Chapter 2
The Growth of Matter Perturbations in the Universe

2.1 Numerical Methods

In this chapter we outline some aspects of the N-body simulation code used in this thesis as well as the modifications made to the code to include the effects of various dark energy cosmologies. We also describe how the initial conditions for the simulations are set up.

2.1.1 The Simulation Code

Once a dark matter perturbation approaches the cosmic mean, $\delta \sim 1$, linear theory breaks down and full numerical methods are needed in order to follow the non linear growth of structure. Analytic solutions can be used in special circumstances, for example, the Press-Schechter formalism can be used to predict the number of objects of a certain mass in a given volume assuming spherical collapse (Press and Schechter 1974). Here we present a brief review of the N-body simulation code GADGET- 2. For more information on the code see Springel (2005) and for a comprehensive review of N-body simulations see Bertschinger (1998).

Following the dynamics of dark matter particles under their mutual gravitational attraction requires us to solve the collisionless Boltzmann equation and Poisson's equation simultaneously. Using a method of characteristics (Leeuwin et al. 1993) the solution of the Boltzmann equation can be obtained by sampling the (6 +1) dimensional phase space, $\{\vec{x}, \vec{p}, t\}$, of the initial distribution function, $f(\vec{x}, \vec{p}, t)$. Solving Poisson's equation for N particles, the system can be evolved forward in time using the equations of motion derived from $\partial f/\partial t + [f, H] = 0$, where H, in this instance, is the system's Hamiltonian.

The core of any N-body simulation is the gravity solver. In the PM (particle-mesh) algorithm the density field is realised on a grid and the gravitational potential is constructed by solving Poisson's equation. In this scheme all the particles are

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assigned to a grid using a kernel which splits up the masses and determines the density field, $\rho_{i,j,k}$, at each grid point. The simplest choice of mass assignment scheme is nearest grid point (NGP) where all the mass is allocated to the nearest grid cell. This method leads to significant fluctuations in the evaluated force which can be avoided by using higher order schemes such as the cloud-in-cell (CIC) or triangular shaped cloud (TSC) schemes (Hockney and Eastwood 1981). In the CIC scheme the mass is assigned to the 8 grid points nearest to the particle while the TSC method uses the nearest 27 grid points. The kernel used to construct the density field in the PM part of GADGET- 2 is the CIC assignment scheme. The density field on the grid is then Fourier transformed and the potential on the grid is obtained using the Green's function, $-4\pi G/k^2$, to solve Poisson's equation, $\nabla^2\phi_{i,j,k} = 4\pi G\rho_{i,j,k}$ in Fourier space. Using a grid to estimate the forces in this way results in a lack of short range accuracy on scales comparable to the grid spacing. The Particle-Particle PM scheme (P^{3}M) overcomes the force resolution problem associated with PM methods by adding a direct summation of pairs separated by less than 2 or 3 grid spacings. The combination of mesh based and direct pair summation results in high accuracy forces. However, the algorithm slows down when clustering becomes strong on small scales which degrades the performance of the P^{3}M code.

GADGET- 2 makes use of a TreePM algorithm to compute the gravitational forces accurately. The tree algorithm groups distant particles into larger cells and approximates their potentials using multipole expansions about the centre of mass of the group (Barnes and Hut 1986). The advantage of this method is a scaling in computation time of $\mathcal{O}(N\log N)$, where N is the number of particles, compared to $\mathcal{O}(N^2)$ calculations with a direct summation of the forces. The error on the long range force is then controlled by an opening angle parameter which determines when a multipole expression is used to calculate the forces for a group of particles. A distant cell of mass M, at a distance r and extension l, is considered for opening if

$$\frac{GM}{r^2}\left(\frac{l}{r}\right)^2 \leq \alpha|a| \tag{2.1}$$

where α is a tolerance parameter and a is the total acceleration obtained in the last timestep. The TreePM algorithm employed in GADGET- 2 combines the computational efficiency of the PM code with the short range accuracy of the tree code and splits the gravitational potential into a long and short range component, $\Phi = \phi^{\text{short}} + \phi^{\text{long}}$, where the tree algorithm is used to evaluate the force on small scales and the long range potential is calculated using a mesh. The spatial scale of the force split, r_s, is present in the expression for the short range potential given by

$$\phi^{\text{short}}(\vec{x}) = -G\sum_i \frac{m_i}{r_i}\text{erfc}\left(\frac{r_i}{2r_s}\right), \tag{2.2}$$

where the smallest distance of any of the images of a particle, i, in a periodic box of length L, to the point $\vec{x}$ is given by $r_i = \min[|\vec{x} - \vec{r_i} - \vec{n}L|]$. The force is estimated according to $F_{i,j,k} = -\nabla\Phi_{i,j,k}$ by finite differencing the potential. The force is then interpolated back to the particle positions using the CIC kernel.

