

Effects of the size of cosmological N -body simulations on physical quantities – I. Mass function

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Accepted 2006 May 5. Received 2006 May 3; in original form 2006 January 19

ABSTRACT

N -body simulations are a very important tool in the study of formation of large-scale structures. Much of the progress in understanding the physics of galaxy formation and comparison with observations would not have been possible without N -body simulations. Given the importance of this tool, it is essential to understand its limitations as ignoring these can easily lead to interesting but unreliable results. In this paper, we study the limitations due to the finite size of the simulation volume. We explicitly construct the correction term arising due to a finite box size and study its generic features for clustering of matter and also on mass functions. We show that the correction to mass function is maximum near the scale of non-linearity, as a corollary we show that the correction to the number density of haloes of a given mass changes sign at this scale; the number of haloes at small masses is overestimated in simulations. This overestimate results from a delay in mergers that lead to formation of more massive haloes. The same technique can be used to study corrections to other physical quantities. The corrections are typically small if the scale of non-linearity is much smaller than the box size. However, there are some cases of physical interest in which the relative correction term is of order unity even though a simulation box much larger than the scale of non-linearity is used. Within the context of the concordance model, our analysis suggests that it is very difficult for present-day simulations to resolve mass scales smaller than $10^2 M_{\odot}$ accurately and the level of difficulty increases as we go to even smaller masses, though this constraint does not apply to multiscale simulations.

Key words: gravitation – methods: N -body simulations – methods: numerical – cosmology: theory – dark matter – large-scale structure of Universe.

1 INTRODUCTION

Large-scale structures like galaxies and clusters of galaxies are believed to have formed by gravitational amplification of small perturbations. For an overview and original references, see, e.g. Peebles (1980), Peacock (1999), Padmanabhan (2002) and Bernardeau et al. (2002). Initial density perturbations were present at all scales that have been observed (Hawkins et al. 2003; Spergel et al. 2003; Pope et al. 2004). Understanding evolution of density perturbations for such initial conditions is essential for the study of formation of galaxies and large-scale structures. The equations that describe the evolution of density perturbations in an expanding universe have been known for a long time (Peebles 1974) and these are easy to solve when the amplitude of perturbations is small. These equations describe the evolution of density contrast defined as $\delta(\mathbf{r}, t) = [\rho(\mathbf{r}, t) - \bar{\rho}(t)]/\bar{\rho}(t)$. Here $\rho(\mathbf{r}, t)$ is the density at point \mathbf{r} and time t , and $\bar{\rho}$ is the average density in the universe at

time t . These are densities of non-relativistic matter, the component that clusters at all scales and is believed to drive the formation of large-scale structures in the universe. Once density contrast at relevant scales becomes large, i.e. $|\delta| \geq 1$, the perturbation becomes non-linear and coupling with perturbations at other scales cannot be ignored. The equation for evolution of density perturbations cannot be solved for generic perturbations in this regime. N -body simulations (Bagla & Padmanabhan 1997b; Bertschinger 1998; Bagla 2005) are often used to study the evolution in this regime. Alternative approaches can be used if one requires only a limited amount of information and in such a case either quasi-linear approximation schemes (Zel'dovich 1970; Gurbatov, Saichev & Shandarin 1989; Matarrese et al. 1992; Brainerd et al. 1993; Bagla & Padmanabhan 1994; Sahni & Coles 1995; Hui & Bertschinger 1996; Bernardeau et al. 2002) or scaling relations (Davis & Peebles 1977; Hamilton et al. 1991; Nityananda & Padmanabhan 1994; Peacock & Dodds 1994; Jain, Mo & White 1995; Padmanabhan 1996; Padmanabhan et al. 1996; Peacock & Dodds 1996; Ma 1998; Kanekar 2000; Smith et al. 2003) suffice.

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In cosmological N -body simulations, we simulate a representative region of the universe. This is a large but finite volume and periodic boundary conditions are often used. Almost always, the simulation volume is taken to be a cube. Effect of perturbations at scales smaller than the mass resolution of the simulation, and of perturbations at scales larger than the box is ignored. Indeed, even perturbations at scales comparable to the box are undersampled.

It has been shown that perturbations at small scales do not influence collapse of perturbations at much larger scales in a significant manner (Peebles 1974, 1985; Little, Weinberg & Park 1991; Bagla & Padmanabhan 1997a; Couchman & Peebles 1998) if we study the evolution of the correlation function or power spectrum at large scales due to gravitational clustering in an expanding universe. This is certainly true if the scales of interest are in the non-linear regime (Bagla & Padmanabhan 1997a). Therefore, we may assume that ignoring perturbations at scales much smaller than the scales of interest does not affect results of N -body simulations. However, there may be other effects that are not completely understood at the quantitative level (Bagla, Prasad & Ray 2005) even though these have been seen only in somewhat artificial situations.

Perturbations at scales larger than the simulation volume can affect the results of N -body simulations. Use of periodic boundary conditions implies that the average density in the simulation box is same as the average density in the universe, in other words we ignore perturbations at the scale of the simulation volume (and at larger scales). Therefore, the size of the simulation volume should be chosen so that the amplitude of fluctuations at the box scale (and at larger scales) is ignorable. If the amplitude of perturbations at larger scales is not ignorable then clearly the simulation will not be a faithful representation of the model being studied. It is not obvious as to when fluctuations at larger scales can be considered ignorable, indeed the answer to this question depends on the physical quantity of interest, the model being studied and the specific length/mass scale of interest as well.

The effect of a finite box size has been studied using N -body simulations and the conclusions in this regard may be summarized as follows.

(i) If the amplitude of density perturbations around the box scale is small ($\delta < 1$) but not much smaller than unity, simulations underestimate the correlation function though the number density of small mass haloes does not change by much (Gelb & Bertschinger 1994a,b). In other words, the formation of small haloes is not disturbed but their distribution is affected by non-inclusion of long wave modes.

(ii) In the same situation, the number density of massive haloes drops significantly (Gelb & Bertschinger 1994a,b; Bagla & Ray 2005).

(iii) Effects of a finite box size modify values of physical quantities like the correlation function even at scales much smaller than the simulation volume (Bagla & Ray 2005).

(iv) The void spectrum is also affected by finite size of the simulation volume if perturbations at large scales are not ignorable (Kauffmann & Melott 1992).

(v) It has been shown that properties of a given halo can change significantly as the contribution of perturbations at large scales is removed to the initial conditions but the distribution of most internal properties remain unchanged (Power & Knebe 2005).

In some cases, one may be able to devise a method to ‘correct’ for the effects of a finite box size (Colombi, Bouchet & Schaeffer 1994), but such methods cannot be generalized to all statistical measures or physical quantities.

The effects of perturbations at scales larger than the box size can be added using mode adding procedure (MAP) after a simulation has been run (Tormen & Bertschinger 1996). This method makes use of the fact that if the box size is chosen to be large enough then the contribution of larger scales can be incorporated by adding displacements due to the larger scales independently of the evolution of the system in an N -body simulation. The motivation for development of such a tool is to enhance the range of scales over which results of an N -body simulation can be used by improving the description at scales comparable to the box size. Such an approach ignores the coupling of large-scale modes with small-scale modes and this again brings up the issue of what is a large enough scale for a given model such that the effects of mode coupling can be ignored. Large scales contribute to displacements and velocities, and variations in density due to these scales modify the rate of growth for small-scales perturbations (Cole 1997).

