Particle-Mesh code for cosmological simulations

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Abstract

Particle-Mesh (PM) codes are still very useful tools for testing predictions of cosmological models in cases when extra high resolution is not very important. We release for public use a cosmological PM N-body code. The code is very fast and simple. We provide a complete package of routines needed to set initial conditions, to run the code, and to analyze the results. The package allows you to simulate models with numerous combinations of parameters: open/flat/closed background, with or without the cosmological constant, different values of the Hubble constant, with or without hot neutrinos, tilted or non-tilted initial spectra, different amount of baryons.

Routines are included to measure the power spectrum and the density distribution function in your simulations, and a bound-density-maxima code for halo finding. We also provide results of test runs. A simulation with 256^3 mesh and 128^3 particles can be done in a couple of days on a typical workstation (about 70Mb of memory is needed). To run simulations with 800^3 mesh and 256^3 particles one needs a computer with 1Gb memory and 1Gb disk space. The code has been successfully tested on an HP workstation and on a Sun workstation running Solaris, but we expect it should work on other systems.

The package can be downloaded from http://astro.nmsu.edu/∼aklypin/PM/PMcode.tar.gz A PostScript version of this manual can be obtained from http://astro.nmsu.edu/∼aklypin/PM/PMcode.ps.gz

We provide this tool as a service to the astronomical community, but we cannot guarantee results.

1 Introduction

There are many different numerical techniques to follow the evolution of a system of many particles. For earlier reviews see Hockney & Eastwood (1981) and Sellwood (1987). The most frequently used methods for cosmological applications fall in three classes: Particle Mesh (PM) codes, Particle-Particle/Particle-Mesh (P^3M) codes, and TREE codes. All methods have their advantages and disadvantages.

PM codes use a mesh for the density and potential. As a result, their resolution is limited by the size of the mesh. The largest simulations done by the author have been on a 800^3 mesh with $3 \times 256^3 = 1.5 \times 10^8$ particles. The SP2 parallel supercomputer at Cornell has been used to run simulations with a $1600^3 = 4.096 \times 10^9$ mesh (Gross, 1997). There are two advantages of the method: i) it is fast (the smallest number of operations per particle per time step of all the other methods), ii) it typically uses very large number of particles. The latter can be crucial for some applications. There are a few variants of PM codes. A "plain-vanilla" PM was described by Hockney & Eastwood (1981), and this includes a Cloud-In-Cell density assignment and a 7-point discrete analog of the laplacian operator. Higher order approximations improve the accuracy on large distances, but degrade the resolution (e.g. Gelb (1992)). In an effort to reduce the order of approximation and to increase the resolution, Melott (1986) introduced the staggered mesh. It gives a better resolution on cell-size distances, but particles get self-forces (an isolated particle experiences a force from itself), which might be not a welcome feature.

P^3M codes are described in detail in Hockney & Eastwood (1981) and in Efstathiou et al.(1985). They have two parts: a PM part, which takes care of large-scale forces, and a PP part, which adds a small-scale particle-particle contribution. The simulations usually have 64^3–100^3 particles. Because of strong clustering at late stages of evolution, the PP part becomes prohibitively expensive once large objects start to form

in large numbers. Significant speed is achieved in a modified version of the code which introduces subgrids (next levels of PM) in areas with high density (AP^{3}M code of Couchman (1991)). With modification this code runs as fast as TREE code even for heavily clustered configurations (Couchman 1991).

TREE codes are the most flexible code in the sense of the choice of boundary conditions (Appel 1985, Barnes & Hut 1986, Hernquist 1987). They are also more expensive than PM: it takes 10-50 times more operations. Bouchet & Hernquist (1986) and Hernquist, Bouchet & Suto (1991) have extended the code for the periodical boundary conditions, which are important for simulating large-scale fluctuations.

Multigrid methods were introduced long ago, but only recently have they started to show a potential to produce real results (Anninos, Norman & Clarke 1994, Suisalu & Saar 1995, Kravtsov et al.1997). At present the most advanced and fastest multigrid code has been developed by Kravtsov et al.(1997).

2 Equations and dimensionless variables

The equations of motion of particles in expanding coordinates, which are used in our PM code, were presented by Kates et al.(1991). Different numerical effects (including resolution) were discussed in Klypin et al.(1996). We use comoving coordinates ofr particles $\mathbf{x} = \mathbf{x}(t)$, which are related to proper coordinates by $\mathbf{r} = a(t)\mathbf{x}$, where $a(t) = (1+z)^{-1}$ is the expansion parameter. Instead of using peculiar velocity $\mathbf{v}_{\rm pec} = a\dot{\mathbf{x}}$ we write the equations for particle momenta $\mathbf{p}$:

$$\mathbf{p} = a^2\dot{\mathbf{x}}, \quad \mathbf{v}_{\rm pec} = \mathbf{p}/a \tag{1}$$

This choice of "velocity" simplifies the equations of motion by removing a few terms with $\dot{a}/a$. It is also convenient to change the time variable from time t to the expansion parameter a. The equations governing the motion of particles are:

$$\frac{d\mathbf{p}}{da} = -\frac{\nabla\phi}{\dot{a}}, \quad \frac{d\mathbf{x}}{da} = \frac{\mathbf{p}}{\dot{a}a^2} \tag{2}$$

$$\nabla^2\phi = 4\pi G\Omega_{\rm m}(t)a^2\rho_{\rm cr}(t)\delta = 4\pi G\Omega_0\rho_{\rm cr,0}\frac{\delta}{a}, \quad \delta \equiv \frac{\rho(\mathbf{x})-\rho_b}{\rho_b}, \tag{3}$$

$$\dot{a}\sqrt{a} = H_0\sqrt{\Omega_0 + \Omega_{\rm curv,0}a + \Omega_{\Lambda,0}a^3}, \quad \Omega_0 + \Omega_{\rm curv,0} + \Omega_{\Lambda,0} = 1, \tag{4}$$

where $\Omega_0 = \Omega_m(z=0)$, $\Omega_{\rm curv,0}$, and $\Omega_{\Lambda,0}$ are the density of the matter, effective density of the curvature, and the cosmological constant in units of the critical density at $z = 0$. The curvature contribution is positive for negative curvature.

