R(\bar{R}_0) \). It is
common to assume that the HS model follows (4.21) for all $R$.

In addition to this assumption, it is common to assume that the background expansion history of the model follows that of $\Lambda$CDM. As shown in Section 4.2, this is well justified for $|\bar{f}_{R0}| < 10^{-4}$. In this case the background Ricci scalar evolves according to

$$\bar{R}(a) = 3\Omega_m H_0^2 \left( a^{-3} + 4 \frac{1 - \Omega_m}{\Omega_m} \right)$$  \hspace{1cm} (4.22)

where it is assumed that relativistic matter components of the energy density are negligible.

If we assume that the power-law form, (4.21), holds for all regimes of interest we can write the background value of $f_R$ as

$$\bar{f}_R(a) = \bar{f}_{R0} \left( \frac{1 + \frac{1 - \Omega_m}{\Omega_m}}{a^{-3} + 4 \frac{1 - \Omega_m}{\Omega_m}} \right)^{n+1}$$  \hspace{1cm} (4.23)

and the perturbation of the Ricci scalar as

$$\delta R = \bar{R}(a) \left[ \left( \frac{\bar{f}_R(a)}{f_R} \right)^{\frac{1}{n+1}} - 1 \right].$$  \hspace{1cm} (4.24)

See Fig: 4.2 for the level of agreement between the full form of the model and the power-law approximation.

### 4.4.2 Designer Model

In the designer model (Song, Hu & Sawicki, 2007; Pogosian & Silvestri, 2008) the expansion history is exactly that of a $\Lambda$CDM universe. The exact form of $f(R)$ in the designer model is that of a hypergeometric function (see Eq. 1.69). In the literature there are three different approximations for the form of $f_R(R)$.

The simplest approximation one could make is to approximate $f_R$ as a power-law in $R$ (He, Li & Jing, 2013),

$$f_R(R) = D \left( \frac{3\Omega_m H_0^2}{R} \right)^{p_+},$$  \hspace{1cm} (4.25)
Figure 4.3: Top: The approximate forms of $R(f_R)$ proposed to emulate the designer model. In this plot we take $\Omega_m = 0.316$ and $\bar{f}_{R0} = -10^{-5}$ We have also scaled $R$ by $4\Lambda$ so it is clear where the models deviate from the exact function (shown in black). The blue, magenta and red lines correspond to the approximate forms studied by [He, Li & Jing (2013), He et al. (2014) and [He, Li & Hawken (2015)] respectively. Bottom: The fractional error in $R$ relative to the exact form. It is clear that the [He, Li & Jing (2013)] model fails to reproduce the exact solution in low curvature regimes. The other two models are significantly better at reproducing the exact function in low curvature regimes.

where $D$ is a constant that determines the normalisation ($\bar{f}_{R0}$) of the model and $p_+ = (5 + \sqrt{73})/12$. While this makes the model easily invertible it does significantly differ from the exact model at low curvature. [He et al. (2014)] improved upon this approximation by considering a broken power-law

$$f_R(R) = D \left( \frac{3\Omega_m H_0^2}{R - 12\alpha (1 - \Omega_m) H_0^2} \right)^{p_+}$$

where $\alpha$ is a parameter that is to be fit for before the simulation is run. For $\Omega_m = 0.316$
the value $\alpha = 0.9436$ is recommended (He et al., 2014). He, Li & Hawken (2015) further improved the accuracy of the approximate model by introducing an exponential correction

$$R(f_R) = 12\alpha (1 - \Omega_m) H_0^2 + 3\Omega_m H_0^2 \left[ \left( \frac{D}{f_R} \right)^{\frac{1}{\eta}} - \eta \exp \left( - \left( \frac{f_R}{D} \right)^{\alpha} \right) \right]$$ (4.27)

where $\eta = 1.3038$ and $\alpha = 0.3733$ for $\Omega_m = 0.316$. While this form is closer in relation to the true form of $R(f_R)$, it is not readily invertible and the authors do not state how they compute $f_R(R)$ from (4.27).

The above models are catalogued in Table 4.1. The agreement between each of the three approximations and the true form of the model is shown in Fig. 4.3. One can see that power-law approximation is a substantially worse approximation than the other two. He et al. (2014) found that the minimum value of $\beta = R/4\Lambda - 1$ in their simulations was $\sim 3.4 \times 10^{-2}$ and they concluded that their model was sufficient for their purposes. The effect that making these approximations have on the matter power spectrum will be discussed in Section 5.3.
<table>
<thead>
<tr>
<th>Name</th>
<th>$R(u_{i,j,k})$</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power-law</td>
<td>$\tilde{R}(a) e^{-u_{i,j,k}/(n+1)}$</td>
<td>Oyaizu (2008)</td>
</tr>
<tr>
<td>Spline</td>
<td>$\exp (\log R_{\text{spline}})$</td>
<td>This Work</td>
</tr>
<tr>
<td>He-13</td>
<td>$3\Omega_m H_0^2 \left( \frac{D}{f_{R(a)}} \right)^{\frac{1}{p+}} \exp \left( -\frac{u_{i,j,k}}{p+} \right)$</td>
<td>He, Li &amp; Jing (2013)</td>
</tr>
<tr>
<td>He-14</td>
<td>$12\alpha (1 - \Omega_m) H_0^2 + 3\Omega_m H_0^2 \left( \frac{D}{f_{R(a)}} \right)^{\frac{1}{p+}} \exp \left( -\frac{u_{i,j,k}}{p+} \right)$</td>
<td>He et al. (2014)</td>
</tr>
<tr>
<td>He-15</td>
<td>$12\alpha (1 - \Omega_m) H_0^2 + 3\Omega_m H_0^2 \left[ \left( \frac{D}{f_{R(a)}} \right)^{\frac{1}{p+}} \exp \left( -\frac{u_{i,j,k}}{p+} \right) - \eta \exp \left( -\left( \frac{f_{R(a)}}{D} \right)^{\alpha} \exp (\alpha u_{i,j,k}) \right) \right]$</td>
<td>He, Li &amp; Hawken (2015)</td>
</tr>
</tbody>
</table>

Table 4.1: Form of $R$ term used in each of the simulations. In the Power-law model, $n$ is the power-law index. In the He models $\eta$ and $\alpha$ are constants determined by the value of $\Omega_m$ whereas $D$ is only dependent on the value of $f_{R0}$. 
4.5 Numerical Methodology

In this section we describe the numerical methods we use to simulate $f(R)$ gravity in the non-linear regime. In particular we solve (4.12) on a regular grid using a multigrid algorithm before solving the modified Poisson equation, (4.17), for the potential via the PM algorithm (Oyaizu, 2008). This procedure has been implemented in the MPI parallel GADGET-2 code. We name our implementation MIRAGE (ModifIed gRavity gAdGEt).

Similar codes have previously been presented in the literature. The first $N$-body simulations of $f(R)$ gravity were conducted by Oyaizu (2008). In this early work the dynamics were solved on a regular grid and the code was parallelised using OpenMP. Later work by Zhao, Li & Koyama (2011) used AMR techniques to achieve increased force resolution in their simulations. This code was limited to serial processing since it was based on the MLAPM (Knebe, Green & Binney, 2001) $N$-body code.

The most recent codes presented in the literature are MPI parallel and are adaptive in spatial resolution. ECOSMOG (Li et al., 2012) is based on the RAMSES (Teyssier, 2002) $N$-body code and is the successor of the Zhao, Li & Koyama (2011) code. Puchwein, Baldi & Springel (2013) presented the MG-GADGET code, a modified gravity version of the GADGET-3 code (itself an update of GADGET-2). In order to solve the $f(R)$ equations of motion the MG-GADGET code uses a modified version of the TreePM algorithm. The most recent modified gravity $N$-body code is ISIS (Llinares, Mota & Winther, 2014). This code, like ECOSMOG, is based on RAMSES. ISIS differs from the other codes in the literature because it performs calculations in the Einstein frame (as opposed to the Jordan frame).

While the MIRAGE code is not AMR enabled, it is capable of correctly simulating $f(R)$ gravity over a range of scales. In addition, there are two novel features which have been implemented to make the code readily adaptable to different $f(R)$ models. Firstly, the $f_R(R)$ and $R(f_R)$ functions are stored using a numerical spline instead of being hard coded. As will be shown in Chapter 5, this enables us to run simulations
with both the designer and HS models. The second novel feature of our implementation is that we have modified the underlying GADGET-2 code to run with any supplied $w(a)$. We will also return to this in the next chapter.

### 4.5.1 Solving for the Scalar Field

In this section we describe the multigrid technique we use to solve the trace equation for the scalar field $f_R$. In our implementation we solve for the field on a grid of fixed spatial resolution using a hierarchy of lower resolution grids. Unlike other PDE solution methods, multigrid methods require an initial guess for the value of the field at every point in space before carrying out an iterative update process to reach a solution. We start by defining our update rule before outlining the Full Approximation Storage algorithm. Finally, we describe the criteria used to evaluate when the field has sufficiently converged.

**Update Rule**

The range of values that $|f_R|$ can take in a cosmological volume is known to vary over many orders of magnitude. It therefore makes sense to calculate it as

$$u = \ln \left( \frac{f_R}{f_R(a)} \right)$$

where $f_R = \bar{f}_R(a) \exp(u)$. In these units the field $u$ is of order unity for all redshifts and environments we consider. Importantly this redefinition also ensures that the value of $f_R$ remains negative to avoid nonphysical gravitational dynamics. We store all values of $u$ in double precision. In the above units, (4.28), the discretised version of the trace equation can be written in the form

$$\mathcal{L}^h(u^h) = f^h$$

where the superscript $h$ indicates that a field is discretised on a grid with cell spacing $h$. In the above equation $\mathcal{L}^h(u^h)$ is a non-linear differential operator and $f^h$ is the source term.
The differential operator at cell $i, j, k$ is
\[
L^h(u^h)_{i,j,k} = (\nabla^2 e^u)^h_{i,j,k} + \frac{1}{3c^2 f_R(a)} \left( \bar{R}(a) - R(u^h_{i,j,k}) \right) \tag{4.30}
\]
while the source term is
\[
f^h_{i,j,k} = \frac{8\pi G}{3 f_R(a)} \left( \bar{\rho}(a) - \frac{m^h_{i,j,k}}{h^3} \right) \tag{4.31}
\]
where $m^h_{i,j,k}$ is the mass assigned to cell $(i, j, k)$. Following Oyaizu (2008) we express $\nabla^2 e^u$ as
\[
(\nabla^2 e^u)_{i,j,k} = \frac{1}{h^2} \left[ b_{i+1/2,j,k} u_{i+1,j,k} + b_{i-1/2,j,k} u_{i-1,j,k} + (b_{i-1/2,j,k} + b_{i+1/2,j,k}) u_{i,j,k} \right]
+ \frac{1}{h^2} \left[ b_{i,j+1/2,k} u_{i,j+1,k} + b_{i,j-1/2,k} u_{i,j-1,k} + (b_{i,j-1/2,k} + b_{i,j+1/2,k}) u_{i,j,k} \right]
+ \frac{1}{h^2} \left[ b_{i+1/2,j,k} u_{i,j-1/2} + b_{i,j+1/2,k} u_{i,j+1/2} - (b_{i,j-1/2,k} + b_{i,j+1/2,k}) u_{i,j,k} \right],
\tag{4.32}
\]
where
\[
b_{i+1/2,j,k} = \frac{1}{2} (e^{u_{i,j,k}} + e^{u_{i+1,j,k}}) \tag{4.33}
\]
and
\[
b_{i-1/2,j,k} = \frac{1}{2} (e^{u_{i,j,k}} + e^{u_{i-1,j,k}}). \tag{4.34}
\]
We use the Newton-Raphson method to update the value associated with each cell.
In this scheme the value of cell $u_{i,j,k}$ on the $(m + 1)$th iteration is
\[
u_{i,j,k}^{m+1} = u_{i,j,k}^m - \frac{\left( L^m(u^m)_{i,j,k} - f_{i,j,k} \right)}{L'(u_{i,j,k})}. \tag{4.35}
\]
where $L'(u_{i,j,k}) = dL^m(u^m)_{i,j,k}/du_{i,j,k}$ and we have dropped the $h$ superscripts for clarity. The update rule in (4.35) is a generalisation of the root-finding method used for a single equation.