Effects of a finite box size modify values of physical quantities even at scales much smaller than the simulation volume (Bagla & Ray 2005) (BR05, hereafter). In BR05, we suggested use of the fraction of mass in collapsed haloes as an indicator of the effect of a finite box size. We found that if the simulation volume is not large enough, the fraction of mass in collapsed haloes is underestimated. As the collapsed fraction is less sensitive to box size as compared to measures of clustering, several other statistical indicators of clustering to deviate significantly from expected values in such simulations. A workaround for this problem was suggested in the form of an ensemble of simulations to take the effect of convergence due to long wave modes into account (Sirko 2005), the effects of shear due to long wave modes are ignored here. It has also been shown that the distribution of most internal properties of haloes, e.g. concentration, triaxiality and angular momentum do not change considerably with the box size even though properties of a given halo may change by a significant amount (Power & Knebe 2005).

There is a clear need to develop a formalism for estimating the effect of perturbations at large scales on a variety of physical quantities. Without such a formalism, we cannot decide in an objective manner whether a simulation box size is sufficiently large or not. In this paper, we generalize the approach suggested in BR05 and write down an explicit correction term for a number of statistical indicators of clustering. This approach allows us to study generic properties of the expected correction term in any given case, apart of course from allowing us to evaluate the magnitude of the correction as compared to the expected value of the given statistical indicator. We apply this technique to mass functions in this paper.

2 BASIC EQUATIONS

Initial conditions for N -body simulations are often taken to be a realization of a Gaussian random field with a given power spectrum, for details see, e.g. Bagla & Padmanabhan (1997b), Bertschinger (1998) and Bagla (2005). The power spectrum is sampled at discrete points in the k -space between the scales corresponding to the box size (fundamental mode) and the grid size (Nyquist frequency/mode). Here k is the wave vector. Sampling of the power spectrum in initial conditions of N -body simulations is dense towards the Nyquist mode, but is sparse for modes near the fundamental mode. Power spectra for density, potential and the velocity field are related to each other in the linear regime.¹ The power spectra can be used to compute the

¹ Density and potential are related through the Poisson equation and hence the knowledge of power spectrum of one can be used to compute the power

second moment; either two-point functions or rms fluctuations. In view of the sampling of the power spectrum in initial conditions, the second moment can be expressed as a sum over power spectrum at these points, weighted by an appropriate window function.

In the peak picture, most quantities of interest can be related to the two-point correlation function (Bardeen et al. 1986), therefore a method for estimating box-size correction to the second moment can be used as a base for computing correction for other physical quantities.

2.1 Clustering amplitude

We now present our approach for estimating the effects of a finite box size on physical quantities in the linear limit. We will illustrate our approach using rms fluctuations in mass $\sigma(r)$, but as shown below, the basic approach can be generalized to any other quantity in a straightforward manner. In general, $\sigma(r)$ may be defined as follows:

$$\sigma^2(r) = \int_0^\infty \frac{dk}{k} \frac{k^3 P(k)}{2\pi^2} W^2(kr). \quad (1)$$

Here $P(k)$ is the power spectrum of density contrast, r is the comoving length scale at which rms fluctuations are defined, $k = \sqrt{k_x^2 + k_y^2 + k_z^2}$ is the wave number and $W(kr)$ is the Fourier transform of the window function used for sampling the density field. The window function may be a Gaussian or a step function in real or k -space. We choose to work with a step function in real space where $W(kr) = 9(\sin kr - kr \cos kr)/(k^6 r^6)$, see e.g. section 5.4 of Padmanabhan (1993) for further details. In an N -body simulation, the power spectrum is sampled only at specified points in the k -space. In this case, we may write $\sigma^2(r)$ as a sum over these points.

$$\begin{aligned} \sigma^2(r, L_{\text{box}}) &= \frac{9}{V} \sum_k P(k) \left(\frac{\sin kr - kr \cos kr}{k^3 r^3} \right)^2 \\ &\simeq \int_{2\pi/L_{\text{box}}}^{2\pi/L_{\text{grid}}} \frac{dk}{k} \frac{k^3 P(k)}{2\pi^2} 9 \left(\frac{\sin kr - kr \cos kr}{k^3 r^3} \right)^2 \\ &\simeq \int_{2\pi/L_{\text{box}}}^\infty \frac{dk}{k} \frac{k^3 P(k)}{2\pi^2} 9 \left(\frac{\sin kr - kr \cos kr}{k^3 r^3} \right)^2 \\ &= \int_0^\infty \frac{dk}{k} \frac{k^3 P(k)}{2\pi^2} 9 \left(\frac{\sin kr - kr \cos kr}{k^3 r^3} \right)^2 \\ &\quad - \int_0^{2\pi/L_{\text{box}}} \frac{dk}{k} \frac{k^3 P(k)}{2\pi^2} 9 \left(\frac{\sin kr - kr \cos kr}{k^3 r^3} \right)^2 \\ &= \sigma_0^2(r) - \sigma_1^2(r, L_{\text{box}}). \end{aligned} \quad (2)$$

Here $\sigma_0^2(r)$ is the expected level of fluctuations in mass at scale r for the given power spectrum and $\sigma^2(r, L_{\text{box}})$ is what we get in an N -body simulation at early times. We have assumed that we can approximate the sum over the k modes sampled in initial conditions by an integral. Further, we make use of the fact that small scales do not influence large scales to ignore the error contributed by the upper limit of the integral. This approximation is valid as long as the scales of interest are more than a few grid lengths.

spectrum for the other quantity. These quantities at late times are obtained through evolution in which mode-coupling is significant and hence the effects of missing modes are not easy to quantify. The sampling of initial conditions is, in our considered view, more relevant and easier to quantify than the effects of missing mode-coupling terms. Therefore, in our discussion, we deal with the initial or the linearly evolved power spectra of various quantities.

In the approach outlined above, the value of σ^2 at a given scale is expressed as a combination of the expected value σ_0^2 and the correction due to the finite box size σ_1^2 . Here σ_0^2 is independent of the box size and depends only on the power spectrum and the scale of interest. It is clear that $\sigma^2(r, L_{\text{box}}) \leq \sigma_0^2(r)$ and also $\sigma_1^2(r, L_{\text{box}}) \geq 0$. It can also be shown that for hierarchical models, $d\sigma_1^2(r, L_{\text{box}})/dr \leq 0$, i.e. $\sigma_1^2(r, L_{\text{box}})$ increases or saturates to a constant value as we approach small r .