Dimensionless variables (shown with tildas below) are defined by introducing the length of a cell of the grid x_0 and by measuring the time in units of $1/H_0$:

$$\mathbf{x} = x_0\tilde{\mathbf{x}}, \quad t = \tilde{t}/H_0, \tag{5}$$

$$\mathbf{v}_{\rm pec} = (x_0H_0)\tilde{\mathbf{p}}/a, \quad \phi = \tilde{\phi}(x_0H_0)^2 \tag{6}$$

$$\rho = \frac{\tilde{\rho}}{a^3}\frac{3H_0^2}{8\pi G}\Omega_0 \tag{7}$$

Equations (2–5) can be rewritten in terms of dimensionless variables:

$$\frac{d\tilde{\mathbf{p}}}{da} = -F(a)\tilde{\nabla}\tilde{\phi}, \quad \frac{d\tilde{\mathbf{x}}}{da} = F(a)\frac{\tilde{\mathbf{p}}}{a^2} \tag{8}$$

$$\tilde{\nabla}^2\tilde{\phi} = \frac{3}{2}\frac{\Omega_0}{a}(\tilde{\rho} - 1), \tag{9}$$

where

$$F(a) \equiv H_0/\dot{a} = \left(\frac{\Omega_0 + \Omega_{\rm curv,0}a + \Omega_{\Lambda,0}a^3}{a}\right)^{-1/2}. \tag{10}$$

Equations (8 – 9) are solved numerically by the PM code.

If L is the length of the computational box at $z = 0$, $N_{\rm grid}$ is the number of grid cells in one direction, and $N_{\rm row}$ is the number of particles in one direction, which contribute a fraction Ω_0 of the critical density, then the transformations from dimensionless variables given by the code to dimensional variables are given by

$$x = x_0\tilde{x}, \quad x_0 = \frac{L}{N_{\rm grid}} = 7.8{\rm kpc}\left(\frac{L_{\rm Mpc}}{N_{\rm grid}/128}\right), \tag{11}$$

$$v_{\rm pec} = (x_0 H_0)\frac{\tilde{p}}{a} = 0.781\frac{\rm km}{\rm s}\cdot\frac{\tilde{p}}{a}\cdot\frac{L_{\rm Mpc}h}{N_{\rm grid}/128}, \tag{12}$$

$${\rm Mass} = N_{\rm particles}\cdot m_1, \quad m_1 = \Omega_0\rho_{\rm cr,0}\left(\frac{L}{N_{\rm row}}\right)^3 = 1.32\cdot 10^5(\Omega_0 h^2)\left(\frac{L_{\rm Mpc}}{N_{\rm row}/128}\right)^3 \tag{13}$$

3 Scheme of integration

Equations (8 – 9) are solved using finite differences with a constant step in space $\Delta x = \Delta y = \Delta z = 1$ and a constant step in the expansion parameter Δa. We use the "leap-frog" scheme to advance coordinates and velocities from one moment to another. (In the following we drop tildas for all dimensionless variables.) At any moment $a_n = a_0 + n\Delta a$, we have the coordinates $\mathbf{x}_n$ and the potential ϕ_n. Velocities $\mathbf{p}_{n-1/2}$ are defined at $a_{n-1/2} = a_n - \Delta a/2$. The coordinates and the velocities for the next moment are found using:

$$\begin{aligned} \mathbf{p}_{n+1/2} &= \mathbf{p}_{n-1/2} - F(a_n)\nabla\phi_n\Delta a, \\ \mathbf{x}_{n+1} &= \mathbf{x}_n + \frac{F(a_{n+1/2})}{a^2_{n+1/2}}\mathbf{p}_{n+1/2}\Delta a \end{aligned} \tag{14}$$

In order to solve eq.(9) we approximate the Laplacian operator using the 7-point "crest" template:

$$\nabla^2\phi \approx \phi_{i\pm1,j,k} + \phi_{i,j\pm1,k} + \phi_{i,j,k\pm1} - 6\phi_{i,j,k}, \tag{15}$$

where $(i, j, k) = 1, ..., N_{\rm grid}$. This leads to a large system of linear equations relating unknown variables $\phi_{i,j,k}$ with known right-hand side of the discrete form of the Poisson equation $3\Omega_0(\rho_{i,j,k} - 1)/2a$. The system of equations is solved exactly by the FFT technique.

The density on the mesh $\rho_{i,j,k}$ is obtained from particle positions using the Cloud-In-Cell method. In order to find the "acceleration" $\mathbf{g} = -\nabla\phi$ for each particle, the gravitational potential is differentiated on the mesh:

$$g_x = -(\phi_{i+1,j,k} - \phi_{i-1,j,k})/2, \quad g_y = ..., \quad g_z = ... \tag{16}$$

Then the acceleration is interpolated to the position of the particle using a three-linear interpolation. This scheme for the force interpolation (the same interpolation as in the density assignment) is very important because it does not produce a force acting on the particle itself. (Thus, an isolated point does not produce a force at the position of the particle). While this might sound like a natural condition for any realistic method, only two methods – PM and TREE – do not have this self-force. In P^3M the effect is minimized. In the case of multigrid methods the self-force cannot be excluded – only minimized. Typically this is achieved by placing extended buffer zones around regions with high resolution (e.g. Kravtsov 1997). No precautions were made in AP^3M method, which might result in spurious effects in regions were multi-level grids are introduced.

Thus, the main scheme of the PM method consists of the following four blocks repeated every time step:

- Find density on the mesh using the Cloud-In-Cell technique.
- Solve the Poisson equation using two three-dimensional FFTs.
- Advance velocities and coordinates of the particles.
- Advance time and print results.

4 Format of data

In order to have the best possible resolution, most of the available computer memory is allocated to the density/potential grid. The Poisson solver is organized in such a way that only one large mesh is needed. Particle coordinates and velocities are kept on disk and are read into memory in large portions when necessary. This reading/writing of particles results in a small overhead – typically 5-10% of the total cpu time. If this overhead is an issue, the code can be easily adjusted to keep all particles in memory. This is always the case for a parallel version of the code. Particles are divided into "species" with constant mass of a particle for each species. Each species is kept in a separate file. Information which describes the run (such as the number of particles, omegas, and current time) is written in a separate header file.