Updates are performed in red-black Gauss-Seidel update sweeps. A Gauss-Seidel sweep is where the current value of $u_{i,j,k}$ is overwritten in place and so the update process can use $u_{i,j,k}$ as soon as it becomes available. This avoids retaining an extra copy of the grid in memory. In order to optimise the Gauss-Seidel sweep it is common
4: SIMULATING $F(R)$ GRAVITY

Figure 4.4: Left: Schematic of a two dimensional red-black sweep. Right: Schematic of a V-cycle. Note that the finest grid is at the top of the figure and the algorithm progresses from left to right with relaxation sweeps being carried out on each level.

to update every second cell on a grid in the first half of the sweep before returning for the other cells. This is known as red-black iteration (as from the checkers board).

Together, this procedure is known as the Newton-Raphson-Gauss-Seidel (NRGS) update. Applying the above update rule ensures that the $u$ field iterates towards the correct solution. Small scale errors in the initial guess field are typically removed within a few update sweeps.

In other codes described in the literature (Oyaizu, 2008; Li et al., 2012; Puchwein, Baldi & Springel, 2013; Llinares, Mota & Winther, 2014; He, Li & Hawken, 2015), the function $R(u)$ is hard-coded to one of the approximate models described in Section 4.4. We do not limit the utility of our code in this manner. Instead we allow the user to choose from one of the hard coded approximate models or to input a tabulated form of $f_R(R)$. In particular our code can read in a table of $\ln(R[H_0^2])$ and $\ln(f_R/\bar{f}_R)$ values and use a cubic order spline to compute $R(u)$. Our code uses the GNU Scientific Library (GSL; Gough, 2009) interpolation routines and an associated accelerator object to improve the interpolation lookup time.

We tested our technique by running the suite of analytic tests described in Section 4.6.1 with the power-law model, with and without the spline routine. The tabulated data used with the code contained $10^6$ points equally spaced in $\ln(R[H_0^2])$ between

102  Simulations with Modified Gravity
Figure 4.5: A schematic of slab-based domain decomposition. At the top of the diagram the $x - y$ plane of the global 8 by 8 (by 8) grid is shown. Each colour represents a different MPI task, in this case there are four. The bottom part of the figure shows the memory used on each MPI task. Each task holds the cell field values for a region of space as well as a buffer of cells from bordering regions. The buffer cells for task 0 are those of tasks 1 and 3 because the domain boundary is periodic. Note that on each MPI task $N_{\text{thick}} = 2$ and there is an 8 by 8 square of buffer cells on each side of the slab.

0.01 and 150. While there was a 10 per cent increase in the time taken to compute a sweep (in addition to the time required to read in the 48MB file), the results were identical down to machine precision. Using an alternative library, such as [NAG](2002), for spline creation and lookup may reduce the performance overhead, however we deem the GSL library acceptable for our purposes.

We decompose the regular grid into slabs of thickness $N_{\text{thick}}$ along the $x$ axis and distribute the domains among the MPI tasks as shown in Fig. 4.5. When updating a
cell the field value from nearby cells is required. In order to avoid the overhead of a large number of small communications between tasks we opt to store the value of nearby cells in buffer regions and perform a small number of larger communications. The total number of cells on the global grid is \( N_{\text{cell}} = N_c \times N_c \times N_c \) where \( N_c \) is the number of cells along a single axis. Each task holds \( N_{\text{thick}} \times N_c \times N_c \) cells and \( 2N_c^2 \) buffer cells in memory. These buffer cells contain the field value of cells on the edge of the computational domains controlled by nearby tasks. For example, if there are 4 MPI tasks active then buffer cells for Task 1 will be from Task 0 and Task 2. We will demonstrate the computational advantages and limitations of this domain decomposition in Section 4.6.2.

During each Gauss-Seidel sweep there are two points where the buffer cells need to be updated from the adjacent tasks: after updating the red cells and after updating the black cells. To further reduce communication overhead, only the updated cells are sent to the adjacent tasks buffer regions.

**FAS Scheme**

In terms of computational resources, it is prohibitively expensive to correctly solve for large features in the \( u \) field on a single grid (see Fig. 4.6). To this end we apply multigrid techniques in order to reduce the number of NRGS update sweeps required to reach a given convergence level.

Unfortunately the differential operator is non-linear: \( L^h(u^h + v^h) \neq L^h(u^h) + L^h(v^h) \). This means we cannot use standard multigrid techniques nor the Fourier techniques used in the PM algorithm. Instead we utilise the Full Approximation Storage (FAS) algorithm ([Press et al., 1992], [Briggs, Henson & McCormick, 2000], [Brandt & Livne, 2011]). FAS is named as such because the value of \( u \) is used on each grid level rather than just correction terms. This algorithm is particularly suited to solving the non-linear boundary condition partial differential equations such as (4.12).

We will outline the algorithm below with respect to two regular grids, \( \Omega_h \) with cell spacing \( h \) and \( \Omega_{2h} \) which has cell spacing of \( 2h \). We also note that the algorithm is

---

4: SIMULATING F(R) GRAVITY

Simulations with Modified Gravity
Figure 4.6: The convergence rates of applying the NRGS update scheme on a single grid (blue) and on multiple grids via the FAS scheme (red). Here we are demonstrating the sinusoid test from Section 4.6 run with $256^3$ cells but we find a similar trend regardless of the test chosen. Here we measure convergence of the field as the $L_2$ norm of the residual (see Eq: 4.39) and plot this as a function of the wall-clock time expended. These tests were conducted with 4 MPI tasks on an Intel Core i5 chipset. The V-cycle method outlined in the text is obviously vastly superior in terms of achieving convergence as it reaches machine precision within 65 seconds. We note that the time taken to reach machine precision depends on the problem chosen.

There are two important grid transfer operators of note. Firstly, $I_{2h}^h$ is a restriction operator which transfers a field defined on fine grid with spacing $h$ onto a coarser grid with spacing $2h$. The second operator of interest is the prolongation operator $I_{2h}^h$ which interpolates a field defined on grid with space between cells of $2h$ onto a finer grid with cell spacing $h$. There is no formal requirement for the transfer operators to be duals of
4: SIMULATING $F(R)$ GRAVITY

each other, i.e. it is not necessarily true that $u^h = I_{2h}^h I_{2h}^{2h} u^h$. We will give details of our implementation in the section below.

The FAS algorithm to solve $\mathcal{L}^h(u^h) = f^h$ is as follows,

1. Perform $N_{\text{sweep}}$ Newton-Raphson-Gauss-Seidel sweeps on $\Omega_h$ (pre-smoothing)

2. Compute $\tau^{2h} = \mathcal{L}^{2h}(I_{2h}^{2h} u^h) - I_{2h}^{2h} \mathcal{L}^h(u^h)$ on $\Omega_{2h}$

3. Solve $\mathcal{L}^{2h}(u^{2h}) = \tilde{f}^{2h}$ on $\Omega_{2h}$, where $\tilde{f}^{2h} = I_{2h}^h f^h + \tau^{2h}$

4. Correct the fine grid solution $u^h \rightarrow u^h + I_{2h}^h (u^{2h} - I_{2h}^{2h} u^h)$

5. Perform $N_{\text{sweep}}$ Newton-Raphson-Gauss-Seidel sweeps on $\Omega_h$ (post-smoothing)

6. Check convergence criteria.

Steps 1. and 5. are the same operation and are labeled as pre-smoothing and post-smoothing to indicate that by performing the update sweeps we are reducing the amplitude of high frequency errors in the solution. We stress that there is no explicit smoothing operation being carried out. By performing the update procedure the (unknown) error field, $e = \mathcal{L} - f$, becomes smoother and smaller in amplitude.

We emphasise that this algorithm is recursive, particularly step 3. This is known as a V-cycle algorithm (see the right hand panel of Fig. [4.4]). By performing Gauss-Seidel update sweeps on grids with a number of different resolutions we improve the quality of the solution on a number of different length scales. While sweeps using coarse grids are not capable of improving the solution on scales below a grid cell they do reduce errors on larger scales. There exist other similar algorithms of various complexity, e.g. W-cycles and the Full-Multigrid method, which attempt to improve the efficiency of the solution process. We have chosen to implement a V-cycle procedure because of its relative simplicity.

In the above $\tau^{2h}$ is known as the relative truncation error (defined on grid $\Omega_{2h}$ relative to $\Omega_h$) and can be thought of as the correction to the source term $f^{2h}$ that makes the solution on $\Omega_{2h}$ equal to the solution on $\Omega_{2h}$. The multigrid recursion is carried
4.5: NUMERICAL METHODOLOGY

Figure 4.7: Schematic of cell-centred grid hierarchies. Left: A two dimensional example. The diagram shows four finer grid cells within a single coarse grid cell. The centre of the coarser grid cell is shown as a solid black dot while the centres of the $\Omega_h$ cells are indicated by circles. Important scales such as the grid size and the separation between cell centres are indicated. Right: A three dimensional schematic of a single coarse grid cell and how it can be subdivided into eight finer cells. Each subcell is denoted with a “+” or “−” according to whether its centre is above or below the coarse grid cell centre in each dimension. For example the cell in the lower right of the diagram is denoted as $u^h_{++−}$.

out until the number of grid cells in each dimension reaches $N_{\text{base}}$. The hierarchy of additional grids add a mere $\sim15\%$ to the overall memory footprint of the program. We will discuss the convergence criteria later in this section.

Grid Transfer Operators

We have chosen to use the cell-centred formalism (as opposed to the vertex-centred formalism) where the value of a field stored in each cell corresponds to the average value of the field within the cell region. This has the advantage of being conceptually simple. It has also been shown that some cell-centred solvers require lower order (and therefore less computationally expensive) grid transfer routines in order to achieve
4: SIMULATING $F(R)$ GRAVITY

convergence (Mohr & Wienands, 2004). However, unlike the vertex-centred description, coarser versions of a grid cannot be formed from a subset of the fine grid points (see Fig. 4.7 for schematics in two and three dimensions). Instead, eight fine cells can be united to form a single coarse cell. While this does not affect the grid storage requirements it does complicate the form of the prolongation and restriction operators.