If the scale of interest is much smaller than the box size L_{box} then,

$$\begin{aligned} \sigma_1^2(r, L_{\text{box}}) &= \int_0^{2\pi/L_{\text{box}}} \frac{dk}{k} \frac{k^3 P(k)}{2\pi^2} 9 \left(\frac{\sin kr - kr \cos kr}{k^3 r^3} \right)^2 \\ &\simeq \int_0^{2\pi/L_{\text{box}}} \frac{dk}{k} \frac{k^3 P(k)}{2\pi^2} \\ &\quad - \frac{r^2}{5} \int_0^{2\pi/L_{\text{box}}} \frac{dk}{k} \frac{k^5 P(k)}{2\pi^2} \\ &\quad + \frac{3r^4}{175} \int_0^{2\pi/L_{\text{box}}} \frac{dk}{k} \frac{k^7 P(k)}{2\pi^2} + \mathcal{O}(r^6) \\ &= C_1 - C_2 r^2 + C_3 r^4 + \mathcal{O}(r^6). \end{aligned} \quad (3)$$

The small parameter in the expansion is r/L_{box} . This expansion is useful if $k^3 P(k)$ goes to zero as we approach $k = 0$. It is interesting to note that the first term is scale independent. The numerical values of C_i can be used to estimate the scale below which σ_1 can be approximated by a constant. Later terms are scale dependent and the noteworthy feature is that modes closer to $2\pi/L_{\text{box}}$ contribute more significantly to the integral for most models.

It is noteworthy that the first term, C_1 , has the same value for all choices of window functions that approach unity at small k . By virtue of this fact, C_1 is also the correction for the two-point correlation function $\xi(r)$ at sufficiently small scales.

At large scales $\sigma_0^2(r)$ and $\sigma_1^2(r, L_{\text{box}})$ have a similar magnitude and the rms fluctuations in the simulation become negligible compared to the expected values in the model. As we approach small r the correction term $\sigma_1^2(r, L_{\text{box}})$ is constant and for most models it becomes insignificant in comparison with $\sigma_0^2(r)$. In models where $\sigma_0^2(r)$ increases very slowly at small scales or saturates to a constant value, the correction term σ_1^2 can be significant at all scales. This can be seen from the expression for C_1 for power-law models [$P(k) = Ak^n$]:

$$C_1 = \frac{1}{n+3} \frac{A}{2\pi^2} \left(\frac{2\pi}{L_{\text{box}}} \right)^{n+3}. \quad (5)$$

Clearly, this term becomes more and more significant as $n \rightarrow -3$. Fig. 1 illustrates this point, here C_1 is shown as a function of $n+3$. We fix A by choosing a scale of non-linearity r_{nl} such that $\sigma_0(r_{\text{nl}}) = 1$. Curves are plotted for three values of $L_{\text{box}}/r_{\text{nl}}$: $L_{\text{box}}/r_{\text{nl}} = 16$ (dot-dashed curve), $L_{\text{box}}/r_{\text{nl}} = 128$ (dashed curve) and $L_{\text{box}}/r_{\text{nl}} = 512$ (solid curve). As σ_0 is unity at the scale of non-linearity and C_1 is the first-order correction, clearly we require $C_1 \ll 1$ for the error due to box size to be small and hence ignorable. If we fix $C_1 \leq 0.1$ then we can simulate $n = -1$ with $L_{\text{box}}/r_{\text{nl}} = 16$ but for more negative indices we require a larger separation between the box size and the scale of non-linearity. We can just about manage $n = -2.3$ with $L_{\text{box}}/r_{\text{nl}} = 128$ with the same threshold on error, and with $L_{\text{box}}/r_{\text{nl}} = 512$ we can go up to $n = -2.5$. As N -body simulations are most useful for studying non-linear evolution, even the largest simulations possible today are left with a small range of scales over which $\sigma_0 \geq 1$ for $n \leq -2.0$. This shows the pitfalls of simulating models with $n \simeq -3$ over the entire range of scales.

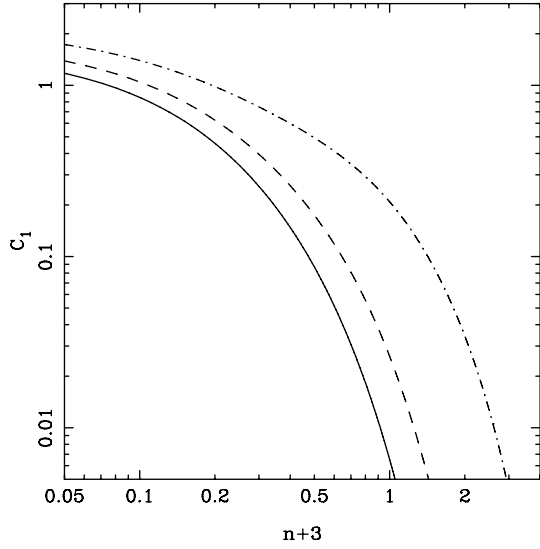


Figure 1. This figure shows the first correction term C_1 (see equation 5) for power-law models with index n normalized such that $\sigma_0^2(r_{\text{nl}}) = 1$. The curves here are for $L_{\text{box}}/r_{\text{nl}} = 16$ (dot-dashed curve), $L_{\text{box}}/r_{\text{nl}} = 128$ (dashed curve) and $L_{\text{box}}/r_{\text{nl}} = 512$ (solid curve). C_1 is plotted as a function of $n + 3$ and we find that the correction term increases as $n + 3 \rightarrow 0$. See text for more details.

Fig. 2 (top panel) shows lines of constant C_1/σ_0^2 in the $L_{\text{box}}-r$ plane for the Λ cold dark matter (Λ CDM). We chose $n = 1$, $h = 0.7$, $\Omega_\Lambda = 0.7$, $\Omega_{\text{nr}} = 0.3$ and $\sigma_8 = 0.9$. We ignored the effects of Baryons on the power spectrum. From top to bottom, the lines correspond to $C_1/\sigma_0^2 = 0.01, 0.03, 0.1, 0.3$ and 0.5 . It is noteworthy that a box size smaller than 0.5 Mpc is precluded if we insist on $C_1(L_{\text{box}})/\sigma_0^2(r) \leq 0.1$, irrespective of the scale of interest. This implies that we cannot expect to simulate scales smaller than about 0.5 kpc in the Λ CDM model without considerable improvement in the dynamic range of cosmological N -body simulations. As we are using linearly evolved quantities for our argument, the comments on box size are valid irrespective of the redshift up to which the simulation is run. The contours do not change if we use σ_1^2 instead of C_1 .

The lower panel of the same figure shows the scale of non-linearity for the Λ CDM model as a function of redshift.

This formalism can be used to estimate corrections for other estimators of clustering. For reference, we have given expressions equivalent to equation (4) for the correction to ξ and $\bar{\xi}$ in Table 1.

2.2 Velocities

We can use the method outlined above to estimate finite box corrections to the velocity field. Velocities and density contrast are related to one another (Peebles 1980) in the linear regime. The power spectra for these two are related as $P_v(k) \propto P(k)/k^2$. Thus, bulk velocities at any given scale get a larger contribution from the power spectrum at large scales (small k) than density fluctuations. This implies that the correction term must be more significant for velocities than the equivalent correction for the clustering amplitude. We will discuss the corrections in velocity field in detail in a follow-up paper.