Each file with particle data is a FORTRAN direct-access file with the number of records equal to the number of particles in one direction $N_{\rm row}$. Each record has coordinates and velocities for a "page" of particles $N_{\rm page} = N_{\rm row}^2$. The "page" of particles is read into a common block, which has the structure: $X(N_{\rm page}), Y(N_{\rm page}), Z(N_{\rm page}), V_x(N_{\rm page}), V_y(N_{\rm page}), V_z(N_{\rm page})$ The particle files and the header file are needed for continuation of the run or for the data analysis. The following diagram shows the structure and names of the data files:

C3CRD.DAT	Header		Text-of-Header, a, $a_{\rm init}$, Δa, Step,...
C3crs0.DAT	Set 0	Page 1	$x_1, x_2, \ldots x_{\rm Npage}$, $y_1, \ldots$ $z_1, \ldots$ $V_{x1}, \ldots$ $V_{z{\rm Npage}}$
		Page 2	$x_1, x_2, \ldots x_{\rm Npage}$, $y_1, \ldots$ $z_1, \ldots$ $V_{x1}, \ldots$ $V_{z{\rm Npage}}$
		...	...
		...	...
		Page $N_{\rm row}$	$x_1, x_2, \ldots x_{\rm Npage}$, $y_1, \ldots$ $z_1, \ldots$ $V_{x1}, \ldots$ $V_{z{\rm Npage}}$
C3crs1.DAT	Set 1	Page 1	$x_1, x_2, \ldots x_{\rm Npage}$, $y_1, \ldots$ $z_1, \ldots$ $V_{x1}, \ldots$ $V_{z{\rm Npage}}$
		Page 2	$x_1, x_2, \ldots x_{\rm Npage}$, $y_1, \ldots$ $z_1, \ldots$ $V_{x1}, \ldots$ $V_{z{\rm Npage}}$
		Page $N_{\rm row}$	$x_1, x_2, \ldots x_{\rm Npage}$, $y_1, \ldots$ $z_1, \ldots$ $V_{x1}, \ldots$ $V_{z{\rm Npage}}$
...			

File Name — Description — Content of the file

Not a part of the file

Thus, the memory required to run the code is about $N_{\rm grid}^3 + 6N_{\rm row}^2$ memory words or 64Mb$(N_{\rm grid}/256)^3$ +0.375Mb$(N_{\rm row}/128)^2$ if single precision arithmetic is used. The total amount of disk space is 48Mb$(N_{\rm row}/128)^3$ per each set of "species".

5 Initial conditions: CDM and CHDM models

We use the Zeldovich approximation to set initial conditions. The approximation is valid in mildly nonlinear regime and is much superior to the linear approximation. We slightly rewrite the original version of the approximation to incorporate cases (like CHDM) when the growth rates $b(t)$ depend on the wavelength of the perturbation $|k|$. In the Zeldovich approximation the comoving and the lagrangian coordinates are related in the following way:

$$\mathbf{x} = \mathbf{q} - \alpha \sum_{\mathbf{k}} b_{|k|}(t) \mathbf{S}_{|k|}(\mathbf{q}), \quad \mathbf{p} = -\alpha a^2 \sum_{\mathbf{k}} b_{|k|}(t) \left(\frac{\dot{b}_{|k|}}{b_{|k|}} \right) \mathbf{S}_{|k|}(\mathbf{q}), \tag{17}$$

where the displacement vector $\mathbf{S}$ is related to the velocity potential Φ and the power spectrum of fluctuations $P(|k|)$:

$$\mathbf{S}_{|k|}(\mathbf{q}) = \nabla_q \Phi_{|k|}(\mathbf{q}), \quad \Phi_{|k|} = \sum_{\mathbf{k}} a_{\mathbf{k}} \cos(\mathbf{kq}) + b_{\mathbf{k}} \sin(\mathbf{kq}), \tag{18}$$

where a and b are gaussian random numbers with the mean zero and dispersion $\sigma^2 = P(k)/k^4$:

$$a_{\mathbf{k}} = \sqrt{P(|k|)} \cdot \frac{Gauss(0,1)}{|k|^2}, \quad b_{\mathbf{k}} = \sqrt{P(|k|)} \cdot \frac{Gauss(0,1)}{|k|^2}. \tag{19}$$

The parameter α, together with the power spectrum $P(k)$, define the normalization of the fluctuations.

We estimate the power spectrum $P(k)$ for a wide range of cosmological models using a Boltzman code (Holtzman 1989). As compared with the original version of the code, the current version allows for more accurate estimates at high wavenumbers. For each cosmological model the numerical data points were fitted using the following fitting formula:

$$P(k) = \frac{k^n \exp(P_1)}{(1 + P_2 k^{1/2} + P_3 k + P_4 k^{3/2} + P_5 k^2)^{2P_6}}. \quad (20)$$

The coefficients P_i are presented in the file **cdm.fit** for a variety of models. The errors of the fits are smaller than 5% in the power spectrum. The top panel in Figure 1 shows the errors of the fits for CDM models ($\Omega_0 = 1$) with a Hubble constant $H = 50$km/s/Mpc. Errors at a level of $\sim 2\%$ level at $k \sim 3h$ Mpc^{-1} and at $k \sim 30h$ Mpc^{-1} are due to small mismatch in approximations used at high wavenumbers. The fits smooth out the jumps and, thus, provide better approximations to the real power spectra at those large wavenumbers. The waves around $k \sim 0.1h$ Mpc^{-1} are due to acoustic oscillations in baryons. They are larger for larger Ω_b/Ω_0 ratios. For very small Ω_b/Ω_0 the errors introduced by using the fits are extremely small. Thus, if one can neglect (or smooth out) the acoustic oscillations, the maximum errors of our fits are expected to be smaller than 1–2% in the power. The comparison of some of our power spectra with the results from COSMICS (Bertschinger 1996) support our conclusion. We recommend the use of the fits whenever it is possible.

The power spectrum of cosmological models is often approximated using a fitting formula given by Bardeen et al.(1986, BBKS):

$$P(k) = k^n T^2(k), \quad T(k) = \frac{\ln(1 + 2.34q)}{2.34q}[1 + 3.89q + (16.1q)^2 + (5.4q)^3 + (6.71q)^4]^{-1/4}, \quad (21)$$

where $q = k/(\Omega_0 h^2$ Mpc$^{-1})$. Unfortunately, the accuracy of this approximation is not great. Peacock & Dodds (1994) modified the fit using another relation between q and k:

$$q = k/(\Omega_0 h^2 \exp(-2\Omega_b)\ \text{Mpc}^{-1}). \quad (22)$$

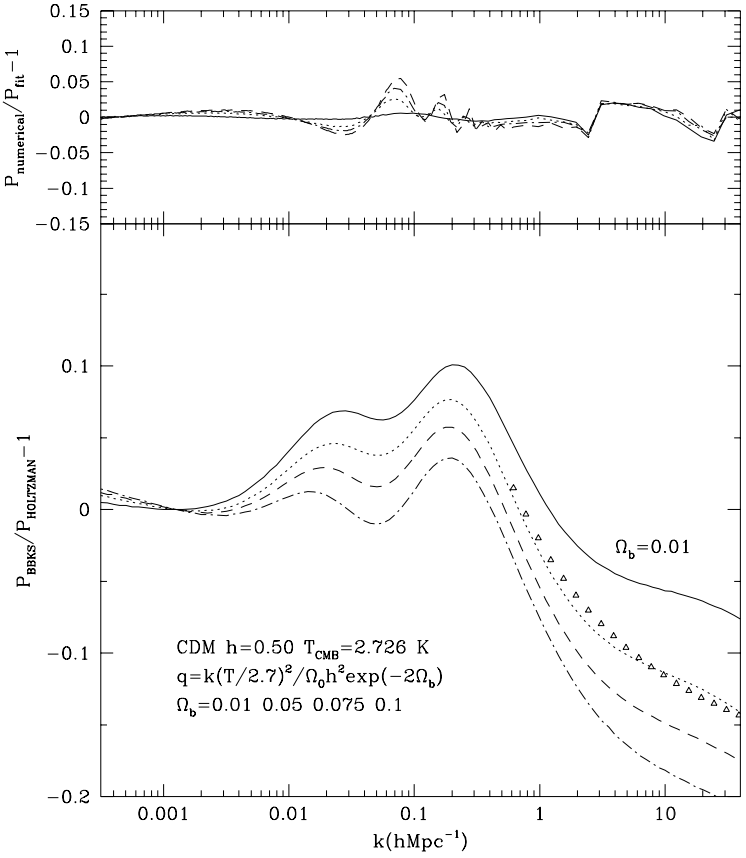
This approximation was criticized by Sugiyama (1995), who introduced a better scaling for low-Ω_0 cases:

$$q = \frac{k(T_{\rm CMB}/2.7K)^2}{\Omega_0 h^2 \exp(-\Omega_b - \sqrt{h/0.5}\Omega_b/\Omega_0)\ \text{Mpc}^{-1}}. \quad (23)$$

These approximations have been frequently used in a number of publications (e.g. Liddle et al.1996). The bottom panel of Figure 1 shows the ratio of the power spectrum given by this approximation to the power spectrum obtained from our fits for several choices of baryon fraction. For comparison, we also present the error of the eqs.(21-23) relative to the power spectrum obtained by COSMICS for $\Omega_b = 0.05$ (triangles), showing the good agreement of our results with those of COSMICS. In all cases, there is a large decline (around 20% in power) between a peak at $k = 0.2h$ Mpc^{-1} and small scales $k \sim (10 - 30)h$ Mpc^{-1}. This decline was noticed by Hu & Sugiyama (1996), who studied the small-scale perturbations. Note that if we take $T_{\rm CMB} = 2.70$K instead of 2.726K, than the peak of the error at $k = 0.2$ increases up to 15%. The error in the power is rather small for small $k < 0.1h$ Mpc^{-1} and for a realistic amount of baryons $\Omega_b \sim 0.07$. One can easily miss it if instead of an error of the power spectrum, one plots the transfer function in a double logarithmic scale. But the error is very significant for galactic-scale events. It can result in serious errors in the epoch of galaxy formation or in the amount of gas in damped Ly-α clouds at high redshifts.

Hu & Sugiyama (1996) recommend changing the last parameter in the BBKS fit from 6.71 to 6.07. We do not find that this correction gives an accurate fit to our spectrum. We find that the following approximation, which is a combination of a slightly modified BBKS fit and the Hu & Sugiyama (1996) scaling with the amount of baryons, provides errors in the power spectrum smaller than 5% for the range of wavenumbers $k = (10^{-4} - 40)h$ Mpc^{-1} and for $\Omega_b/\Omega_0 < 0.1$:

Figure 1: (Top) Errors of the fits eq.(20) for the CDM models ($\Omega_0 = 1$) with a Hubble constant $H = 50$km/s/Mpc. Errors at the $\sim 2\%$ level at $k \sim 3h$ Mpc^{-1} and at $k \sim 30h$ Mpc^{-1} are due to a small mismatch in approximations used at high wavenumbers. The fits smooth out the jumps and, thus, provide better approximations to the real power spectra at these large wavenumbers. The waves around $k \sim 0.1h$ Mpc^{-1} are due to acoustic oscillations in baryons. (Bottom) The differences between the power spectrum given by the BBKS approximation and the power spectrum obtained from our fits. Triangles show results obtained using COSMICS for $\Omega_b = 0.05$



$$
\begin{aligned}
P(k) &= k^n T^2(k), \\
T(k) &= \frac{\ln(1+2.34q)}{2.34q}[1+13q+(10.5q)^2+(10.4q)^3+(6.51q)^4]^{-1/4}, \\
q &= \frac{k(T_{\rm CMB}/2.7K)^2}{\Omega_0 h^2 \alpha^{1/2}(1-\Omega_b/\Omega_0)^{0.60}}, \qquad \alpha = a_1^{-\Omega_b/\Omega_0} a_2^{-(\Omega_b/\Omega_0)^3} \\
a_1 &= (46.9\Omega_0 h^2)^{0.670}[1+(32.1\Omega_0 h^2)^{-0.532}], \quad a_2 = (12\Omega_0 h^2)^{0.424}[1+(45\Omega_0 h^2)^{-0.582}]
\end{aligned} \tag{24}
$$

Figures 2 and 3 show errors of the fits for the CDM and for the ΛCDM models.

6 Finding Halos with Bound Density Maxima code

Finding halos in dense environments is a challenge. The most widely used halo-finding algorithms – the friends-of-friends (e.g., Efstathiou et al.1985) and the spherical overdensity algorithm (e.g., Lacey & Cole 1994; Klypin 1996) – are not acceptable (Gelb & Bertschinger 1994, Summers et al.1995). The friends-of-friends (FOF) algorithm merges together apparently distinct halos if the linking radius is too large or misses some of the halos if the radius is small. Adaptive FOF (van Kampen 1995) seems to work better. But we find that it is difficult to find an optimal scaling of the linking radius with the density. We have developed a related algorithm (Klypin, Gottlober, Kravtsov 1997), which we call "hierarchical friends-of-friends". Because it uses all linking radii, it does not have the problem that the adaptive FOF algorithm has. The algorithms, either adaptive or hierarchical, can not work because they pick up many fake halos in very dense environments. Klypin et al.(1997) supplement the hierarchical FOF algorithm with an algorithm which checks if halos existed at previous moments. The algorithm which finds halos as maxima of mass inside spheres of a given overdensity works better than plain FOF, but no fixed overdensity limit can find halos in both low and high density environment. The DENMAX algorithm (Gelb & Bertschinger 1994) and its offspring, SKID (Governato et al.1997), make significant progress – they remove unbound particles, which is important for halos in groups and clusters. Recently, Summers et al.(1995) tried to perfect the idea of Couchman & Carlberg (1992) to trace the history of halo merging and to use it for halo identification. Starting at an early epoch, Summers et al.identify halos using the FOF algorithm with a linking radius corresponding to the "virial overdensity" of 200 and then trace particles belonging to halos at later times. It appears that it is impossible to make a working algorithm because halos interact too violently. A large fraction of mass is tidally stripped from some halos and a large fraction of mass is accreted. Some of the problems that any halo finding algorithm faces are not numerical. They exist in the real Universe. We select a few typical difficult situations.