For the $I_{2h}^h$ operator we choose a trilinear interpolation. In one dimension, the linear interpolation of function $u$ that is uniformly sampled at rate $2h$ is given by

$$u(x) = u_i + \frac{m_x}{2h} (x - x_i) \tag{4.36}$$

where $u_i$ is the sampled field value at $x_i$ and $m_x = \frac{1}{2} (u_{i+1} - u_{i-1})$. In the grid transfer operation we aim to compute the interpolated field values onto the finer grid. That is, we are interested in the value at $x_\pm = x_i \pm \frac{h}{2}$ where we refer the reader to Fig. 4.7. In this case

$$u^h_{\pm} = u^{2h}_i \pm m_x. \tag{4.37}$$

One can readily generalise this to two and three dimensions, i.e. by calculating $m_y$ and $m_z$.

The restriction operator $I_{h}^{2h}$ is much simpler in design. In terms of the cell-centred grids, the value of a coarse cell is an average of the eight finer cells within the spatial extent of the coarse cell. Using the notation in Fig. 4.7,

$$u^{h}_{i,j,k} = \frac{1}{8} (u_{+++} + u_{++-} + u_{+--} + u_{---} + u_{++-} + u_{+-+} + u_{-++} + u_{---}). \tag{4.38}$$

Both the restriction and prolongation operations can usually be carried out locally on each MPI task (although the buffer cells must be updated after each operation). When dealing with very coarse grids on a large number of MPI tasks it is not uncommon for $N_{\text{task}} \geq N_{\text{thick}}$. This is sub-optimal so we enforce that $N_{\text{thick}} > 2$ on every task. If this condition is not satisfied, i.e. there are as many boundary cells being held on a task as regular cells, then the global grid is redistributed on a factor of 2 fewer MPI tasks. This down-stepping condition is also applied in reverse when interpolating to a finer grid on a small number of the potential MPI tasks.
The optimal choice of grid transfer operators is sometimes problem specific (Brandt & Livne, 2011). In the literature there are other schemes which aim to achieve similar levels of accuracy while using fewer computational resources (see e.g. Wesseling 1988; Kwak 1999). The operators we use represent a choice of accuracy over computational efficiency.

**Convergence Criteria**

The obvious question one can ask when using any iterative algorithm such as FAS is “how do we know that the solution has converged?”. The first possible measure of convergence is the norm of the defect

\[
||d^h|| = ||L^h(u^h) - f^h||
\]  

where \( ||x|| \) is the L₂ norm of \( x \). Setting a requirement that \( ||d^h|| < \epsilon_c \), where \( \epsilon_c \) is a small numerical constant, is a viable criterion. One could also construct criteria based on the maximum value or the distribution of \( d^h = L^h(u^h) - f^h \).

Alternatively one could consider setting a limit on the local truncation error \( \tau^{2h} \). It has been argued that, in general, setting \( ||d^h|| < \alpha ||\tau^h|| \) with \( \alpha = 1/3 \) should ensure that the solution converges to the numerical limit of the discretisation.

Bose, Hellwing & Li (2015) argued that when solving the \( f(R) \) equations one should use a fixed value of \( \epsilon_c = 10^{-8} \) to ensure convergence. We will test the above convergence criteria in Section 4.6.

**4.5.2 Modifications to GADGET-2**

As described above, the calculation of the scalar field at each time step is carried out using the fixed grid. In our attempt to modify the underlying GADGET-2 code as little as possible we use a copy of the PM grid as the finest grid in our multigrid calculation.

---

1. \( ||x|| = \sqrt{\sum_{i,j,k} |x_{i,j,k}|^2} \)

2. See Press et al. (1992) for a derivation and the assumptions on the behaviour of \( L^h(u^h) \) made.
Figure 4.8: The fractional error in the power spectrum caused by omitting the tree algorithm from the TreePM gravity calculation. Each line represents the fractional difference between a set of 5 ΛCDM simulations utilising the TreePM method and 5 ΛCDM simulations utilising the PM method. The colour of the line indicates the comoving size of the volume ($L = 64$, 128, 256, 400 and 512 $h^{-1}$Mpc runs are shown in blue, green, red, orange and cyan respectively). Each run was carried out using $256^3$ particles and $512^3$ PM cells. The horizontal lines indicate the 1 and 5 per cent error margins.

We make two additional function calls in the PM algorithm. The first is taken after the particles are smoothed to the grid (using the CIC charge assignment scheme) and it is here that the multigrid method is enacted. At this point the source term $f^h$ is computed on the finest grid. The gridded density field used for the PM calculation is unchanged at this point.

The second function call is taken directly after the multigrid calculation of $u$ is complete. This function calculates the effective density and adds the contribution to
the matter density. The matter density held in the PM grid (after scaling by numerical
constants) is then the source term of the equation

$$\nabla^2 \Psi = 4\pi G \left( \delta \rho + \delta \rho_{\text{eff}} \right).$$  \hspace{1cm} (4.40)

It is worthy of note that $\delta \rho_{\text{eff}}$ contains the non-linearities in the $f(R)$ gravity force law
(i.e. it encapsulates the chameleon mechanism). This is the only point where we alter
the values in memory that are used for the PM calculation.

In order to avoid complications with force resolution we are forced to disable the
tree calculation from the TreePM algorithm within the GADGET-2 code (see Puchwein, Baldi & Springel 2013 for an advanced technique that uses the tree calculation as an
adaptive mesh). Our calculations are limited by the spatial resolution of the fixed grid.
In this situation we can compute the limitations of our methods in terms of a cut off in
the power spectrum by running two $\Lambda$CDM simulations, one with the full TreePM and
the other using only the PM. In Fig. 4.8 we show the fractional error in the power
spectrum that we induce by removing the tree calculation. For each simulation we
run we can compute the range of $k$ over which the matter power spectrum is correctly
calculated to precision $\epsilon$. We will typically conservatively take $\epsilon \approx 0.01$.

4.6 Static Examples

In this section we test the correctness, the resolution limitations, convergence criteria
and the computational performance of our solver. In order to validate the code and test
its performance, we construct a number of analytically-solvable problems. We start
with the desired $f_R$ field we wish to recover e.g. $f_R = X(x, y, z)$ and analytically
compute the required density field that would induce this field. Note that these density
fields are often not physically meaningful as cosmological volumes, e.g. in some prob-
lems $\delta \leq 0$ for all $x, y, z$. The test of the code is whether (or how fast can) it recover
the expected $f_R$ field given the density field $\delta$.

In this section we will take the HS model with $n = 1$ unless otherwise stated. All
4: SIMULATING $F(R)$ GRAVITY

tests performed in this section have been made using the version of the code that uses a spline for $R(u)$. That is, the error in the distributions below include any originating from the fact that we are using an interpolation of a tabulated function. Note also that although the forms of $\delta \rho$ we choose are sometimes one dimensional functions these tests have been performed in three dimensions.

4.6.1 Analytic Examples

There are a number of analytic test cases in the literature that have been used to validate $f(R)$ solvers (e.g. Oyaizu 2008; Li et al. 2012; Puchwein, Baldi & Springel, 2013). In this section we validate the multigrid solver in the MIRAGE code in four static scenarios: a homogeneous field, an isolated point mass, a Gaussian field and a sinusoidal field.

Homogeneous Field

The simplest test of our code is the case where $\rho = \bar{\rho}$ for all space. One can easily show that the solution is $u_{i,j,k} = 0$ for all $i,j,k$. Usually the code is set to take a uniform field as an initial guess, however for this test we take a uniformly random field centred on $u = 1$ with a range of 8. Note that since $u \propto \ln(f_R)$ this corresponds to an initial guess field that varies over orders of magnitude. Fig. 4.9 shows the initial guess field and final field along the $x$ axis after 5 V-cycles. Note that since the slab based domain decomposition is performed along the $x$ axis, any errors originating from the parallelisation should be apparent. The fractional error, in this case $f_R/\bar{f}_R - 1$, is below $10^{-12}$ for all cell values.

Point Mass

In this section we aim to test whether the weak field behaviour of the $f_R$ field can be recovered. To this end we place a point mass in a uniform density background (Oyaizu).
Figure 4.9: The $f_R$ field along the $x$ axis for a uniform density field. The initial guess for the $f_R$ field is shown in blue while the final field after 5 V-cycles is shown in green. The error on the solution was reduced after each V-cycle, for an example of the possible convergence rate see Fig. 4.6. For this example we have taken $f_{R0} = -10^{-6}$, a cubic box size of 100 $h^{-1}$ Mpc and performed the calculation at $z = 0$.

\[2008; \text{Puchwein, Baldi & Springel} \ (2013)\]. The $\delta \rho$ field in cell $i, j, k$ is given by

\[
\delta \rho_{i,j,k} = \begin{cases} 
A (N_{\text{cell}} - 1) \bar{\rho} & : \text{if } i, j, k = \hat{i}, \hat{j}, \hat{k} \\
-A \bar{\rho} & : \text{otherwise}
\end{cases}
\quad (4.41)
\]

where $A$ is the amplitude of the point mass (for this test we will follow \text{Puchwein, Baldi & Springel} \ (2013) and take $A = 10^{-4}$), $N_{\text{cell}}$ is the total number of cells in the grid and the point mass is positioned at $\hat{i}, \hat{j}, \hat{k}$. For the test shown in Fig. 4.10 we take $N_{\text{cell}} = 128^3$ within a 256 $h^{-1}$ Mpc box.

In this limit of $\delta f_R \ll \bar{f}_R$, the analytic solution of this setup is given by

\[
\delta f_R = \frac{2Gm e^{-\mu r}}{3c^2 r}
\quad (4.42)
\]
Figure 4.10: The $\delta f_R$ field around a point mass for $|f_R| = 10^{-4}$, $10^{-5}$ and $10^{-6}$ shown in blue, green and red respectively. The solid lines indicate the analytic solution of the linearised equation while the dots are the field found by our code. This test is exactly the same set up as described in Puchwein, Baldi & Springel (2013).

where

$$\mu = \sqrt{\frac{1}{3c^2} \frac{dR}{df_R}}_{f_R=f_R}$$

(4.43)

and $m$ is the mass value within cell $\hat{i}, \hat{j}, \hat{k}$. Noting that

$$\frac{df_R}{dR} = \frac{n + 1}{R} |f_R|,$$

(4.44)

one can express $\mu$ as

$$\mu = \sqrt{\frac{H_0^2}{c^2} \frac{(\Omega_m a^{-3} + 4\Omega_\Lambda)}{(n + 1) |f_R|}}$$

(4.45)

where we have used the value of the background Ricci scalar in a $\Lambda$CDM cosmology from Eq: (4.22).