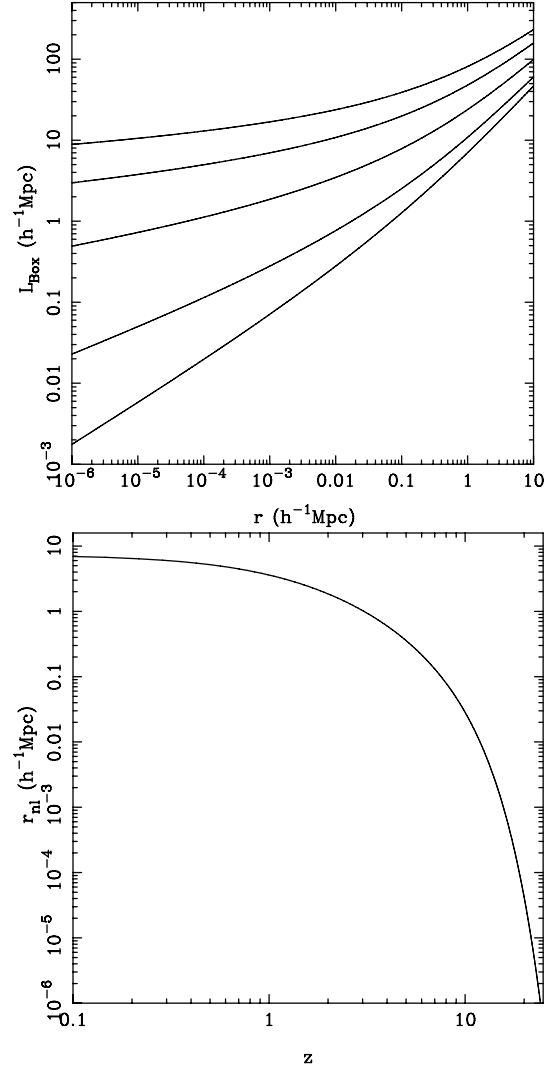


Figure 2. The top panel shows curves of constant $C_1(L_{\text{box}})/\sigma_0^2(r)$ on the $r-L_{\text{box}}$ plane for the Λ CDM model (see text for details). Lines mark $C_1/\sigma_0^2 = 0.01, 0.03, 0.1, 0.3$ and 0.5 , from top to bottom. The lower panel shows the scale of non-linearity r_{nl} as a function of redshift for the Λ CDM model.

Table 1. This table lists corrections due to a finite box size to indicators of clustering in the limit $r \ll L_{\text{box}}$. These expressions are equivalent to equation (4) and constants C_i are the same as in that equation.

Indicator	Correction
$\xi(r)$	$C_1 - \frac{5}{6}C_2r^2 + \frac{35}{72}C_3r^4 + \mathcal{O}(r^6)$
$\bar{\xi}(r)$	$C_1 - \frac{1}{2}C_2r^2 + \frac{5}{24}C_3r^4 + \mathcal{O}(r^6)$

2.3 Mass function

We can use the explicit correction for rms fluctuations (σ) to estimate the correction for mass functions of haloes. We use the Press-Schechter approach (Press & Schechter 1974; Bond et al. 1991), but we also give results for the Sheth-Tormen mass function (Sheth & Tormen 1999; Sheth, Mo & Tormen 2001) in order to demonstrate that our results are generic in nature.

The mass fraction in collapsed haloes with mass greater than M is given in the Press–Schechter model by

$$\begin{aligned} F(M, L_{\text{box}}) &= \text{erfc} \left[\frac{\delta_c}{\sigma(M, L_{\text{box}})\sqrt{2}} \right] \\ &= \frac{2}{\sqrt{\pi}} \int_{\delta_c/\sigma(M, L_{\text{box}})\sqrt{2}}^{\infty} \exp(-x^2) dx. \end{aligned} \quad (6)$$

Where $\delta_c (\simeq 1.68$ for Einstein-de Sitter cosmology) is a parameter² and M is related to the scale r through the usual relation. We can write F as the contribution expected in the limit $L_{\text{box}} \rightarrow \infty$ and a correction due to the finite box size.

$$\begin{aligned} F(M, L_{\text{box}}) &= \frac{2}{\sqrt{\pi}} \int_{\delta_c/\sigma_0(M)\sqrt{2}}^{\infty} \exp(-x^2) dx \\ &\quad - \frac{2}{\sqrt{\pi}} \int_{\delta_c/\sigma_0(M)\sqrt{2}}^{\delta_c/\sigma(M, L_{\text{box}})\sqrt{2}} \exp(-x^2) dx \\ &= F_0(M) - F_1(M, L_{\text{box}}). \end{aligned} \quad (7)$$

The correction to $F(M)$ due to the finite box size always leads to an underestimate as $F_1(M, L_{\text{box}})$ is always positive. This is consistent with what we found in BR05. However, $F_1(M, L_{\text{box}})$ is not a monotonic function of M as it goes to zero at small as well as large M . At small M ($M \ll M_{\text{nl}}$),³ the limits of the integral differ by a very small amount. This difference ($\delta_c \sigma_1^2 / 2\sqrt{2}\sigma_0^3$) keeps on decreasing as we get to small M while the integrand remains finite. Therefore, we expect F_1 to decrease at small M . At these scales, we can write an approximate expression for $F_1(M)$:

$$F_1(M) \simeq \frac{\delta_c}{\sqrt{2\pi}} \frac{\sigma_1^2}{\sigma_0^3} \exp\left(-\frac{\delta_c^2}{2\sigma_0^2}\right). \quad (8)$$

This clearly decreases as we go to small M : σ_1 goes over to the constant C_1 and σ_0 keeps increasing.

At large M ($M \gg M_{\text{nl}}$), both $\sigma(M, L_{\text{box}})$ and $\sigma_0(M)$ are small and the limits of the integral cover the region where the integrand is very small. Thus, we expect $F_1(M, L_{\text{box}})$ to become smaller as we go to larger M in this regime. At these scales, we also expect F_0 and F_1 to become almost equal while $F(M)$ goes to zero faster than either term. Therefore, $F_1(M, L_{\text{box}})$ must have a maxima at an intermediate scale. The scale at which the maxima occurs can be found by solving the following equation.

$$\begin{aligned} \frac{d \log \sigma_1^2}{d \log \sigma_0^2} &= -\frac{\sigma_0^2}{\sigma_1^2} \left[\frac{\sigma}{\sigma_0} \left(1 - \frac{\sigma_1^2}{\sigma_0^2} \right) \exp\left(\frac{\delta_c^2 \sigma_1^2}{2\sigma^2 \sigma_0^2}\right) - 1 \right] \\ &\simeq \frac{3}{2} - \frac{\delta_c^2}{2\sigma_0^2}. \end{aligned} \quad (9)$$

Here, the second equation is obtained if $\sigma_1 \ll \sigma_0$. If $L_{\text{box}} \gg r_{\text{nl}}$, where r_{nl} is the scale of non-linearity then σ_1 is very well approximated by the Taylor series equation (4) around this scale and σ_1 is a very slowly varying function of scale. Thus $F_1(M, L_{\text{box}})$ has a maxima at $\sigma_0 = \delta_c^2/3 \sim 1$ if the first term in equation (4) is a good approximation for σ_1 . If scale-dependent terms in equation (4) are not ignorable then the maxima of $F_1(M, L_{\text{box}})$ shifts to smaller scales (larger σ_0) in a manner that depends on the power spectrum and box size L_{box} .