1. *A large galaxy with a small satellite.* Examples: LMC and the Milky Way or the M51 system. Assuming that the satellite is bound, do we have to include the mass of the satellite in the mass of the large galaxy? If we do, then we count the mass of the satellite twice: once when we find the satellite and then when we find the large galaxy. This does not seem reasonable. If we do not include the satellite, then the mass of the large galaxy is underestimated. For example, the binding energy of a particle at the distance of the satellite will be wrong. The problem arises when we try to assign particles to different halos in an effort to find masses of halos. This is very difficult to do for particles moving between halos. Even if a particle at some moment has negative energy relative to one of the halos, it is not guaranteed that it belongs to the halo. The gravitational potential changes with time, and the particle may end up falling onto another halo. This is not just a precaution. This actually was found very often in real halos when we compared contents

Figure 2: Errors of the approximation eqs.(24) for the CDM models with different Hubble constants and amount of baryons.

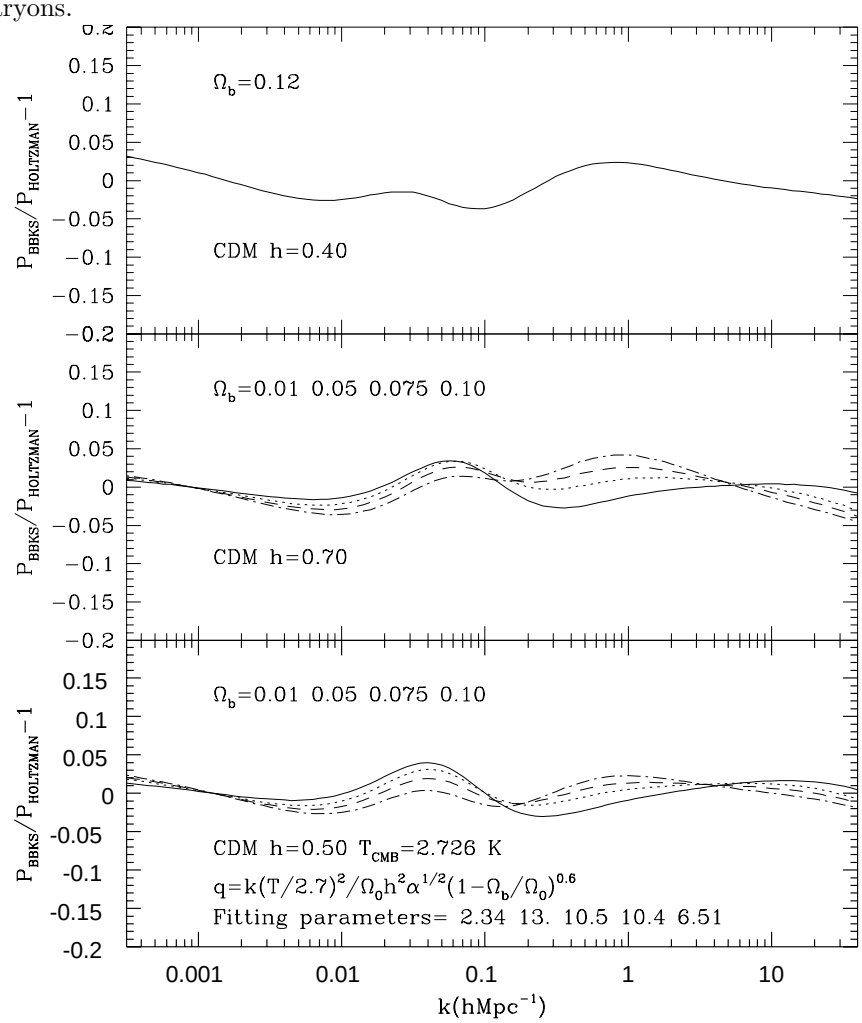
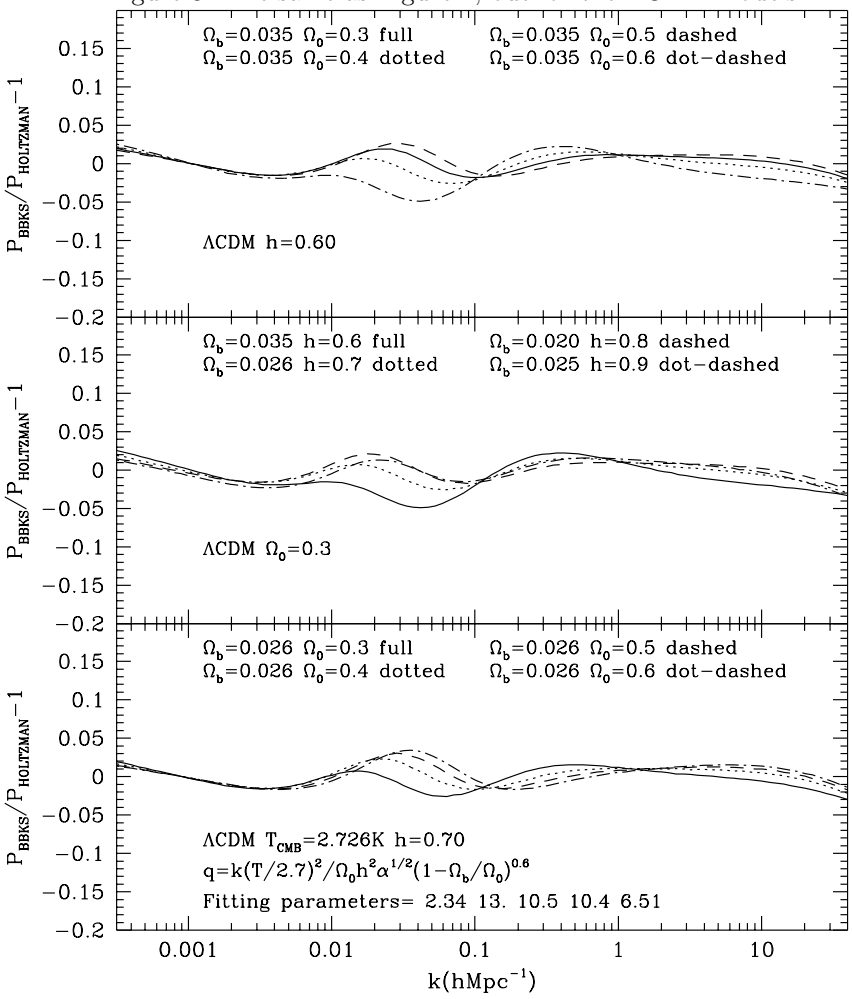