One can see from Fig. 4.10 that the approximate solution is recovered well in the $|\tilde{f}_{R0}| = 10^{-4}$ and $10^{-5}$ cases. We also do not expect the numerical solution to cap-
Figure 4.11: The $\delta f_R$ field around a point mass of mass $m$ for $|f_{R0}| = 10^{-5}$. The simulations in this plot were conducted with varying box sizes ($L = 256$, 512 and 1024$h^{-1}$Mpc shown in blue, green and red respectively) and a fixed number of grid cells ($N_{cell} = 256^3$). Note that the scale on the $x$ axis is different to that in Fig. 4.10.

The nature of the solution within a few grid cells of the point mass because of discretisation errors.

The $|f_{R0}| = 10^{-6}$ simulation fails to reproduce the approximate solution. This is because the approximate solution has regions where $\delta f_R > \bar{f}_R$, i.e. where $f_R > 0$. This behaviour is unphysical and is not permitted in our numerical scheme. In this linearised solution the chameleon mechanism is not active. The correct $\delta f_R$ profile is being exhibited by our solver. Puchwein, Baldi & Springel (2013) showed that by extending the extent of the source it is possible to match numerical solution to the linearised solution.

Furthermore, the linearised solution is not valid at large separations, where boxsize effects are important. In the analytic solution, vacuum conditions are assumed whereas
periodic boundaries are used in our test simulations. To see this further we conduct the 
\( |\tilde{f}_{R0}| = 10^{-5} \) point mass test again with \( L = 256, 512 \) and \( 1024 \, h^{-1}\text{Mpc} \) while keeping 
\( m \) constant (see Fig.4.11). We perform each of these simulations with the same number 
of grid cells \( (256)^3 \) so to point out two effects. Firstly, in agreement with [Puchwein, 
Baldi & Springel (2013)] we find that our numerical solution agrees with the linearised 
solution to larger radii when we conduct the test in a larger volume. Secondly, when 
the point mass is poorly resolved (as in the \( L = 1024 \, h^{-1}\text{Mpc} \) case) the behaviour of 
\( f_{R} \) at small radii is not correctly captured.

**Gaussian Spike**

In this case we aim to recover

\[
f_R(x) = -A \left[ 1 - \alpha \exp \left( \frac{-(x-x_0)^2}{w^2} \right) \right]
\]  
(4.46)

where \( A \) is a normalisation and \( \alpha \) is a constant close to unity. This distribution has 
minima at \( x = x_0 \) and a width of \( w \). In one dimension the corresponding density field 
is

\[
\delta \rho(x) = \frac{R(a)}{8\pi G} \left( \frac{A}{f_R} \left[ 1 - \alpha \exp \left( \frac{-(x-x_0)^2}{w^2} \right) \right] \right)^{-\frac{1}{2}} - 1 \\
+ \frac{3c^2}{8\pi Ga} \frac{2\alpha A}{w^4} \left( w^2 - 2x_0^2 + 4x_0x - 2x^2 \right) \exp \left( \frac{-(x-x_0)^2}{w^2} \right)
\]  
(4.47)

For this test we place the peak in the middle of a \( 256h^{-1}\text{Mpc} \) box \( (x_0 = 128h^{-1}\text{Mpc}) \) and set \( w = 15h^{-1}\text{Mpc} \). We also set \( \alpha = 0.99999 \) and \( A = 2.7 \times 10^{-5} \) so to compare 
with the test of [Puchwein, Baldi & Springel (2013)]. In order to demonstrate that our 
code produces high resolution results that are consistent with the lower resolution runs 
we carry out this test three times with different \( N_{\text{cell}} \). One can see from Fig.4.12 that 
the expected \( f_R \) distribution is recovered. In the \( N_{\text{cell}} = 128^3 \) case the sharp spike is 
not well resolved but increasing the number of cells improves the quality of the solution 
around \( x = 128h^{-1}\text{Mpc} \). Note that the general error level is expected to drop with 
resolution as errors associated with the discretisation are smaller for smaller \( h \).
Figure 4.12: Numerical results from the $L = 256h^{-1}\text{Mpc}$ Gaussian spike test. The parameters of the test are detailed in the text below. The results from the $N_{\text{cell}} = 128^3$, $256^3$ and $512^3$ runs are shown in blue, green and red respectively. Top: The $|f_R|$ field along the $x$ axis with the exact solution shown in black. Bottom: The fractional error $|f_R/f_{R,\text{exact}} - 1|$. 
Figure 4.13: The resultant $|f_R|$ as a function of $x$ for the sine field test. The blue, green and red lines correspond to the $|f_{R0}| = 10^{-4}$, $10^{-5}$ and $10^{-6}$ respectively. The level of error ($|f_R/f_{R,\text{exact}} - 1|$) is below $10^{-5}$ for all $x$.

Sine-varying Field

The $f_R$ field in this case is

$$f_R(x) = |\bar{f}_R| \left( \sin \left( \frac{2n\pi x}{L} \right) - 2 \right)$$ \hfill (4.48)

where $n$ is an integer. Note that again the field only depends on the $x$ coordinate. In effect, this is a one dimensional problem solved on a three dimensional grid. The corresponding density field is given by

$$\delta \rho(x) = \frac{1}{8\pi G} \left[ R(a) \left( \frac{1}{\sqrt{2 - \sin(\frac{2n\pi x}{L})}} - 1 \right) + \frac{3c^2}{a^2} |\bar{f}_R| \left( \frac{2n\pi}{L} \right)^2 \sin \left( \frac{2n\pi x}{L} \right) \right].$$ \hfill (4.49)

The results of our first tests, where we take $n = 1$, $L = 256h^{-1}\text{Mpc}$ and use $N_{\text{cell}} = 256^3$, are shown in Fig. 4.13. As expected, the $|f_R|$ field is recovered in each case.
4.6.2 Computational Performance

In this section we test the scalability of the code. First we test the strong scaling by taking a problem of fixed size and time how long it takes the code to solve it on a varying number of computational cores. We then test the weak scaling by fixing the number of grid cells allocated to each processor. In this section we will use the terms MPI task and CPU core interchangeably since we always set $N_{\text{Task}}$ equal to the number of effective cores we wish to use.

**Strong Scaling**

We test the strong scaling of our code by performing a fixed number of V-cycles (10) on a $512^3$ grid with a varying number of cores. By comparing the total time taken, $t$, we can determine whether or not the code achieves linear scaling. The speedup relative to running on 8 MPI tasks, $t/t_{N_{\text{Task}}=8}$, is shown in Fig 4.14.

We have run the above tests on the COSMA4 machine which consists of nodes with $6 \times 2$ effective CPU cores. Therefore we naively expect a drop in performance between 8 and 16 cores due to the increased communications overhead of sending and receiving data outside a single node. However, we do not observe a deviation from linear scaling. This relative increase in performance is due to the slabs of the distributed grid becoming small enough to fit into each processors cache memory as $N_{\text{Task}}$ is increased.

The observed deviation from linear scaling at larger $N_{\text{Task}}$ is a consequence of our choice of domain decomposition. As $N_{\text{Task}}$ increases, the thickness of each slab decreases but the number of buffer cells remains the same. Therefore the ratio of the active cells to the buffer cells decreases. This leads to each task dedicating a greater proportion of its CPU cycles to communicating the buffer cells rather than updating the active cells.

The number of cores on which linear scaling breaks down is dependent on the number of grid cells, the system architecture and the number of V-cycles required. Since...
Figure 4.14: The speed up in the code as a function of $N_{\text{Task}}$ for 10 V-cycles being performed on a $512^3$ grid.

the number of V-cycles required to reach convergence cannot be known in advance we cannot easily calculate the optimal number of MPI tasks on which the code should be run.

**Weak Scaling**

We test the weak scaling of our code by performing simulations with a fixed value of $N_{\text{cell}}/N_{\text{Task}}$. Increasing the total number of active cells by a factor of 8 while increasing the number of MPI tasks by the same factor keeps the load on each core constant. In particular, we carry out test simulations with $N_{\text{cell}} = 128^3$, $256^3$ and $512^3$ on $N_{\text{Task}} = 1$, 8 and 64. In each run 10 V-cycles were performed (regardless of whether 10 cycles are required in order to reach convergence). We measure the wall clock time, $t$, required to complete the calculation.

The results of our tests are shown in Fig. 4.15. Perfect weak scaling would result
4.6: STATIC EXAMPLES

Figure 4.15: Weak scaling efficiency, $\eta$, of the MIRAGE code. The results from runs on the COSMA4 machine are shown in blue while the results from COSMOS are shown in red. Each processing unit was assigned $128^3$ cells and 10 V-cycles were performed.

in a constant value of $t$ with respect to $N_{\text{Task}}$. We plot the weak scaling efficiency $\eta = t_1/t$ where $t_1$ is the time taken for on a single processing unit. The intermediate cases ($8 < N_{\text{Task}} < 64$) cannot be tested since the V-cycle routines have been written to work where $N_{\text{Task}}$ and $N_{\text{cell}}^{1/3}$ are powers of 2.

From Fig. 4.15 we can see that $\eta$ drops as a function of $N_{\text{Task}}$. We attribute this to the necessary overheads involved in MPI communication: the greater the number of processors the greater the time required to perform global communication processes.

While the slab-based domain decomposition is based on using point-to-point communications (which would generally lead to good weak scaling), the processing units are required to be synchronised in the restriction and prolongation routines. While the behaviour of $\eta$ with respect to $N_{\text{Task}}$ is not optimal, the benefits of parallelisation (larger problem sizes, reduced wall-clock times) still outweigh the overheads for $N_{\text{Task}} \leq 64$. 

Samuel Cusworth
We began this chapter by computing the background expansion history of the Hu & Sawicki (2007) model for various values of $f_{R0}$. It was shown that for $f_{R0} = -10^{-3}$ the effective equation of state, $w_{\text{eff}}$, did not differ from $-1$ by more than 0.003 for any redshift. Decreasing the value of $f_{R0}$ below this value or increasing $n$ led to a $w_{\text{eff}}$ that was indistinguishable from the $\Lambda$CDM result at the 0.3 per cent level.

In Section 4.3 the equations of motion for $f(R)$ gravity were derived under the quasi-static approximation. Later, in Section 4.4 we outlined the approximate forms of the HS and designer model that have been used in the literature. For the HS model it was shown that for $n = 1$ and $|f_{R0}| = 10^{-4}$ the fractional error in the Ricci scalar, $\Delta R/R$, is below $2 \times 10^{-4}$ for all values of $f_{R}$. On the other hand, the approximations to the designer model do not agree with the exact form as well. In particular, for $\bar{f}_{R0} = -10^{-4}$ the model of He, Li & Jing (2013) does not capture the features of the designer model for $|f_{R}| \geq 10^{-6}$. The approximations of He et al. (2014) and He, Li & Hawken (2015) are much better approximations to the exact form of the designer model: the former agreeing to within 10 per cent for $|f_{R}| < 2 \times 10^{-5}$ and the later to within 4 per cent for $|f_{R0}| < 10^{-4}$.

Our methodology for solving the equations of motion in $f(R)$ gravity was set out in Section 4.5. There was particular emphasis on the application of multigrid techniques to this problem. We also described how our implementation was integrated into the MPI parallel GADGET-2 $N$-body code.