² In the spherical collapse model, this is the linearly extrapolated density contrast at which we expect the halo to virialize (Gunn & Gott 1972).

³ M_{nl} is the mass corresponding to the scale where $\sigma_0 = 1$ and we will assume that L_{box} is much larger than this scale.

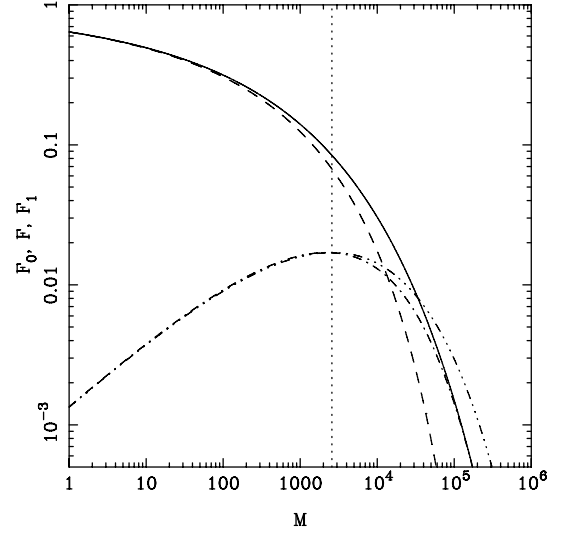


Figure 3. The Press–Schechter mass function and correction terms are plotted as a function of mass. $F_0(M)$ (solid curve), $F(M)$ (dashed curve) and $F_1(M)$ (dot–dashed curve) are shown here. The scale where $\sigma_0 = \delta_c/\sqrt{3}$ is marked with a vertical dotted line, we see that this estimate coincides with the maximum of $F_1(M)$. The correction term $F_1(M)$ is more than 10 per cent of $F_0(M)$ at this scale. Also shown is the approximate expression equation (8) for $F_1(M)$ (dot–dot–dot–dashed curve) and we note that it follows the actual curve to masses greater than M_{nl} . Mass here is plotted in units of mass of each particle and we assumed that the scale of non-linearity is 8 grid lengths.

Fig. 3 shows the Press–Schechter mass function $F(M)$ for a power-law model with $n = -2$, $L_{\text{box}}/r_{\text{nl}} = 16$. We have plotted $F_0(M)$ (solid curve), $F(M)$ (dashed curve) and $F_1(M)$ (dot–dashed curve) as a function of M . The scale where $\sigma_0 = \delta_c/\sqrt{3}$ is marked with a vertical dotted line, we see that this estimate is close to the maximum of $F_1(M)$. The correction term $F_1(M)$ is more than 10 per cent of $F_0(M)$ at this scale. Also shown is the approximate expression equation (8) for $F_1(M)$ (dot–dot–dot–dashed curve) and we note that it follows the actual curve to masses greater than M_{nl} . This figure illustrates all the generic features of corrections to mass function that we have discussed above.

The multiplicity function f is often defined as the fraction of mass in a logarithmic interval in mass:

$$\begin{aligned} f(M, L_{\text{box}}) d \log M &= -\frac{\partial F(M, L_{\text{box}})}{\partial \log M} d \log M \\ \Rightarrow f(M, L_{\text{box}}) &= -\frac{dF_0(M)}{d \log M} + \frac{\partial F_1(M, L_{\text{box}})}{\partial \log M} \\ &= f_0(M) - f_1(M, L_{\text{box}}). \end{aligned} \quad (10)$$

It is not possible to reduce this expression further while writing the correction term due to the finite box size separately. We can, however, ascertain generic properties of the correction term $f_1(M, L_{\text{box}})$ from our understanding of $f_1(M, L_{\text{box}})$. At large M , f_1 is positive as $f_1(M, L_{\text{box}})$ decreases with increasing M . Thus, the mass fraction of haloes in this mass range is underestimated in simulations. For typical models and simulations, this is the most significant effect of a finite box size.

We know that f_1 has a zero near the scale of non-linearity as F_1 has a maxima here. Thus, there is a scale where corrections for the multiplicity function due to a finite box size vanish. At smaller scales, the slope of F_1 and hence f_1 changes sign and the correction to mass fraction in haloes is positive. A finite box size leads to an

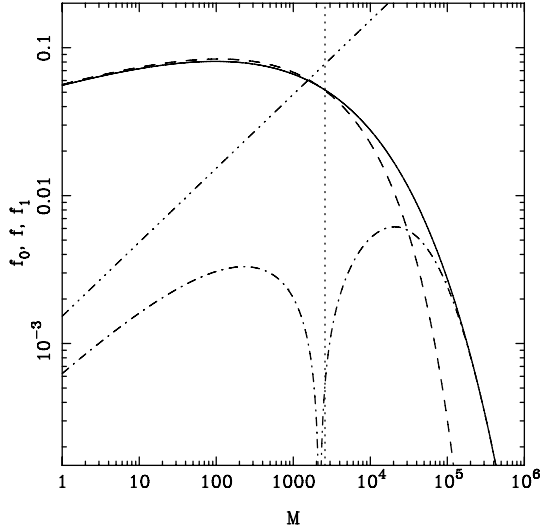


Figure 4. The Press–Schechter multiplicity function and correction terms are plotted as a function of mass. $f_0(M)$ (solid curve), $f(M)$ (dashed curve) and $f_1(M)$ (dot–dashed curve) are shown here. The scale where $\sigma_0 = \delta_c/\sqrt{3}$ is marked with a vertical dotted line, we see that this estimate coincides with change of sign for $f_1(M)$. At scales below this, the correction term $f_1(M)$ is positive and hence there are more haloes in simulation than expected in the model. Also shown is the approximate expression for $f_1(M)$ (dot-dot-dot–dashed curve). Mass here is plotted in units of mass of each particle and we assumed that the scale of non-linearity is 8 grid lengths.

overestimate of number of low-mass haloes. This overestimate is caused by absence of long wave modes, as the low-mass haloes do not merge to form the high-mass haloes.

The magnitude of overestimate depends on σ_1 , and hence on the slope of the power spectrum and L_{box} . In the limit of $M \ll M_{\text{nl}}$, we can use equation (8) to compute the magnitude of overestimate:

$$f(M) \simeq f_0(M) + \frac{3\delta_c}{\sqrt{2\pi}} \frac{C_1}{\sigma_0^4} \left| \frac{d\sigma_0}{d \log M} \right|. \quad (11)$$

Here, we have ignored the contribution of the exponential term in equation (8). The correction term scales as $M^{(n+3)/2}$ for power-law models, thus it is significant even at small mass scales if $n \simeq -3$. Clearly, the term is also large for CDM like power spectra if the slope of the power spectrum is close to -3 at all scales in the simulation volume.