Figure 3: The same as Figure 2, but for the ΛCDM models.



of halos at different redshifts. Interacting halos exchange mass and lose mass. We try to avoid the situation: instead of assigning mass to halos, we find the maximum of the "rotational velocity", $\sqrt{GM/R}$, which is observationally a more meaningful quantity.

2. *A satellite of a large galaxy.* The previous situation is now viewed from a different angle. How can we estimate the mass or the rotational velocity of the satellite? The formal virial radius of the satellite is large: the big galaxy is within the radius. The rotational velocity may rise all the way to the center of the large galaxy. In order to find the outer radius of the satellite, we analyze the density profile. At small distances from the center of the satellite the density steeply declines, but then it flattens out and may even increase. This means that we reached the outer border of the satellite. We use the radius at which the density starts to flatten out as the first approximation for the radius of the halo. This approximation can be improved by removing unbound particles and checking the steepness of the density profile in the outer part.

3. *Tidal stripping.* Peripheral parts of galaxies, responsible for extended flat rotation curves outside of clusters, are very likely tidally stripped and lost when the galaxies fall into a cluster. The same happens with halos: a large fraction of halo mass may be lost due to stripping in dense cluster environments. Thus, if an algorithm finds that 90% of mass of a halo identified at early epoch is lost, it does not mean that the halo was destroyed. This is not a numerical effect and is not due to "lack of physics". This is a normal situation. What is left of the halo, given that it still has a large enough mass and radius, is a "galaxy".

We have developed our halo-finding algorithm (Klypin et al.1997) having in mind all these problems. The bound-density-maxima (BDM) algorithm stems from the DENMAX algorithm (Gelb & Bertschinger 1994). Just as in DENMAX, the BDM algorithm first finds positions of the density maxima on some scale and then removes unbound particles inside the halo radius. However, the algorithm finds maxima and removes unbound particles in a way different from DENMAX. The algorithm can work by itself or in conjunction with the hierarchical FOF. In the latter case, it takes positions of halos from the hierarchical friends-of-friends, and then removes unbound particles and finds parameters of halos.

In order to find positions of halos we choose a radius r_{sp} of a sphere for which we find maxima of mass. This defines the *scale* of objects we are looking for, but not exact radii or masses of halos. The radius of a halo can be either larger or smaller than r_{sp}, but distances between halos cannot be smaller than r_{sp}. We place a large number of spheres in the simulation box. The number of the spheres is typically an order of magnitude or more larger than the expected number of halos. For each sphere we find the mass inside the sphere and the center of the mass. The center of the sphere is displaced to the center of mass and the new mass and the center of mass is found. The process is iterated until convergence. Depending on specific parameters of the simulations, the number of iterations ranges from 10 to 100. This process finds local maxima of mass within sphere of radius r_{sp}.

The efficiency of finding local maxima of mass depends on how the spheres are chosen. In the present version of the code two algorithms were implemented. (1) A small fraction of all particles are chosen as centers of the spheres. The code asks you to enter N_{seed}, the "Number of particles for initial seeds". Then it will select every $N_{particles}/N_{seed}$ particle as a center of a sphere. (2) Additional spheres will be placed in regions with relatively low density. The whole simulation box is divided into a mesh of large cells. The size of the cells is defined by the variable "Cell" in **PMhalos.f**. The "Cell" is typically equal to one or two PM cells. If a cell has many particles in it ("neighbors"), than some of them (not more than 3) will be chosen as centers of spheres. The code asks you to enter the minimum number of neighbors: "Number of neighbors for a seed".

In some cases one would need to improve the location of the halo. An example is if one is looking for groups of "galaxies" but also would like to have the groups always centered on a galaxy. The search radius for the groups may be chosen to be, say 500 kpc. Additional iterations with a smaller radius of the sphere will find the galaxy-size halo closest to the center of mass of the group and place the center of the group at

the "galaxy". In the BDM code this option is realized in the following way. The code asks you to enter the "smaller radius for final halos". If this radius r_{small} is not equal to the search radius r_{sp}, the code will do additional iterations by gradually changing the search radius from r_{sp} to r_{small}. If $r_{small} = r_{sp}$, no additional iterations are made.

Some of the density maxima will be found many times because in the process of maximizing the mass some of spheres converge on the same local maximum. Spheres which find the same maximum are called "duplicates". We remove duplicates and keep only one halo for each maximum. Halos with too small number of particles (typically 5–10) and halos with too low central overdensity are removed from the final list. Parameters which control the removal are supplied by the user.

Once centers of potential halos are found, we start the procedure of removing unbound particles and finding the structure of halos. We place concentric spherical shells around each center. For each shell we find the mass of the dark matter particles, the mean velocity, the velocity dispersion relative to the mean, and the maximum of the rotational velocity $V_{\rm max} = \sqrt{GM(r)/r}\mid_{max}$. In order to determine whether a particle is bound or not, we estimate the escape velocity at the distance r of the particle from the halo center:

$$V^2_{\rm escape}(r) \approx (2.15 \times V_{\rm max})^2 \frac{\ln(1+2r/r_{max})}{(r/r_{max})}, \tag{25}$$

where r_{max} is the radius of the maximum of the rotational velocity. This expression for the escape velocity is valid for a halo with the Navarro-Frenk-White density profile. If the velocity of a particle is larger than the escape velocity, it is assumed to be unbound. We estimate the maximum rotational velocity V_{max} and radius of the maximum r_{max} using the density profile for the halo. Because V_{max} and r_{max} must be found before the unbound particles are removed and because the mean velocity is also found using all particles (bound and unbound), the whole procedure cannot be done in one step. We start by artificially increasing the value of the escape velocity by a factor of three. Only particles above the limit are removed. We find a new density profile, new mean velocities, and new V_{max} and r_{max}. The escape velocity is again increased, but this time by a smaller factor. The procedure is repeated 6 times. The last iteration does not have any extra factors for the escape velocity: all unbound particles are removed. Examples of halos identified by the code are presented in Klypin et al.(1997).