Finally in this chapter we have validated our implementation by running the code on static test cases for which the $f_{R}$ field solution is known. In particular the code was able to correctly solve for a homogeneous field, the case of an isolated point mass, a Gaussian field and a sine-varying field. We also performed scaling tests to demonstrate the limitations of the slab-based domain decomposition scheme.
Chapter 5

Structure formation in the $f(R)$ Universe

5.1 Introduction

This chapter pertains to the formation of structure in the $f(R)$ cosmology. The formation of structure in $f(R)$ models has been studied in detail by many in the literature (see reviews by Baldi, 2012; Koyama, 2015).

Some probes, such as the CMB, are primarily sensitive to linear physics because of the small overdensities involved. One can solve the modified linear equations of motion to compute observables such as the CMB power spectrum, lensing power spectra and predictions for the underlying matter power spectrum. A popular code for doing so is MGCAMB (Zhao et al., 2009; Hojjati, Pogosian & Zhao, 2011), an extension of the CAMB code (Lewis, Challinor & Lasenby, 2000). In principle, there are multiple observables which can be used to place constraints on the value of $\bar{f}_{\text{R0}}$ including CMB temperature anisotropies (Marchini et al., 2013; Marchini & Salvatelli, 2013; Hu et al., 2013), the abundance of dwarf galaxies (Jain & VanderPlas, 2011; Vikram et al., 2013) and the properties of galaxy clusters (Terukina et al., 2014; Wilcox et al., 2015).

However, a number of the most powerful probes require detailed predictions in the
non-linear regime (Lombriser et al., 2012c; Lombriser, 2014). It is possible to make analytic predictions for the halo mass function in \( f(R) \) gravity. Various approaches have been attempted including extending the spherical top hat collapse model (Li & Efstathiou, 2012; Lombriser et al., 2013; Kopp et al., 2013). \( N \)-body simulations are the obvious approach to improve theoretical predictions. For some observables, the insight provided by the results of \( N \)-body simulations is vital.

The vast majority of the literature concerning \( N \)-body simulations with \( f(R) \) gravity have been limited to the HS model with \( n = 1 \) (see Section 4.4.2 for details of alternative models). The primary statistic of interest is the fractional change in the matter power spectrum (Oyaizu, Lima & Hu, 2008; Zhao, Li & Koyama, 2011; Li et al., 2012; Puchwein, Baldi & Springel, 2013; Llinares, Mota & Winther, 2014)

\[
\frac{\Delta P}{P} = \frac{P(k) - P_{\Lambda CDM}(k)}{P_{\Lambda CDM}(k)}
\]

where \( P(k) \) and \( P_{\Lambda CDM}(k) \) are the power spectra from the \( f(R) \) and \( \Lambda \)CDM simulations respectively. A version of the halo model HALOFIT has been recalibrated using the simulated matter power spectra (Zhao, 2014).

There has also been work analysing the simulated halo mass function (e.g. Schmidt et al., 2009; Ferraro, Schmidt & Hu, 2011; Zhao, Li & Koyama, 2011; Li & Hu, 2011), halo density profiles (Lombriser et al., 2012b; Corbett Moran, Teyssier & Li, 2014), halo concentrations (Lombriser et al., 2012a), velocity dispersions (Schmidt, 2010; Lombriser et al., 2012a; Lam et al., 2012; Hellwing et al., 2014; Arnold, Puchwein & Springel, 2014) and clustering statistics (Hellwing et al., 2013). Other work has focused on reproducing observed astrophysical phenomena including the integrated Sachs-Wolfe effect (Cai et al., 2014), redshift space distortions (Jennings et al., 2012) and the impact of screening on the fifth force in galaxy clusters (Corbett Moran, Teyssier & Li, 2014). In addition, semi-analytic models of galaxy formation have been applied to the \( N \)-body simulations (Fontanot et al., 2013).

Constraints on \( \bar{f}_{R0} \) made using power spectrum information can be evaded (in the most part) by including the effects of massive neutrinos (Baldi et al., 2014). In this
case the relative increase in power due to modified gravity can be cancelled out by the influence of neutrinos which act to decrease the amplitude on small scales. Baldi et al. (2014) showed that the power spectrum of the HS model with $|f_{R0}| = 10^{-4}$ could be made compatible with $\Lambda$CDM predictions to 10% by including massive neutrinos with $\sum_i m_{\nu,i} = 0.4$ eV.

In addition, the details of baryonic physics in the $f(R)$ cosmology are expected to complicate predictions on sufficiently small scales. Recently, there have been attempts to include baryonic physics in $f(R)$ gravity $N$-body simulations (Arnold, Puchwein & Springel, 2014; Hammami et al., 2015; He & Li, 2015).

At the time of writing, the highest resolution $f(R)$ simulation run to $z = 0$ was conducted by Shi et al. (2015). The authors simulated a small region to high resolution with the $f_{R0} = -10^{-6}$ model, a model they term as being on the “borderline” between being cosmologically interesting and being ruled out by current observations. In this chapter we do not attempt to reach the very high resolution of Shi et al. (2015). Nor will we concern ourselves with any explicit attempt to constrain $f_{R0}$. Instead, we focus on the important assumptions that have been made in the simulations and the consequences for measurements of large scale structure.

The most obvious assumption that we could relax is the quasi-static approximation (see Section 4.3.1). Given that Bose, Hellwing & Li (2015) have shown that including time derivatives of $f_R$ in the equations of motion had minimal effect on the resulting matter power spectrum we will continue to make the quasi-static approximation in our simulations. Instead we will test the validity of the use of approximate models in this area (see Section 4.4).

In this chapter we present results from cosmological volumes that have been simulated using the MIRAGE code described in the previous chapter. We start in Section 5.2 by validating the power spectrum results of our code against others in the literature. In Section 5.3 we simulate the designer $f(R)$ model and compare our results against the results of using the approximate forms of $R(f_R)$. The Hu & Sawicki (2007) model is investigated in Section 5.4. A discussion of the results and our conclusions are pre-
5. STRUCTURE FORMATION IN THE $f(R)$ UNIVERSE

sent in Section 5.5.

5.2 Validation of the MIRAGE Code

In this section we perform simulations to confirm that our modified gravity $N$-body code produces results consistent with others in the literature. We start by testing the power-law version of the HS model by taking part in a code comparison project. In the later subsection we run simulations of the designer $f(R)$ model using approximations presented in the literature.

5.2.1 Winther et al. (2015) Code Comparison

To date, a single formal code comparison project has been presented in the literature. Winther et al. (2015) used a single set of initial conditions and compared the outputs of running several modified gravity codes. Three classes of modified gravity were chosen: $f(R)$, DGP (Dvali, Gabadadze & Porrati 2000) and Symmetron (Hinterbichler & Khoury 2010) models. For the purposes of this comparison we will focus on $f(R)$ gravity. The $f(R)$ gravity codes that were compared were ECOSMOG (Li et al. 2012), MG-GADGET (Puchwein, Baldi & Springel 2013) and ISIS (Llinares, Mota & Winther 2014). All three used the HS model with $n = 1$ and $|f_R| = 10^{-5}$. The common set of initial conditions were generated using 2LPT via the MUSIC (Hahn & Abel 2011) package with the cosmological parameters labeled Winther in Table 1.2. A total of $512^3$ dark matter particles were set up within a $250h^{-1}$Mpc box at $z_i = 49$.

Overall there was broad agreement in the resulting $P(k)$ produced by the modified gravity solvers (up to 1% on scales $k < 1h$Mpc$^{-1}$). Most of the differences in the $P(k)$ were attributed to the difference in the underlying Newtonian gravity solvers: ISIS and ECOSMOG are based on RAMSES while MG-GADGET is based on the GADGET-3 code. It is worthy of note that even when using a single codebase, e.g. GADGET, the choice of timestepping parameters, smoothing lengths and number of grid cells can make a
5.2: VALIDATION OF THE MIRAGE CODE

Figure 5.1: Fractional matter power spectrum measurements from the MIRAGE, ISIS and ECOSMOG codes are shown in purple, red and green respectively. These simulations were performed as part of the [Winther et al. (2015)] code comparison project. For MIRAGE we plot the results from the standard resolution simulation ($N_{cell} = 512^3$) in dashed lines and the results from a higher resolution simulation ($N_{cell} = 1024^3$) as a full line. Note that in this plot, the ISIS and ECOSMOG simulations were performed without using refinements in their respective meshes ($N_{cell} = 1024^3$). The linear theory prediction from MGCAMB is also shown in black.

large difference to small scale structure ([Sembolini et al., 2015]).

Comparison to fixed grid results

In Fig. 5.1 we show the results from running the MIRAGE code (using the power-law model with $n = 1$) on the [Winther et al. (2015)] initial conditions to $z = 0$. We also plot the results from versions of the ISIS and ECOSMOG codes. These other codes have an obvious advantage in this test: they are capable of adaptively refining their respective mesh grids in regions of high density. In order to negate this advantage the ISIS and
Figure 5.2: Comparison of the fractional matter power spectrum results of the ECOSMOG and ISIS modified gravity codes with the results of MIRAGE at multiple redshifts. Note that this measure includes the errors originating from the underlying N-body code. Again, as in Fig. 5.1, the ISIS and ECOSMOG runs were performed using a fixed resolution.

ECOSMOG simulations were run without refinements, that is on a fixed grid. Unfortunately, the modified TreePM algorithm used in MG-GADGET cannot be truncated in this manner. For this reason we do not include this code in our comparisons until the end of this section.

The power spectra from the different runs in Fig. 5.1 are in excellent agreement. Differences at large $k$ are expected due to the numerical noise introduced by the fact that there is a finite number of cells in each grid. In order to demonstrate the effect of finite spatial resolution we have simulated the MIRAGE run with two different numbers of grid cells, $N_{\text{cell}} = 512^3$ and $N_{\text{cell}} = 1024^3$. One can see that the two MIRAGE simulations are in good agreement on large scales. At higher $k$ however, the higher resolution grid captures the correct behaviour of $\Delta P/P$ over a larger range of modes.
5.2: VALIDATION OF THE MIRAGE CODE

For the remainder of this code comparison we will use the results from the \( N_{\text{cell}} = 1024^3 \) simulation.

In Fig. 5.1 we also plot the expected fractional difference in the linear power spectrum. As expected, the simulated \( P(k) \) is in agreement with the linear prediction on large scales and deviates on smaller scales where non-linear collapse has taken place.

In Fig. 5.2 we compare the fractional power spectra of the different codes at multiple redshifts. There is excellent agreement (5% for \( z < 1 \)) between the fractional power spectra for \( 0.05 \leq k/[h\text{Mpc}^{-1}] \leq 0.3 \). Note that all measurements of \( \Delta P/P \) are in agreement to within 10 per cent. We therefore conclude that the results from the MIRAGE code are comparable to the outputs of the ISIS and ECOSMOG codes when run without grid refinements.

Comparison to AMR results

We now compare the results of the MIRAGE code with the results of the three adaptive mesh enabled codes used in the comparison project. It is expected that there will be significant differences between the fractional power spectra on small scales. This is simply because the MIRAGE code is limited in spatial resolution to a \( N_{\text{cell}}^{1/3} \times N_{\text{cell}}^{1/3} \times N_{\text{cell}}^{1/3} \) grid. The ISIS, ECOSMOG and MG-GADGET codes on the other hand are capable of adaptively refining their respective base grids in regions of high density.