Fig. 4 shows the Press–Schechter multiplicity function and correction terms as a function of mass for the model used in Fig. 3. (Power-law model with $n = -2$, $L_{\text{box}}/r_{\text{nl}} = 16$.) The expected multiplicity function $f_0(M)$ (solid curve), what is expected in the simulation $f(M)$ (dashed curve) and the correction term $f_1(M)$ (dot–dashed curve) are shown here. The scale where $\sigma_0 = \delta_c/\sqrt{3}$ is marked with a vertical dotted line, we see that this almost coincides with change of sign for $f_1(M)$.⁴ At scales below this, the correction term $f_1(M)$ is positive and hence there are more haloes in the simulation than expected in the model. The relative magnitude of the correction term is large for $M > M_{\text{nl}}$ and this is the most significant effect of a finite box size on the mass function. The overestimate of the multiplicity function is typically a subdominant effect, as it is for the model shown here. However, as we will see below, this effect

⁴ The change of sign happens at $\sigma_0 = 1$ instead of $\sigma_0 = 0.97$ drawn here with $\delta_c = 1.68$.

can be very significant in some situations. Also shown in the figure is the approximate expression for $f_1(M)$ (dot–dot–dot–dashed curve) in the limit $M \ll M_{\text{nl}}$. Unlike the approximation for $f_1(M)$ which is accurate over a large range of scales, this is expected to be valid only in the limit of $M \ll M_{\text{nl}}$ and indeed, is off by about a factor of 2 at the smallest scales shown here. However, it is a good approximation if we go to even smaller masses. We note that for this model, the overestimate of multiplicity function due to the finite box is small and therefore is difficult to detect. For this model, $C_1/\sigma_0^2 \simeq 0.2$ at the scale of non-linearity and is smaller than 0.1 at scales where the overestimate in $f(M)$ is maximum. At small scales, f_1/f_0 is typically of the same order of magnitude as C_1/σ_0^2 .

2.3.1 Sheth–Tormen mass function

We now give corresponding formulae for the Sheth–Tormen mass function (Sheth & Tormen 1999; Sheth et al. 2001). The definition of mass function (equation 6) is modified to:

$$F(M, L_{\text{box}}) = \frac{2}{\sqrt{\pi}} \int_{\delta_c/\sigma(M, L_{\text{box}})/\sqrt{2}}^{\infty} A(1+x^{-2q}) \exp(-x^2) dx. \quad (12)$$

In the limit of $A = 0.5$ and $q = 0$ this is identical to the usual Press–Schechter mass function (equation 6). The maxima of the correction term [$F_1(M, L_{\text{box}})$] occurs when the following equation is satisfied:

$$\begin{aligned} \frac{d \log \sigma_1^2}{d \log \sigma_0^2} &= -\frac{\sigma_0^2}{\sigma_1^2} \left[\frac{\sigma}{\sigma_0} \left(1 - \frac{\sigma_1^2}{\sigma_0^2} \right) \right. \\ &\quad \left. \exp \left(\frac{\delta_c^2 \sigma_1^2}{2\sigma^2 \sigma_0^2} \right) \frac{1 + \left(\frac{\delta_c}{\sqrt{2}\sigma_0} \right)^{-2q}}{1 + \left(\frac{\delta_c}{\sqrt{2}\sigma} \right)^{-2q}} - 1 \right] \\ &\simeq \frac{3}{2} - \frac{\delta_c^2}{2\sigma_0^2} - q \left(\frac{\delta_c}{\sqrt{2}\sigma_0} \right)^{-2q}. \end{aligned} \quad (13)$$

As before, this reduces to the expression in the Press–Schechter case (equation 9) in the limit $q = 0$. The qualitative features of the finite box correction to mass function are the same for the two prescriptions and may be considered to be generic. For reference, we write approximate expressions for correction to the mass function $F(M)$:

$$F_1 \simeq \frac{\delta_c}{\sqrt{2\pi}} \frac{\sigma_1^2}{\sigma_0^2} \exp \left(-\frac{\delta_c^2}{2\sigma_0^2} \right) A \left[1 + \left(\frac{\delta_c}{\sqrt{2}\sigma_0} \right)^{-2q} \right] \quad (14)$$

and the multiplicity function $f(M)$:

$$f_1 = \frac{3\delta_c}{\sqrt{2\pi}} \frac{C_1}{\sigma_0^4} \left(\frac{d\sigma_0}{d \log M} \right) A \left[1 + \left(1 - \frac{2q}{3} \right) \left(\frac{\delta_c}{\sqrt{2}\sigma_0} \right)^{-2q} \right] \quad (15)$$

for the Sheth–Tormen mass function.

2.3.2 N-body simulations

We present here some preliminary results of a comparison of our results with N -body simulations. We do not try to fit either the Press–Schechter or the Sheth–Tormen mass functions to simulations here, instead we use a simulation with a larger L_{box} as reference and compare the number density of haloes as a function of mass with another simulation run using a smaller L_{box} . More detailed results obtained from N -body simulations will be presented in a later publication.

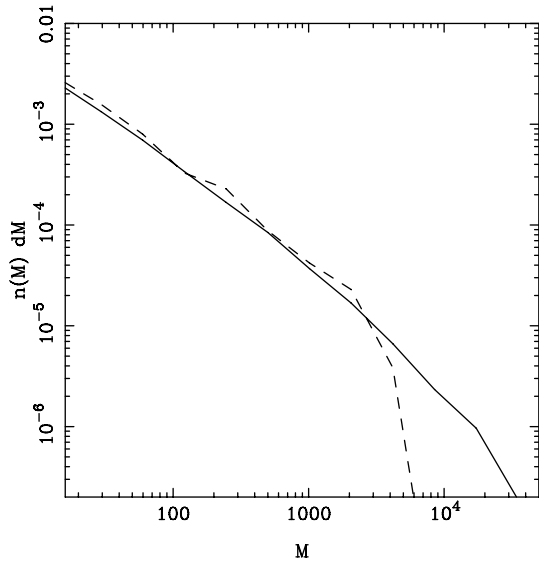


Figure 5. Shown here is the number density of haloes $n(M) dM$ in the mass range $M - M + dM$ for these two simulations. The solid line shows the number density of haloes in the reference simulation ($L_{\text{box}} = 256$). Number density of haloes in the simulation with $L_{\text{box}} = 64$ Mpc is shown by the dashed line.

We simulated the $n = -2$ power-law model in an Einstein-de Sitter universe with the normalization $r_{\text{nl}} = 8$ Mpc at the final epoch. We chose one grid length of the simulation to equal 1 Mpc. The simulation was run with two values of the box size: $L_{\text{box}} = 64$ and 256 Mpc, with the latter being the reference. The simulations were run using the TreePM method (Bagla 2002; Bagla & Ray 2003). The parallel TreePM code was used for the 256^3 simulation (Ray & Bagla 2004).