To avoid a singularity in the force calculation when particle separations are close to zero, it is common to introduce a softening parameter which softens the force and limits the maximum relative velocity during close encounters between particles. This softening also prevents the artificial formation of binaries in the simulation. The equations of motion in an expanding Universe are obtained by integrating Hamilton's equations

$$\frac{\mathrm{d}\vec{x}}{\mathrm{d}t} = \frac{\vec{p}}{a^2}, \tag{2.3}$$

$$\frac{\mathrm{d}\vec{p}}{\mathrm{d}t} = -\frac{\nabla\Phi}{a}, \tag{2.4}$$

where $\vec{p} = a^2 m\dot{\vec{x}}$ is the canonical momentum and Φ is the interaction potential. In GADGET-2 these equations are discretized and integrated using 'kick' and 'drift' operators in a second order accurate leap frog integrator scheme (Springel 2005). The drift and kick operators are the time evolution operators of the kinetic and potential components of the Hamiltonian of the N-body problem. The drift operator leaves the momentum unchanged and advances the position of each particle, while the kick operator leaves the position unchanged and updates the momentum. In one time step a combination of these is used, for example the drift-kick-drift (DKD) leapfrog integrator. For each particle the timestep in GADGET-2 is given by

$$\Delta t = \min\left[\Delta t_{\mathrm{max}}, \left(\frac{2\eta\varepsilon}{a}\right)^{1/2}\right], \tag{2.5}$$

where ε is the gravitational softening, η is an accuracy parameter, a is the particle's acceleration and Δt_{max} can be set to a fraction of the dynamical time of the system. We discuss the initial conditions of the N-body code in Sect. 2.1.3.

2.1.2 Modifying Gadget-2

In this thesis we will determine the impact of quintessence dark energy on the growth of cosmological structures through a series of large N-body simulations. These simulations were carried out at the Institute of Computational Cosmology using a memory efficient version of the TreePM code `Gadget-2`, called `L-Gadget-2` (Springel 2005). As our starting point, we consider a ΛCDM model with the following cosmological parameters: $\Omega_{\mathrm{m}} = 0.26$, $\Omega_{\mathrm{DE}} = 0.74$, $\Omega_{\mathrm{b}} = 0.044$, $h = 0.715$ and a spectral index of $n_{\mathrm{S}} = 0.96$ (Sánchez et al. 2009). The linear theory rms fluctuation in spheres of radius 8 h^{-1} Mpc is set to be $\sigma_8 = 0.8$.

Within the code of `L-Gadget-2`, under the assumption that the dark energy is a smooth background, the only place where dark energy needs to be accounted for within the code of `L-Gadget-2`, is in the calculation of the Hubble factor. This is needed, for example, when converting from the internal time variable, $\log a$ to a physical time, t, or when converting to physical quantities in the equations of motion. The Hubble parameter for dynamical dark energy in a flat universe is given by

$$\frac{H^2(z)}{H_0^2} = \left(\Omega_{\rm m}\,(1+z)^3 + (1-\Omega_{\rm m})e^{3\int_0^z {\rm d}\ln(1+z')\,[1+w(z')]}\right), \tag{2.6}$$

where H_0 and $\Omega_{\rm m} = \rho_{\rm m}/\rho_{\rm crit}$ are the values of the Hubble parameter and dimensionless matter density, respectively, at redshift $z = 0$ and $\rho_{\rm crit} = 3H_0^2/(8\pi G)$ is the critical density. The details of the dark energy equation of state, $w(z)$, for each quintessence model are given in Chap. 3.