It is obviously important that the MIRAGE code captures the behaviour of \( \Delta P/P \) over an expected range of \( k \). The fact that MIRAGE uses the PM algorithm to compute gravitational forces means we can estimate the range of \( k \) over which we expect the \( \Lambda \)CDM power spectrum to be correctly captured. By comparing the power spectra from \( \Lambda \)CDM simulations using the TPM and PM algorithms (see Section 4.5.2) we can place an upper limit in \( k \) on the modes that we trust.

The results of the fully adaptive versions of the ISIS, ECOSMOG and MG-GADGET codes are compared to the output of the MIRAGE code in Fig. 5.3. We also plot dashed vertical lines to indicate where the TPM and PM GADGET-2 simulations differed by greater than 1 and 5 per cent. It is worthy of note that although the MIRAGE \( \Delta P/P \)
Figure 5.3: Fractional difference in the $z = 0$ matter power spectrum as calculated using the MIRAGE, ISIS, ECOSMOG and MG-GADGET codes shown in purple, red, green and blue respectively. For comparison we also plot the linear theory $\Delta P/P$ from MGCAMB in black. The dashed vertical lines indicate where the TPM and PM GADGET-2 simulations differed by greater than 1 and 5 per cent.

The prediction broadly agrees with the other results at $k > 0.3h\text{Mpc}^{-1}$ the higher $k$ prediction is not expected to be robust in general. Since the resolution issues related to the PM algorithm are present in both the $f(R)$ and $\Lambda$CDM simulations the net effect appears to cancel out in the fractional power spectrum. This is obviously not valid in general since the gravitational forces are not being solved correctly on small scales.

From Fig. 5.3 we conclude that the MIRAGE code is capable of producing results consistent with the AMR $f(R)$ codes over a range of $k$. As a caveat to this we add that we have only shown this for the power-law version of the $n = 1$ [Hu & Sawicki (2007)] model. We also conclude that our method for estimating the trusted range of $k$ is successful.
5.2: VALIDATION OF THE MIRAGE CODE

5.2.2 Approximate Designer Models

Following the successful testing of the MIRAGE code using the power-law model we now test the \( f(R) \) designer model. In particular we have simulated cosmological volumes using the models of \[ \text{He, Li & Jing (2013), He et al. (2014) and He, Li & Hawken (2015).} \] To our knowledge these are the only approaches to running \( N \)-body simulations with the designer model. The reader is referred to Table 4.1 for details of the functional forms of \( R(u) \) used in these models.

All simulations described in this section were performed using the Planck1 cosmological parameter set (see Table 1.2 for details). Here and throughout the remainder of this chapter the cosmological volume initial conditions were generated using L-GENIC, a memory efficient version of the N-GENIC code. The L-GENIC code uses the Zel’dovich approximation (see Sections 1.2.3 and 2.1) when generating the initial conditions. We computed the displacement field on a grid with a factor of \( 2^3 \) more cells than particles, i.e. for \( N = 256^3 \) particles we used a grid with \( N_{\text{cell}} = 512^3 \).

Comparison to He et al. (2013) and He et al. (2014)

We ran 5 realisations of \( L = 150h^{-1}\text{Mpc} \) cosmological regions using the \[ \text{He et al. (2014) model with } |\tilde{f}_{R0}| = 10^{-4}. \] In these simulations we used a cubic order spline to calculate \( f_{R}(R) \) and \( R(u) \). As such, any error originating from the spline calculation is included in the resulting matter power spectrum.

The resulting fractional power spectrum is shown in Fig. 5.4. While we have not used the same sets of initial conditions as \[ \text{He et al. (2014)} \] we have run 5 different realisations which should allow a fair comparison. We note that the work of \[ \text{He et al. (2014)} \] is based on the adaptive mesh capable ECOSMOG code. Therefore, the published work to which we are comparing is expected to resolve the power spectrum to higher values of \( k \). Considering the spatial resolution of the MIRAGE simulations it is clear that there is excellent agreement with the results of \[ \text{He et al. (2014)} \]. We conclude from this that the numerical errors resulting from the cubic spline are unlikely to be problematic.
5: STRUCTURE FORMATION IN THE $F(R)$ UNIVERSE

Figure 5.4: Fractional matter power spectra (relative to $\Lambda$CDM) of cosmological regions run with MIRAGE using the models of He, Li & Jing (2013) and He et al. (2014) in green and blue respectively. The shaded blue region represents the scatter of the 5 realisations and the full line is the average $\Delta P/P(k)$. The black points are the results from He et al. (2014). Note that data from the He, Li & Jing (2013) paper are not plotted here as the authors used a different set of cosmological parameters in their simulations. We also plot a vertical dashed line to indicate where the difference in $P(k)$ in the TPM and PM GADGET-2 runs was greater than 5 per cent. The MIRAGE results for $k > 0.3h\text{Mpc}^{-1}$ are subject to significant numerical noise due to the finite resolution of the grid.

It was previously shown in Fig. 4.3 that the functional form of the He, Li & Jing (2013) model does not capture the features of the exact designer model $R(f_R)$. Given this we ran a single simulation with the model of He, Li & Jing (2013) to demonstrate that the resultant $\Delta P/P$ does not closely resemble that of the He et al. (2014) model (see Fig. 5.4).
5.2: VALIDATION OF THE MIRAGE CODE

Figure 5.5: The fractional matter power (relative to $\Lambda$CDM) spectrum from our 5 realisations of the He, Li & Hawken (2015) model. The red shaded region represents the scatter in the results from the MIRAGE code. Also plotted in black dots are the data from He, Li & Hawken (2015). We also plot a vertical dashed line to indicate where the difference in $P(k)$ in the TPM and PM GADGET-2 runs was greater than 5 per cent.

Comparison to He et al. (2015)

We also ran 5 realisations using the $|\tilde{f}_{R0}| = 10^{-4}$ model of He, Li & Hawken (2015). The resulting fractional matter power spectrum is shown in Fig. 5.5. As per the previous plot, the results from the MIRAGE code are expected to differ from the ECOSMOG based work of He, Li & Hawken (2015) on small scales.

Overall there is excellent agreement between the results of our code and the work presented in the literature. From the results of this section we conclude that the MIRAGE code is capable of reproducing the matter power spectra for the models that have been previously investigated. Our code may be limited by the finite resolution of the grid but we have demonstrated that we understand the numerical limitations of our
5: STRUCTURE FORMATION IN THE F(R) UNIVERSE

| Box size $[h^{-1}\text{Mpc}]$ | # TPM | #PM | # $|f_{R0}| = 10^{-4}$ |
|--------------------------------|-------|-----|---------------------|
| 300                           | 5     | 5   | 5                   |
| 150                           | 5     | 5   | 5                   |
| 75                            | 5     | 5   | 5                   |

Table 5.1: Description of the simulations performed using the $\Lambda$CDM designer model. The TPM and PM simulations were run with the standard $\Lambda$CDM dynamics whereas the simulations labeled with $\tilde{f}_{R0}$ were run using under $f(R)$ gravity.

5.3 $\Lambda$CDM Designer Model

We now investigate the designer model in more detail. In particular we perform simulations using the exact functional form of the model and compare the results to those obtained from simulations run using the approximate forms of $f(R)$ from He et al. (2014) and He, Li & Hawken (2015). To our knowledge these are the first $N$-body simulations to be run using the exact functional form of this model.

5.3.1 Exact Form Results

As we have previously stated, the MIRAGE code is not limited to the case where both $f_R(R)$ and $R(f_R)$ are simple analytic functions. We took the form for $f_R(R)$ for this model from the work of He & Wang (2013)\footnote{We also confirmed that $f_R(R)$ was the same as the one obtained from numerical solution of the modified gravity Friedmann equations.}. Since the background history of this model is exactly that of $\Lambda$CDM, our approach simulates the full designer model under the quasi-static approximation.

As discussed in Section 4.5.2, we are hesitant to trust the resultant $P(k)$ over the whole range of $k$ because of the finite spatial resolution of the PM algorithm. In order
Figure 5.6: Fractional matter power spectrum (relative to ΛCDM) of the designer model. The results from the simulations with $L = 75$, 150 and 300 $h^{-1}$ Mpc are shown in red, blue and green respectively. As before, the shaded region represents the scatter from 5 realisations and the solid line is the average value for each mode. We do not plot the MIRAGE results beyond $k_{5\%}$: where the difference in $P(k)$ in the TPM and PM GADGET-2 runs was greater than 5 per cent for ΛCDM. Note that $k_{5\%}$ is larger for simulations of smaller box size.

to explore a greater range of $k$ in the $f(R)$ power spectrum we run simulations of different box sizes. Since we keep $N_{\text{cell}} = 512^3$ while varying the box size, we are sensitive to different $k$ modes in each simulation. We can simply combine the results of the different simulations in order to measure $P(k)$. A full catalog of the simulations performed using the exact designer model can be found in Table 5.1.

There are important checks that we must perform when combining results in this way. The first is to run multiple realisations of each box size. This gives us an idea of how representative a particular realisation is, i.e. a measure of the cosmic variance.

The second check that we can perform is to run higher resolution versions of the
5: STRUCTURE FORMATION IN THE $F(R)$ UNIVERSE

simulations (in our case $N_{\text{cell}} = 1024^3$ with the same box size). Performing these higher resolution simulations would provide a wider range of $k$ over which the dynamics are correctly captured. They are also a necessary step in confirming the validity of our lower resolution runs. As we will see, the higher resolution runs also allow us to cross-check the results of different simulations against each other.

The power spectrum results from the exact designer model simulations are shown in Fig. 5.6. We note that the largest $k$ modes of $\Delta P/P$ in the simulations with the larger volumes overlap well with the lower $k$ modes of the simulations with smaller volumes. In particular, in the region of $0.1 < k < 0.3$ the results from the $L = 300h^{-1}\text{Mpc}$ simulation agree with those of $L = 150h^{-1}\text{Mpc}$. The larger scatter in the $L = 75h^{-1}\text{Mpc}$ measurement is due to two factors. Firstly, each of the $75h^{-1}\text{Mpc}$ regions is subject to variance. It is questionable whether 5 realisations of $75h^{-1}\text{Mpc}$ are enough to compute a representative $\Delta P/P$. Secondly, it is possible that there are important finite volume effects whereby larger scale modes, which are not present in small volume simulations, affect the dynamics of small scale structure.

5.3.2 Evaluating Approximate Models

We can now evaluate the level of error in $\Delta P/P(k)$ that one induces by making the approximations made in the literature. In Fig. 5.7 we show the ratio of the power spectra of the approximate models and $P(k)$ computed using the exact model. The near uniform $0.3\%$ level of discrepancy between the two approximate models is in agreement with the $< 0.5\%$ error shown in [He, Li & Hawken (2015)]. We can conclude that the fractional error in $P(k)$ that one induces by assuming the approximate model of [He et al. (2014)] or [He, Li & Hawken (2015)] rather than simulating the exact model is around $0.2\%$.  