Fig. 5 shows the number density of haloes $n(M) dM$ in the mass range $M - M + dM$ for these two simulations. Note that following our definitions $n(M) = f(M)/M^2$, where $f(M)$ is the multiplicity function. The solid line shows the number density of haloes in the reference simulation. One can see the approximately power-law variation at small M and a rapid fall-off at large M . Number density of haloes in the simulation with $L_{\text{box}} = 64$ Mpc is shown by the dashed line. As expected from the above discussion, the deviation from power law starts at smaller masses as the number density of very massive haloes is underestimated as compared to the reference simulation. At smaller M , we find about 10 per cent more haloes in this simulation as compared to the reference. It is noteworthy that the number density of low-mass haloes remains above that in the reference simulation at all masses below the rapid drop around $10^2 M_{\odot}$. Both the features follow the predictions in the preceding discussion, indeed we have shown that these features are independent of the specific analytical form for the mass function. Here, we have also shown that the same behaviour is reproduced in N -body simulations. A more detailed comparison is beyond the scope of this paper and the results will be presented in a later publication.

3 DISCUSSION

In the preceding sections, we have described a method to estimate errors in the descriptors of clustering in the linear regime. We have also shown that the key results of the analytical study are borne out by N -body simulations. We have shown that the error is typically small if the scale of interest is sufficiently smaller than the box size.

An implicit requirement is that the scale of non-linearity too should be much smaller than the box size; if this restriction is overlooked then we not only ignore power in modes larger than the simulation box but also the significant effects of mode coupling from scales in the mildly non-linear regime. Therefore, we require $r, r_{\text{nl}} \ll L_{\text{box}}$.

We propose using σ_1^2/σ_0^2 as an indicator of the significance of the finite box size, any descriptor of second moment can be used but σ has the virtue of being positive definite at all scales. Our proposal is that $\sigma_1^2(r)/\sigma_0^2(r), \sigma_1^2[r_{\text{nl}}(z)]/\sigma_0^2[r_{\text{nl}}(z)] \ll 1$, for the finite box-size corrections to be ignorable. All the σ s are evolved linearly here. Conversely, the ratio σ_1/σ_0 at the scale of interest is indicative of the magnitude of correction due to the finite box size. For a given relative magnitude of the correction term (σ_1/σ_0), $L_{\text{box}}/r_{\text{nl}}$ is required to be larger for spectra with more large-scale power. Indeed, the required $L_{\text{box}}/r_{\text{nl}}$ approaches infinity as the slope of the power spectrum approaches -3 .

As a result of finite box-size corrections, the amplitude of density perturbations is not a power law and the range of scales over which it can be approximated by one becomes smaller as we approach $n + 3 \rightarrow 0$. In the linear regime, the radial pair velocity is related directly with ξ (Peebles 1980; Nityananda & Padmanabhan 1994). As ξ is not a pure power law in simulations due to box-size corrections, we expect that the pair velocities must also deviate from expected values. This, in turn leads to deviations from scale invariant growth of density perturbations. This explains the difficulty in getting scale invariant evolution for models like $n = -2$ in N -body simulations (Jain & Bertschinger 1996, 1998). For realistic models like the Λ CDM, the correction term is significant only if the scales of interest are below a few kpc and becomes larger as we move to smaller scales (see Fig. 2). Indeed, at these small scales we may require $L_{\text{box}}/r \sim 10^4$ or even greater in order to manage $C_1/\sigma_0^2 = 0.1$. Of course, a bigger simulation volume is required if we demand better accuracy. On the other hand, if we are interested in scales larger than 10^2 kpc, present-day simulations are sufficient for keeping $C_1/\sigma_0^2 \leq 0.01$.

We have shown that at sufficiently small scales the correction due to a finite box size can be written as a series of progressively smaller terms. The first correction term (C_1) is shown to be positive definite. We have also shown that the first correction term is the same for two-point correlation function and σ^2 , indeed it is the same for all descriptors of the second moment for which the effective window function goes to unity at small k .

As an application of our method, we discussed the correction to mass function and multiplicity function using the Press–Schechter as well as the Sheth–Tormen approach. We have given the explicit form of the correction term due to finite box size in each case. We have also given approximate expressions for the correction term and have shown that the approximation is very good in case of mass function. The mass function is always underestimated in simulations due to finite box-size corrections. Multiplicity function, and hence also the number density of haloes of a given mass are underestimated at $M > M_{\text{nl}}$. At smaller mass scales, however, the multiplicity function is overestimated and we find more haloes in a simulation than expected in the model. The mass scale at which the crossover from underestimate to overestimate occurs is given by equation (10) for Press–Schechter and equation (14) for Sheth–Tormen mass function.

The overestimate at small scales is related to the underestimate of mass in haloes at large-scales. If the full power spectrum had been taken into account, the smaller haloes would have merged to form more massive haloes. In absence of large-scale modes, the formation of massive haloes is slowed down and a larger number of low-mass