Finding a halo radius is straightforward for isolated halos: increase the radius of sphere untill the overdensity inside the sphere is equal to some limiting value provided by the user. For halos inside groups or clusters (halos inside halos) the algorithm is more complicated. It consists of three steps: (i) It starts with finding the radius of given overdensity limit (as for an isolated halo). (ii) Then, the algorithm checks how the mean overdensity inside given radius changes with the radius. It starts going from the very central shell outwards. If the mean overdensity stops declining, the algorithm assigns the radius to the halo radius. (iii) Now the algorithm goes from this radius inwards and checks the slope n of the overdensity profile: $(M(r)/\langle M(r)\rangle) \propto r^{-n}$. If the slope is too shallow (mass increases too fast with the radius), the radius of the halo is decreased because most of the mass at this radius does not belong to the halo. The radius is decreased untill the slope is steep enough. The limit for the slope is equal to $n = 1$. This is a rather mild slope: for an isothermal sphere one expects $n = 2$; for the Navarro-Frenk-White profile $n = 1.7 - 2.5$.

The BDM code will ask you to enter many parameters. A typical dialog may look as follows:

```
Enter Min. Center Overdensity for Halos => 340.          (1)
Enter Overdensity Threshold for Halos   => 340.          (2)
Enter Minimum halo mass in Msun/h       => 5.e+9         (4)
Enter comoving search radius(Mpc/h)     => 0.050         (5)
Enter smaller radius(Mpc/h) of final halos=> 0.030       (6)
```

Enter min.radius for halos(Mpc/h) => 0.030 (7)
Enter fraction of DM particles (1/4,1/2,1)=> 1 (8)
Enter rejection velocity limit (V/Vescape)=> 1.0 (9)
Distance to check for Velocity duplicates => 0.300 (10)
Define duplicates if (v1-v2)/Vrms < 0.10 (11)
Enter Comoving Box size(Mpc/h) => 20. (12)

In lines (1-2), enter the minimum overdensity for halos. If both values are equal, the code will find halos with the overdensity above the limits you provided. You may choose only those halos which have higher central density, if you enter a larger number in the first line. Only halos with mass larger than the value entered in the third line and radius in the line 7 will be kept. For debugging of the code, you may read only 0.25, or 0.5 of all particles (line 8). If you would like to remove unbound particles as described above, enter 1 in line 9. In order to ignore the option (no removing of unbound particles) enter a number larger than 5. Lines 10 and 11 are used for two parameters needed for additional screening of duplicates. In case of very large halos, when the density profile in the center of the halo is rather flat, the iteration of spheres stops when the spheres are still far one from the other. The spheres have found the same object: masses, radii, velocities of the " halos" are very close, but their positions are slightly different. Because the fake halos have very close velocities, they can be identified. The parameter in the line 10 defines the maximum distance (in units of h^{-1}Mpc) within which the code will look for the duplicates. If the difference in velocities $\sqrt{(v_{x1}-v_{x2})^2+(.y)+(.z)}$ is less than the parameter in line (11) as measured in units of maximum of the rms velocities for particles in the halos, only largest will be kept. You may ignore the option by entering two zeros.

7 How to compile and run the code

The code consists of several different FORTRAN programs:

- PM_to_ASCII.f
- PMhalos.f
- PMmain.f
- PMmodelCHDM.f
- PMmodels.f
- PMpower.f
- PMselect.f
- PMstartCDM.f
- PMstartCHDM.f

A Makefile is provided to allow easy compilation of all of the programs. You should edit the Makefile and put in your preferred compilation flags for:

- Optimization. On both our Sun machines running Solaris, and our HP running HPUNIX, we use -O3.

- The routine **PMmodels.f** should be compiled using double precision for all "real" variables and constants. On the Sun, this can be accomplished using the -R8 flag, on the HP with -dbl.

The general scheme for running the code and analyzing results is as follows:

1. Set initial conditions using **PMmodels** and **PMstartCDM**.
2. Run the PM code using **PMmain**.
3. Analyze the results using **PMpower**, and **PMhalos**. **PM_to_ASCII** will scale your results to "normal" units.

More details on each step are provided in subsequent sections.
Some important parameters and variables which are used in the codes, for which you will either be prompted or may wish to change *before compilation*. **Please note the last item which may require you to make a change in the code!**

- AEXPN = expansion parameter ($= 1/(1+z)$). AEXP0 is the expansion parameter at initial moment.
- NROW = number of particles in one dimension ($= 2^n$). The total number of particles is equal to NROW^3. Particles are stored in direct-access files. Each record of the files contains NROW^2 particles.
- NGRID = size of the computational mesh ($= 2^m$). The total number of cells is NGRID^3. If you need to change either NROW or NGRID, the only place where you need to make changes is the file **PMparameters.h**.
- ASTEP = step in the expansion parameter a. Time integration is done with a constant step in the expansion parameter: da =ASTEP.
- ISTEP = current integration step
- Nspecies = number of additional species of particles. This is curretly used for the CHDM models. For plain CDM, ODM, or ΛCDM models Nspecies = 0.
- Om0,Oml0,Ocurv = densities of matter, cosmological constant, and curvature at $z = 0$.
- hubble = the Hubble constant in units of 100km/s/Mpc
- NACCES = length of a record of direct-access files with coordinates and velocities of particles (e.g., PMcrs0.DAT). For some computers the length of the record is counted in bytes, for some it is in machine words. If you get errors when running the code that indicate problems with accessing the data files, multiply NACCES by 4 in file **PMauxiliary.f**, routine RDTAPE, and in files **PMstart...f**. If the length of the data files is too long (it should be $24 \times NROW^3$ bytes), divide NACCES by 4.

8 How to set initial conditions

Two programs need to be run in order to set initial conditions. If the model you are interested in do not have massive neutrinos, the programs are **PMmodels** and **PMstartCDM**. For models with massive neutrinos, the corresponding programs are **PMmodelCHDM** and **PMstartCHDM**. Additionally, if you wish to run the PM code for a model for which the initial power spectrum is not included in the package, it is possible for you (with a bit more work) to specify whatever power spectrum you want.