136 Simulations with Modified Gravity
5.4 Hu & Sawicki (2007) Model

In this section we carry out an investigation of the Hu & Sawicki (2007) model. We have already demonstrated that the MIRAGE code is capable of correctly simulating the power-law model with \( n = 1 \). We will continue to assume a \( \Lambda \)CDM background history in our modified gravity simulations. Here we perform multiple simulations with the power-law \( n = 1 \) model before exploring the case where \( n > 1 \). We also perform simulations using the full functional form of the HS model.

5.4.1 Power-Law, \( n = 1 \)

In Table 5.2 we outline the simulations run with \( N_{\text{cell}} = 512^3 \). In addition, we also ran a single realisation of the \( L = 128h^{-1}\text{Mpc} \) and \( L = 256h^{-1}\text{Mpc} \) simulations.
with $N_{\text{cell}} = 1024^3$. These higher resolution simulations extend the range of $k$ over which the power spectrum results are expected to be reliable. Unfortunately, the higher resolution runs also take significantly longer to run to $z = 0$. This is because the code needs to update a factor of 8 more cells per sweep.

All the simulations presented here were run with $N = 256^3$ particles and a $\Lambda$CDM background was assumed. The cosmological parameter set used here is labeled $PL$ in Table 1.2.

Since the power-law model can be expressed as a linear relation between $\log(R)$ and $\log(f_R)$, we expect there to be minimal numerical noise resulting from the spline calculation. We confirmed that running the code with the model hard coded into the equation gave identical results to the version of the code that used a spline for a representative sample of simulations.

In Fig. 5.8 we show the $z = 0$ fractional matter power spectrum for the power-law model runs with $n = 1$ and $\tilde{f}_{R0} = -10^{-4}$. In the figures in this section we plot $k$ modes larger than $k_L = 2\pi/L$ in order to avoid issues related to the finite size of each simulated volume. We also only show the $\Delta P/P$ over the range of $k$ where the deviation between the TPM and PM versions of the simulations are below 2.5%.

Overall, it is clear from Fig. 5.8 that $\Delta P/P$ increases as a function of $k$ over this range of $k$. This is in broad agreement with previous results in the literature (e.g. Oyaizu, Lima & Hu, 2008; Zhao, Li & Koyama, 2011). We note that the form of $\Delta P/P$ will vary with cosmological parameter sets (Zhao, 2014). Therefore, it is difficult to
Figure 5.8: Fractional matter power spectrum (relative to $\Lambda$CDM) for the power-law version of the HS $n = 1$ model. The results for the case where $\tilde{f}_{R0} = -10^{-4}$ are shown. Each colour represents the power spectrum from a different box size: blue and red correspond to 128 and 256 $h^{-1}$Mpc respectively. The shaded regions show the standard deviation of the standard resolution runs ($N_{\text{cell}} = 512^3$) while the solid lines are the results from higher resolution runs ($N_{\text{cell}} = 1024^3$). The linear theory prediction is shown in black.

We compare the results of our simulations with those using different underlying cosmologies.

The fractional matter power spectrum measured in the high resolution simulations is shown to be in excellent agreement with the lower resolution runs. We attribute the slight discrepancy between the lowest $k$ mode of the $L = 128 h^{-1}$Mpc and the highest $k$ modes of the $L = 256 h^{-1}$Mpc to finite volume effects in the former simulations. There is significantly larger scatter in $\Delta P/P$ in the results from simulations of smaller $L$ compared to the simulations of larger $L$. We attribute this to cosmic variance.

We have also plotted the linear theory prediction for $\Delta P/P$ in Fig. 5.8. As ex-
5: STRUCTURE FORMATION IN THE $F(R)$ UNIVERSE

Figure 5.9: Fractional matter power spectra (relative to $\Lambda$CDM) of the $\bar{f}_{R0} = -10^{-4}$ simulations at multiple redshifts. We show the results of the higher resolution ($N_{\text{cell}} = 1024^3$, $L = 128h^{-1}\text{Mpc}$ and $L = 256h^{-1}\text{Mpc}$) runs. The results from $z = 0$, 0.25, 0.5 and 1 are shown in blue, red, green and purple lines respectively.

As expected, the lowest $k$ modes are in agreement with the linear theory prediction. However, on smaller scales there is notable deviation from the linear theory prediction. This is in agreement with previous findings (Oyaizu, Lima & Hu, 2008).

In Fig. 5.9 we show $\Delta P/P$ at multiple redshifts. For clarity, only the higher resolution results are shown. One can see that the amplitude of $\Delta P/P$ increases as a function of time. It is interesting that the overall shape of $\Delta P/P$ does not significantly vary as a function of $z$. Note that the number of modes plotted in Fig. 5.9 increases with $z$. We attribute this to the fact that small scale structure formation occurs at later times. Since the PM algorithm is limited by the finite resolution scale of the grid it is able to follow the high redshift dynamics better than the lower redshift dynamics.

The results for $\bar{f}_{R0} = -10^{-5}$ are shown in Fig. 5.10. We note that the resultant $\Delta P/P$ is well characterised at low $k$. In addition to the simulations shown here, we...
Figure 5.10: $z = 0$ fractional power spectrum (relative to ΛCDM) for the $\bar{f}_{R0} = -10^{-5}$ power-law $n = 1$ model. The lines are labeled the same way as in Fig 5.8.

ran simulations with $L = 400 h^{-1} \text{Mpc}$ and $L = 512 h^{-1} \text{Mpc}$ with $N_{\text{cell}} = 512^3$. The results of these low spatial resolution runs confirmed that the linear theory prediction is recovered at low $k$.

In Fig. 5.11 we plot $\Delta P/P$ at multiple redshifts. As with the $\bar{f}_{R0} = -10^{-4}$ case, the amplitude of the deviation from ΛCDM increases with scale factor. There are slight discrepancies between the results of the two simulations shown at each redshift. We attribute this to the fact that we are considering modes for which $\Delta P_{\text{PMO}}/P_{\text{TPM}} < 0.025$. Given this level of uncertainty in the underlying ΛCDM power spectrum, we expect there to be errors in the high $k$ modes of each simulation.

5.4.2 Exact, $n = 1$

We now investigate the effect of the power-law approximation made to the HS model. To our knowledge these are the first $N$-body simulations to be run using the exact
Figure 5.11: Fractional matter power spectra (relative to $\Lambda$CDM) of the $\bar{f}_{R0} = -10^{-5}$ simulations at multiple redshifts. Again, we only show the results of the higher resolution $L = 128h^{-1}\text{Mpc}$ and $L = 256h^{-1}\text{Mpc}$ runs. The results from $z = 0, 0.25, 0.5$ and 1 are shown in blue, red, green and purple lines respectively.

We will focus only on the $|f_{R0}| = 10^{-4}$ case since we expect deviations to be greatest for larger values of $|f_{R0}|$. The results from simulations run with $L = 256h^{-1}\text{Mpc}$ and $L = 128h^{-1}\text{Mpc}$ are shown in Fig. 5.12.

Note that the difference between the power spectra of the exact model and the power-law model is negligible ($O(10^{-5})$) over the range of $k$ we study. While there is a small level of discrepancy between the simulations with $L = 256h^{-1}\text{Mpc}$ and $L = 128h^{-1}\text{Mpc}$ at $k \approx 0.1$, the overall amplitude of $\Delta P(k)/P(k)$ is similar. Since the discrepancy between the two functional forms decreases with increased $n$ and decreased $|\bar{f}_{R0}|$ we can conclude that the power-law approximation of the HS model is sufficient for this work.
5.4: HU & SAWICKI (2007) MODEL

Figure 5.12: Fractional difference in the power spectra of simulations using the exact Hu & Sawicki (2007) \( n = 1 \) model and the power law approximation. The results from the \( L = 256 \, h^{-1} \text{Mpc} \) and \( L = 128 \, h^{-1} \text{Mpc} \) simulations are shown in red and blue respectively. We have truncated each power spectrum where the ratio of the TPM and PM simulations differs by more than 2.5 per cent.

5.4.3 Power-Law, \( n \neq 1 \)

While changing the power-law index of the model is technically trivial, this variation of the model has not yet been presented in the literature. Here, we begin to explore the parameter space by performing simulations with \( n = 1.5 \) and \( n = 2 \). We use the same 5 sets of initial conditions that were used in the \( n = 1 \) case and carry out the simulations using \( N_{\text{cell}} = 512^3 \). The value of \( \bar{f}_{R0} = -10^{-4} \) was adopted for these simulations.

The fractional power spectra of our simulations are shown in Fig. 5.13. Note that again we have only plotted each simulation up to the \( k \) mode for which the power spectra of the TPM and PM simulations agree to 2.5\%. One can see from Fig. 5.13...
Figure 5.13: Fractional power spectra (relative to ΛCDM) for the HS model at $z = 0$. The three sets of results, from upper-most in blue to lowest in green, are from the runs with $n = 1$, $1.5$ and $2$ respectively.

that as one increases the power-law index of the model, $n$, the amplitude of $\Delta P/P$ decreases.

In Fig. 5.14 we plot the ratio of the power spectrum from the $n \neq 1$ models and the $n = 1$ case. The ratio $P(k)/P(k)_{n=1}$ is always below unity and decreases as a function of $k$. We note that our investigations have found that the ratio $P(k)/P(k)_{n=1}$ appears to be invariant with respect to time. This merits further study with higher resolution simulations.

### 5.5 Discussion and Conclusions

We have successfully simulated cosmological volumes in the Hu & Sawicki (2007) (HS) and ΛCDM designer models with our MIRAGE $N$-body code. In Section 5.2 we validated the results of the code using cosmological volumes. Firstly, we used the
initial conditions of the Winther et al. (2015) code comparison project and ran our code using the HS model. The MIRAGE code has been found to produce results consistent with codes in the literature (see Fig. 5.1). We attribute the small level of discrepancy to the differences in the underlying N-body codes. Secondly, we ran simulations in the Planck1 cosmology using the approximate models of He et al. (2014) and He, Li & Hawken (2015). The fractional power spectra of these simulations were found to be in excellent agreement with published results.

From our investigations into the designer model in Section 5.3 we make the following conclusions:

- The fractional matter power spectrum, $\Delta P/P$, of the approximate form of the designer model proposed by He, Li & Jing (2013) does not resemble that of the full functional form.

- The $P(k)$ for the exact designer model lies between the results from using the He et al. (2014) and He, Li & Hawken (2015) approximations. The error that one induces from using either of the approximations is $\sim 0.2\%$ over the range of $k$ that we examine.

We have also performed cosmological simulations with the power-law approxi-
mated version of the $n = 1$ HS model. From the work presented in Section 5.4 we have been able to characterise the fractional matter power spectrum of this model. In addition, we have run simulations using the exact functional form of the HS model. Finally, we present the fractional matter power spectra for the $n \neq 1$ case. From this work we conclude:

- The results of the simulations using the exact form of $f_R(R)$ and $R(f_R)$ are very similar to the simulations using the power-law approximation. The error in $P(k)$ induced by making the approximation is $\mathcal{O}(10^{-5})$.