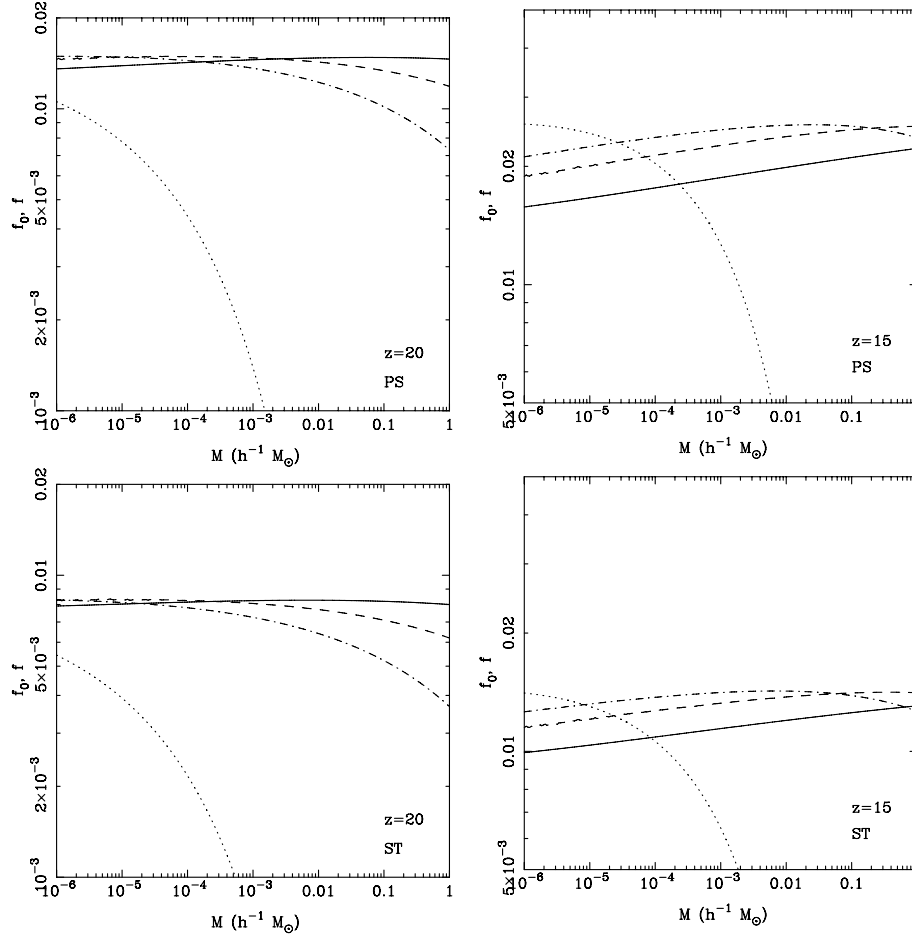


Figure 6. The multiplicity function expected in the Λ CDM model (see text for details). The top row is for Press–Schechter mass function and the lower row is for Sheth–Tormen mass function. The left-hand column is for $z = 20$ and the right-hand column is for $z = 15$. The expected multiplicity function is plotted as a function of mass, shown in each panel by a solid curve. Other curves correspond to multiplicity for a finite simulation box: $L_{\text{box}} = 5 h^{-1}$ kpc (dotted curve), $L_{\text{box}} = 20 h^{-1}$ kpc (dot–dashed curve) and $L_{\text{box}} = 100 h^{-1}$ kpc (dashed curve). These correspond to $C_1/\sigma_0^2 \simeq 0.6, 0.3$ and 0.19 , respectively.

haloes survive. A detailed analysis of the effect of finite box-size correction on merger rates for haloes will be presented in a forthcoming paper. Of significant interest is the impact on rates of major mergers (Cohn, Bagla & White 2001) as these have implications for observations.

We find that the overestimate in multiplicity function is large whenever the ratio $\sigma_1^2(r, L_{\text{box}})/\sigma_0^2(r) \sim C_1(L_{\text{box}})/\sigma_0^2(r)$ is large. To illustrate this correlation, we have plotted the multiplicity function $f_0(M)$ for the Λ CDM model in Fig. 6. This has been plotted for redshift $z = 20$ and 15 and the mass range has been chosen such that very large box size is required to keep $\sigma_1^2(r, L_{\text{box}})/\sigma_0^2(r)$ smaller than 0.1 . We have also plotted $f(M, L_{\text{box}})$ here, with $L_{\text{box}} = 5 h^{-1}$ kpc (dotted curve), $L_{\text{box}} = 20 h^{-1}$ kpc (dot–dashed curve) and $L_{\text{box}} = 100 h^{-1}$ kpc (dashed curve). These correspond to $C_1/\sigma_0^2 \simeq 0.6, 0.3$ and 0.19 , respectively. The top row is for the Press–Schechter mass function and the lower row is for the Sheth–Tormen mass function. An identical x – y range has been used to highlight the differences between the two models for mass function as well. It is noteworthy that the relative error is similar in both the cases even though the multiplicity function itself is different. At $z = 20$, the multiplicity function is underestimated by a large amount for $L_{\text{box}} = 5 h^{-1}$ kpc, even though $L_{\text{box}}/r_{\text{nl}} \simeq 120$ and if we are interested in scales around 1 pc then $L_{\text{box}}/r \simeq 5000$. The situation at small masses is better for

the other two simulation volumes considered here. For $z = 15$, the scale of non-linearity is $r_{\text{nl}} = 1.4 h^{-1}$ kpc, very close to $L_{\text{box}} = 5 h^{-1}$ kpc and hence we do not expect believable results for this box size. Indeed, the two panels on the right demonstrate the large errors and the absurdly incorrect shape of the multiplicity function. The difference in $f(M)$ and $f_0(M)$ at $10^{-6} M_{\odot}$ is about 25 per cent for $C_1(L_{\text{box}})/\sigma_0^2 = 0.3$, in this case $L_{\text{box}} = 20 h^{-1}$ kpc and $L_{\text{box}}/r \simeq 2 \times 10^4$. The error in the multiplicity function is slightly larger than 10 per cent for $L_{\text{box}} = 100 h^{-1}$ kpc even though $L_{\text{box}}/r \simeq 10^5$ and $L_{\text{box}}/r_{\text{nl}} \simeq 67$. The multiplicity function plotted here is the global function, and the conditional mass functions should be used in order to estimate errors in simulations where a high peak is studied at better resolution. Similar results are obtained for other mass functions that have been suggested as a better fit to simulation data (Jenkins et al. 2001; Warren et al. 2005).

The above discussion demonstrates the perils of using simulations where $C_1(L_{\text{box}})/\sigma_0^2(r)$ is close to unity. One may argue that models for mass function have not been tested in this regime where the local slope of the power spectrum is very close to -3 , but the fact that error in amplitude of density perturbations itself is large should be reason enough to worry about reliability of results. Further, the agreement in the magnitude of errors for the several approaches to mass functions also gives us some confidence in results.

Majority of simulations are not affected by such serious errors, as the slope of power spectrum approaches -3 only at very small scales (large wavenumbers). However, high-resolution simulations of earliest structure formation in the Λ CDM model need to have a very large dynamic range before the results can be believed within 10 per cent of the quoted value. Indeed, our work may have some relevance to the ongoing discussion about the Earth mass haloes (Diemand, Moore & Stadel 2005; Moore et al. 2005; Zentner, Koushiappas & Kazantzidis 2005; Zhao et al. 2005a,b).

4 CONCLUSIONS

Conclusions of this work may be summarized as follows.

(i) We have presented a formalism that can be used to estimate the deviations of cosmological N -body simulations from the models being simulated due to the use of a finite box size. These deviations/errors are independent of the specific method used for doing simulations.

(ii) For a given model, the deviations can be expressed as a function of the scale r of interest and L_{box} , the box size of simulations.

(iii) We have applied the formalism to study deviations in rms fluctuations in mass in the initial conditions.

(iv) We find that the errors are small except for models where the slope of the power spectrum is close to -3 at scales of interest.

(v) The errors in case of the Λ CDM model are significant if the scale of interest is smaller than a kpc even if simulations as large as the Millennium simulation (Springel et al. 2005) are used.

(vi) We have studied errors in mass function in the Press–Schechter model, as well as other models.

(vii) The main error due to a finite box size is that the number of high-mass haloes is underestimated.

(viii) The number of low-mass haloes is overpredicted in simulations if the box size effects are important. This happens as low-mass haloes do not merge to form the (missing) high-mass haloes.

(ix) We have verified these trends using N -body simulations.

We note that it is extremely important to understand the sources of errors in N -body simulations and the magnitude of errors in quantities of physical interest. N -body simulations are used to make predictions for a number of observational projects and also serve as a test bed for methods. In this era of ‘precision cosmology’, it will be tragic if simulations prove to be a weak link. We would like to note that our results apply equally to all methods of doing cosmological N -body simulations, save those where techniques like MAP are used to include the effects of scales larger than the simulation volume.

The method for estimating errors due to a finite box size described in this paper can be used for several physical quantities. In this paper, we have used the method to study errors in clustering properties and mass functions. We are studying the effect of finite box size on velocity fields and related quantities, the results will be presented in a later publication.

ACKNOWLEDGMENTS

Numerical experiments for this study were carried out at cluster computing facility in the Harish-Chandra Research Institute (<http://cluster.mri.ernet.in>). This research has made use of NASA’s Astrophysics Data System. We thank the anonymous referee for useful comments.

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