In Chaps. 3 and 4, the simulations use $N = 646^3 \sim 269\times10^6$ particles to represent the dark matter in a computational box of comoving length 1,500 $\rm h^{-1}$ Mpc. These simulations took 3 days to run with typically $\sim$3000 time steps on 38 processors of the Cosmology Machine (COSMA) at Durham university. We chose a comoving softening length of $\varepsilon = 50\,\rm h^{-1}$ kpc. The particle mass in the simulation is $9.02\times10^{11}\,\rm h^{-1}\,M_\odot$ with a mean interparticle separation of $r \sim 2.3\,\rm h^{-1}$ Mpc. The simulation code `L-Gadget-2` has an inbuilt friends-of-friends (FOF) group finder which was applied to produce group catalogues of dark matter particles with 10 or more particles. A linking length of 0.2 times the mean interparticle separation was used in the group finder (Davis et al. 1985).

In Chap. 5 the simulations use $N = 1024^3 \sim 1\times10^9$ particles in a computational box of comoving length 1,500 $\rm h^{-1}$ Mpc. The comoving softening length was $\varepsilon = 50\,\rm h^{-1}$ kpc and the simulations took 5 days to run on 128 processors on COSMA. The `L-Gadget-2` simulation code (Springel 2005) was modified to allow for a time-varying Newton's constant and a dynamical quintessence dark energy. As discussed in the previous section, in this code the gravitational forces are computed using a TreePM algorithm where short-range forces are calculated using a 'tree' method and the long-range part of the force is obtained using mesh based Fourier methods. In the modified gravity simulation, both the long and short-range force computations were modified to include a time-dependent gravitational constant. For both the modified gravity and the quintessence dark energy simulations in Chap. 5 the Hubble parameter computed by the code was also modified (see Chap. 5 for details).

2.1.3 The Initial Conditions

There are two steps needed to set up the initial conditions for an N-body simulation. In the first step an unperturbed Universe is created by setting up a uniform distribution of particles which, in the second step, is perturbed so that the resulting density

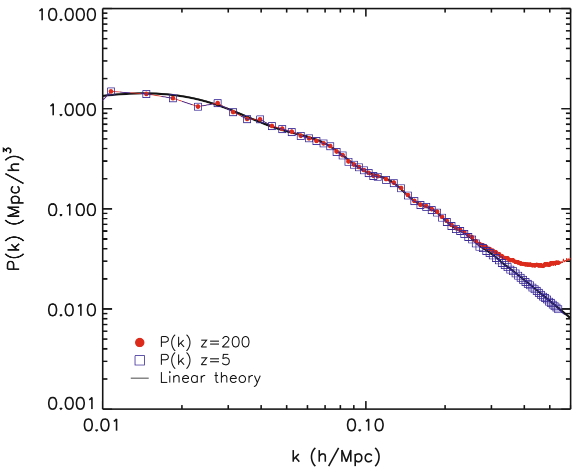

Fig. 2.1 The power spectrum measured from the simulation at $z = 200$ (*circles*) together with the power spectrum at $z = 5$ (*squares*) scaled to $z = 200$ by the squared ratio of the growth rates at the two redshifts. The linear perturbation theory prediction is shown as a *black line*

distribution has the appropriate power spectrum. An initially random distribution of particles will evolve into rapidly growing non linear structures due to the presence of Poisson shot noise on all scales. The initial 'white noise spectrum', in this case, is $|\delta_k|^2 \propto k^n$ where $n = 0$. A better way to generate a uniform distribution is to place the particles on a regular cubic grid, where there is no power above the nyquist frequency of the grid. This method also has its disadvantages as the regularity and size of the grid is imprinted as a characteristic length scale which is visible in the evolved particle distribution. Another method used to generate a uniform distribution of particles which has no regular structure, involves firstly placing the particles at random in a simulation volume. An N-body simulation code, which has been modified by reversing the sign of the acceleration, then follows the motion of the particles in an Einstein de Sitter expanding Universe. As a result the gravitational forces on the particles are repulsive and after many expansion factors they settle down to a 'glass-like' configuration where the distribution is sub-random and shows no order or anisotropy on scales comparable to the mean interparticle spacing (White 1994a; Baugh et al. 1995). The initial conditions of the particle load for the simulations in this thesis were set up with a glass configuration of particles.