- The fractional matter power spectrum of the $n > 1$ models differed from that of the $n = 1$ case. As $n$ is increased, the overall amplitude of $\Delta P/P$ decreases (see Fig. 5.14).

- The ratio of the $n = 1$ and $n > 1$ power spectra decreases as a function of $k$. We found that this ratio was relatively independent of redshift for $z < 1$. 

Simulations with Modified Gravity
Chapter 6

Summary & Future Work

The work in this thesis has been focused on two distinct topics, namely the effect of baryons on the cluster mass function (Chapter 3) and the effect of $f(R)$ gravity on the matter power spectrum (Chapters 4 & 5).

6.1 Baryons and the Cluster Mass Function

Results from the Planck collaboration have shown that cosmological parameters derived from the cosmic microwave background anisotropies and cluster number counts are in tension, with the latter preferring lower values of the matter density parameter, $\Omega_m$, and power spectrum amplitude, $\sigma_8$. Motivated by this, we have investigated the extent to which the tension may be ameliorated once the effect of baryonic depletion on the cluster mass function is taken into account. We use the large-volume Millennium Gas simulations (MGS) in our study, including one where the gas is pre-heated at high redshift and one where the gas is heated by stars and active galactic nuclei (in the latter, the self-gravity of the baryons and radiative cooling are omitted).

Our conclusions from this work are as follows:

- In both generations of the MGS, the cluster baryon fractions are in reasonably good agreement with the data at low redshift, showing significant depletion of
6: SUMMARY & FUTURE WORK

baryons with respect to the cosmic mean.

- The cluster abundance in these hydrodynamic simulations is around 15 per cent lower than the commonly-adopted fit to dark matter simulations by Tinker et al. (2008) for the mass range $10^{14} - 10^{14.5} h^{-1} M_{\odot}$.

- Ignoring baryonic depletion produces a significant artificial shift in cosmological parameters which can be expressed as $\Delta [\sigma_8 (\Omega_m/0.27)^{0.38}] \simeq -0.03$ at $z = 0.17$ (the median redshift of the Planck cluster sample) for the Feedback Only model.

- While this shift is not sufficient to fully explain the Planck discrepancy, it is clear that such an effect cannot be ignored in future precision measurements of cosmological parameters with clusters.

- We outlined a simple, model-independent procedure that attempts to correct for the effect of baryonic depletion. After testing it on the first generation MGS we found that the input cosmological model could not be successfully recovered. From this we conclude that baryons do have a significant influence on the shape of the dark matter mass profile in these models.

6.2 $f(R)$ Gravity and the Matter Power Spectrum

We have presented a modified gravity extension to the massively parallel GADGET-2 $N$-body code which employs a multigrid-accelerated Newton-Raphson-Gauss-Seidel relaxation solver. Our implementation, named MIRAGE, is able to solve the $f(R)$ gravity equations of motion for the scalar field $f_R$. Unlike other modified gravity $N$-body codes in the literature, our code uses a numerical spline to store the $f_R(R)$ and $R(f_R)$ functions. This makes the MIRAGE code readily adaptable to use any model $f(R)$. The modifications to gravity can then be encapsulated by an effective mass density, $\delta \rho_{\text{eff}}$. From this one can then simulate the collapse of structure in $f(R)$ gravity.

In the process of validation we found:
The multigrid solver is capable of recovering the expected $f_R$ field from a density field for a range of commonly used test problems including an isolated point mass, a Gaussian field and a sinusoidally varying field.

The code has also been validated in detail using cosmological density fields. In particular we examined the fractional matter power spectrum, $\Delta P/P$, of the HS $n = 1$ model as part of the Winther et al. (2015) code comparison project. We found excellent agreement with other modified gravity codes in the literature, namely ECOSMOG and ISIS.

Crucially, we were able to confirm that our fixed grid solver predicts $\Delta P/P$ in agreement with the adaptive mesh methods of ECOSMOG, MG-GADGET and ISIS.

The models of He et al. (2014) and He, Li & Hawken (2015) were then implemented in the code and used to reproduce the published $\Delta P/P$ in each case.

After validating the outputs of the code we went on to investigate the $\Lambda$CDM designer and Hu & Sawicki (2007) $f(R)$ models in more detail.

By running simulations of the exact form of the $\Lambda$CDM designer model we were able to evaluate the validity of the three approximate models that have been used in the literature. We found that the He, Li & Jing (2013) model failed to capture the correct form of $\Delta P/P$. On the other hand, the power spectra of the approximate models of He et al. (2014) and He, Li & Hawken (2015) were found to be in agreement with the exact model to within 0.2%.

The use of the power-law approximation of the HS model was evaluated in cosmological simulations. Agreement between the power spectra of the approximate form and the exact form was $O(10^{-5})$ for $n = 1$ and $\tilde{f}_{R0} = -10^{-4}$. It is anticipated that the level of discrepancy will be smaller for smaller values of $|\tilde{f}_{R0}|$ and larger values of $n$. 
6: SUMMARY & FUTURE WORK

- We have conducted, for the first time, $N$-body simulations using the HS model with $n > 1$. The overall amplitude of the fractional power spectrum was found to decrease with increasing $n$. The ratio of the power spectra from the $n \neq 1$ and $n = 1$ cases was found to decrease with increasing $k$. This ratio was found to be largely independent of redshift (for $z \leq 1$).

6.3 Proposed Future Directions

It would be interesting to apply the analysis of Chapter 3 to a new generation of large volume hydrodynamical simulations. While our current simulations are capable of predicting the mass function at lower masses ($10^{14} - 10^{14.5} h^{-1} M_\odot$), we have been unable to make predictions at higher masses with confidence. This is vital for the future success of cluster surveys including the Planck cluster survey which select preferentially for larger mass clusters. Given the computational resources one could run larger volume simulations in order to give insights to the nature of the rarer higher mass clusters.

The results of our simulations using the $\Lambda$CDM designer model could be used to constrain $\bar{f}_{R0}$ from observational data. In particular, incorporating our results into the MG-HALOFIT formalism would enable us to compute forecasts on parameter constraints from future surveys. These surveys include the ongoing Dark Energy Survey (DES; The Dark Energy Survey Collaboration, 2005) and future ventures such as the Large Synoptic Survey Telescope (LSST; LSST Science Collaboration et al., 2009), Euclid (Laureijs et al., 2011) and the Square Kilometer Array (SKA). It would be necessary to run further simulations using at least one other set of underlying cosmological parameters to ensure that the results are robust over a range of cosmologies. Furthermore, it would also be necessary to run simulations with different values of $\bar{f}_{R0}$.

In a similar manner, our current results for the HS model with $n \neq 1$ could be incorporated into the MG-HALOFIT formalism. Again, further simulations would be required to be run with varying cosmological parameter sets. This proposed extension
of HALOFIT would enable one to constrain both $\tilde{f}_{R0}$ and $n$ of this model using current observational data.

Focusing now on the MIRAGE code itself, it would be possible to modify the present solver to investigate a range of different classes of models such as the Galileon (Nicolis, Rattazzi & Trincherini 2009) or Nonlocal gravity (Woodard 2014). These other classes of model have different equations of motion in the background and non-linear regimes. Although we do not make use of it in this thesis, the MIRAGE code is capable of using an arbitrary background history. After computing the background history of a given model, the $w_{\text{eff}}(a)$ function can be stored and accessed using a numerical spline. The most major alterations to the code would be to the solution of scalar field and the way in which $\delta \rho_{\text{eff}}$ is calculated. Numerical formulations for these models have been outlined for the Galileon and Nonlocal gravity models by Barreira et al. (2013) and Barreira et al. (2014) respectively.

While we have shown that our fixed grid solver is capable of correctly determining the $f(R)$ power spectrum it would be advantageous to supplement the fixed grid with adaptively refined meshes. This would be a major undertaking but would allow one to investigate a greater range of spatial scales using a single simulation.
Bibliography


Balaguera-Antolínez A., Porciani C., 2013, JCAP, 4, 22

Baldi M., 2012, Physics of the Dark Universe, 1, 162


Barnes J., Hut P., 1986, Nature, 324, 446

Barreira A., Li B., Hellwing W. A., Baugh C. M., Pascoli S., 2013, JCAP, 10, 27

Baumann D., 2009, ArXiv e-prints


Blas D., Lesgourgues J., Tram T., 2011, JCAP, 7, 34


Bose S., Hellwing W. A., Li B., 2015, JCAP, 2, 34


Brax P., Davis A.-C., Li B., Winther H. A., Zhao G.-B., 2013, JCAP, 4, 29


Carroll S. M., 2004, Spacetime and geometry. An introduction to general relativity


de Felice A., Tsujikawa S., 2010, Living Reviews in Relativity, 13, 3


Hasselfield M. et al., 2013, JCAP, 7, 8

He J.-h., Li B., 2015, ArXiv e-prints

He J.-h., Li B., Jing Y. P., 2013, Phys. Rev. D, 88, 103507
Hockney R. W., Eastwood J. W., 1981, Computer Simulation Using Particles
Hojjati A., Pogosian L., Zhao G.-B., 2011, JCAP, 8, 5
Jain B., VanderPlas J., 2011, JCAP, 10, 32

Samuel Cusworth

157


Komatsu E. et al., 2011, ApJS, 192, 18


Koyama K., 2015, ArXiv e-prints


Laureijs R. et al., 2011, ArXiv e-prints


Li B., Zhao G.-B., Teyssier R., Koyama K., 2012, JCAP, 1, 51
Li Y., Hu W., 2011, Phys. Rev. D, 84, 084033
Llinares C., Mota D. F., 2013, Physical Review Letters, 110, 161101
Lombriser L., 2014, Annalen der Physik, 526, 259
LSST Science Collaboration et al., 2009, ArXiv e-prints
Merz H., Pen U.-L., Trac H., 2005, New Astronomy, 10, 393
BIBLIOGRAPHY


Murray S. G., Power C., Robotham A. S. G., 2013a, Astronomy and Computing, 3, 23


Planck Collaboration et al., 2015a, ArXiv e-prints


Planck Collaboration et al., 2015b, ArXiv e-prints


160 Simulations with Modified Gravity


Schmidt F., 2010, Phys. Rev. D, 81, 103002


Schneider A. et al., 2015, ArXiv e-prints


Sembolini F. et al., 2015, ArXiv e-prints
BIBLIOGRAPHY


Sotiriou T. P., Faraoni V., 2010, Reviews of Modern Physics, 82, 451


Springel V. et al., 2005, Nature, 435, 629


Vikram V., Cabré A., Jain B., VanderPlas J. T., 2013, JCAP, 8, 20

Voit G. M., 2005, Reviews of Modern Physics, 77, 207

Wald R. M., 1984, General relativity


Wesseling P., 1988, Journal of Computational Physics, 1, 85


BIBLIOGRAPHY

Will C., 2001, Living Reviews in Relativity, 4, 4

Winther H. A. et al., 2015, ArXiv e-prints

Woodard R. P., 2014, Foundations of Physics, 44, 213


Simulations with Modified Gravity