8.1 Models without massive neutrinos

A range of initial spectra which have been computed by our Boltzmann code and fit with our fitting function (ea.20) are available. The fitting parameters are tabulated in the file **cdm.fit**. You will need to look in this file and determine the line number of the model which you are interested in. The first program (**PMmodels**) will ask to give you the following parameters:

- Name of a file where it writes parameters of the model and normalized power spectra.
- σ_8 = rms density perturbation in a sphere of radius $8h^{-1}$Mpc and the slope of the power spectrum at long
- Line number in the file **cdm.fit**
- Size of the simulation box, number of particles in 1D, and the redshift at which you would like to start your code (or to get the power spectrum).
- The program will ask you if you need to have a file with all input parameters needed to set initial conditions. If you need the file, answer "Yes", and it will create file **InStart.dat**, which you will give as input to the second code **PMstartCDM**. It will also ask you few questions needed to produce the file. If you answer "No", the code finishes its work by creating the file with the name you gave it in the first line. The file has parameters of the model (all Ω's, the Hubble constant, the age of the universe, growth rate of density δ, and $d(\ln\delta)/d(\ln a)$ at different redshifts. It also gives the bulk velocity of a sphere of radius $50h^{-1}$Mpc and normalized power spectra of dark matter at redshift zero ($a = 1$) and at the redshift you provided.
- If you answered "Yes" for the previous question (you needed to have an input file for **PMstartCDM**), you will be asked to provide the following information:
  - *A string of up to 45 characters ("header").* The header is not used for simulations, but it is useful to label your simulation. You can provide any information you want. This header will stick to your run. All files with snapshots of your simulation and all files with analysis of your simulation will have the header. Experience of running many simulations shows that one never has enough information describing details of a simulation done some time ago to identify that simulation later. Use the header to identify your run.
  - *Step in the expansion parameter da.* This defines how many integration steps the code will do untill it runs to the redshift zero. If you would like to make N steps and you start at redshift z, $da = (1 - \frac{1}{1+z})/N$. The step da should be (significantly) smaller than the initial expansion parameter $a_{init} = -\frac{1}{1+z}$.
  - *Seed for random numbers.* Use any integer number in the range $1-(2^{31}-1)$ ($2^{31} \approx 2.1478 \times 10^9$).

Next you will run **PMstartCDM** which is the program that actually generates initial conditions for the PM code. It will generate two files, which **PMmain** reads and updates: **PMcrd.DAT** (information on the cosmological model and parameters of the run) and **PMcrs0.DAT** (coordinates and velocities of particles). If you run a CHDM simulation, you will have more data files with data for hot neutrinos. **PMstartCDM** will ask you to provide some parameters. If you created file **InStart.dat** using the program **PMmodels**, simply provide the file as input: $PMstartCDM < InStart.dat$.

8.2 Models with massive neutrinos

In order to set initial conditions for a CHDM model, run **PMmodelCHDM** and then **PMstartCHDM**. The codes will ask you similar questions as for non-CHDM models. Because setting initial conditions for the CHDM model is more complicated, we provide only one particular CHDM variant: a model with two equal mass neutrinos with total contribution $\Omega_\nu = 0.20$, $h = 0.5$. Initial conditions can be set only at redshift $z = 30$.

8.3 Initial conditions for arbitrary initial power spectra

There are two ways of building initial conditions for models which are not provided with the package.

1. You may add a line to **cdm.fit** with fitting parameters for your model and with parameters of approximation for the power spectrum. This requires that your model is well fit by our fitting formula (eq. 20). The format of the **cdm.fit** file is described in the file. See also the routine **TRUNF(k)** for details of the approximation of the power spectrum of perturbations.

2. You may change the functions TRUNF in **PMstartCDM.f** and Pk in **PMmodels.f** to return whatever initial spectra you desire.

9 How to run the PM code

After you generate the initial conditions, you can start running the code. Check if two files **PMcrd.DAT** and **PMcrs0.DAT** were generated and are in your directory: **PMmain** will read the files. It will also overwrite the files when it finishes. So, if you need to have the original files, please make copies before you start running **PMmain**.

10 How to get coordinates and velocities of particles

To get the final coordinates and velocities, run **PM_to_ASCII**. This will convert the input files **PMcrd.DAT** and **PMcrs0.DAT** into readable output files. You will specify the output file name.

11 How to get power spectrum and density distribution

You can get the power spectrum and density distribution of your output by running **PMpower**. This will read the raw output files from **PMmain**, **PMcrd.DAT** and **PMcrs0.DAT**. The output will go into a file called **Spectrum.DAT**.

12 How to find halos using the Bound-Density-Maxima code

Run **PMhalos**. The code will ask you many questions. It will produce two files with the final results. "Catalog.DAT" contains detailed information about all halos found by the code. After a rather long preamble, data on the halos follow. Each halo has a "header", which gives global parameters: coordinates, velocities, mass, and so on for the halo (format is given in the preamble). "Catshort.DAT" has a shorter preamble and has only a list of the halo headers.

Tips: The code may miss some halos if one chooses wrong parameters!

1. The number of spheres (seeds) should be very large: 100,000 – 150,000. If it is too small, the code misses some of small halos (but not the big ones).

2. The number of particles in each shell for the halo profile should be large: 5-6 per shell. The code needs the density profile of a halo to find radius, escape velocity and so on. It may get confused if the profile is too noisy.

3. Radius of the first bin for the profile should not be too small: not less than 1/2 of your force resolution. It should also contain few particles (> 2).

4. Outer radius should be large. If density does not decline enough (flat profile), the code thinks that this halo is a fluke. If your radius is too small such that only the central part of a potential halo fits in the radius, and the density gradient is not steep, the code will kill your halo.

13 Examples

We make available two examples of runs of the PM code with data analysis which you can use for comparison with your own results if that is desired. The first example has files for the test with 32^3 particles and 128^3 mesh. The second example is for 128^3 particles and 256^3 mesh. Both tests were done for a ΛCDM model with $h = 0.7$.

These are available as two separate tar files with all results or you can also grab individual result files. Since the output data files for the second example are quite large, the tar file for this case does not include these data files. The full set of files from the 32^3 example can be downloaded from http://astro.nmsu.edu/∼aklypin/PM/TEST32x128.tar.gz. The files from the 128^3 example (without data files) can be downloaded from: http://astro.nmsu.edu/∼aklypin/PM/TEST128x256.tar.gz.

Individual output files from the two cases can be downloaded from: http://astro.nmsu.edu/∼aklypin/PM/TEST32x128 and http://astro.nmsu.edu/∼aklypin/PM/TEST128x256. We recommend looking at the output plots (*.ps.gz).

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