In order to impose the density perturbations on the glass, the particles are perturbed using the Zel'dovich approximation (Zel'Dovich 1970) which moves the initially unperturbed particles to create a discrete density field using

$$\vec{x} = \vec{x_0} - \frac{D(\tau)}{4\pi G\bar{\rho}a^3}\nabla\Phi_0 \tag{2.7}$$

$$\vec{v} = -\frac{1}{4\pi G\bar{\rho}a^2}\frac{a\dot{D}}{D}\nabla\Phi, \tag{2.8}$$

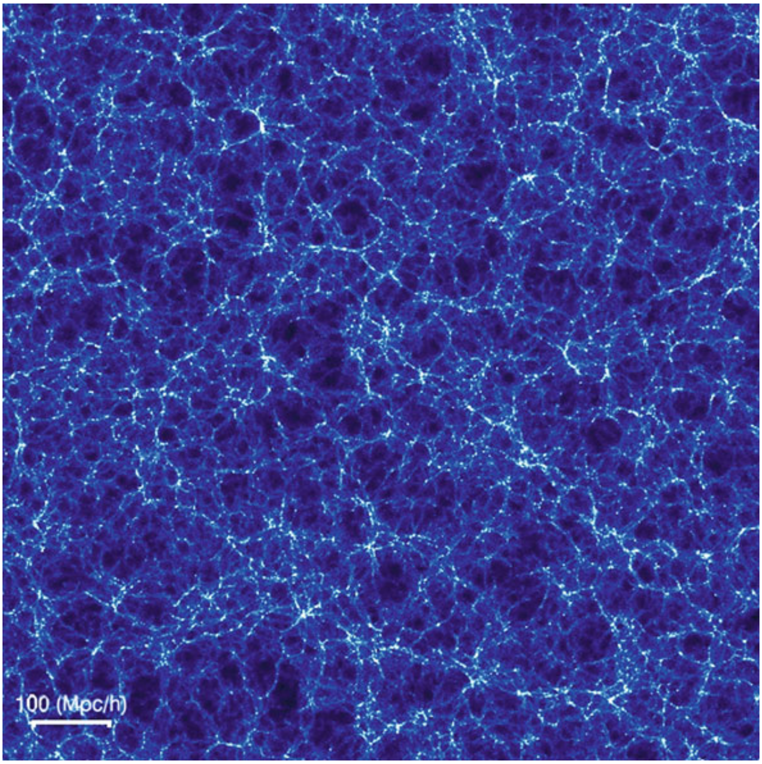

Fig. 2.2 The *dark* matter distribution from a simulation using 646^3 particles to represent the dark matter distribution in box of $1{,}500\,\mathrm{h}^{-1}$ Mpc on a side at redshift $z = 0$

where the Eulerian position, $\vec{x}$, and the peculiar velocity, $\vec{v}$, of each particle are given as a function of its initial Lagrangian position, $\vec{x_0}$, and $D(\tau)$ is the growing mode of linear fluctuations as a function of conformal time, $\mathrm{d}\tau = a^{-1}\mathrm{d}t$ (e.g. Efstathiou et al. 1985; White 1994b). The displacement field, $\nabla\Phi$, is related to a precalculated input power spectrum, $P(k)$, with the desired cosmology. The initially uniform density field is then realised as a Gaussian random field with a random phase. The Zel'dovich approximation can induce small scale transients in the measured power spectrum. These transients die away after $\simeq$10 expansion factors from the starting redshift (Smith et al. 2003). In order to limit the effects of the initial displacement scheme we chose a starting redshift of $z = 200$. In this thesis the linear theory power spectrum used to generate the initial conditions was created using the CAMB package of Lewis and Bridle (2002). The linear theory $P(k)$ output at $z = 0$ was then evolved backwards to the starting redshift of $z = 200$ using the linear growth factor for that cosmology in order to generate the initial conditions for `L-Gadget-2`. The details of the linear power spectra used for each dark energy model is outlined in Chap. 3. The initial power spectrum output at $z = 200$ is shown in Fig. 2.1 (circles) together with the linear perturbation theory (black line) and the power spectrum output at $z = 5$ (squares) scaled to $z = 200$ using the squared ratio of the growth rates at the two redshifts. The power spectrum is drawn from a distribution which results in fluctuations at low k, on large scales, due to the finite number of modes available in the simulation volume. The sample variance fluctuation can be clearly seen in the $z = 200$ and the $z = 5$ power spectra on large scales. The $z = 5$ output agrees very well with linear perturbation theory. In subsequent chapters in this thesis we shall use the $z = 5$ output in ratios to show deviations in growth from linear theory and to remove the sample variance present on large scales. In Fig. 2.2 we plot the dark matter distribution at $z = 0$ in a 2D slice through the simulation with 646^3 particles in a box of 1,500 h^{-1} Mpc in length.

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