Towards quantitative control on discreteness error in the non-linear regime of cosmological N-body simulations

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ABSTRACT
The effects of discreteness arising from the use of the N-body method on the accuracy of simulations of cosmological structure formation are not currently well understood. In the first part of this paper, we discuss the essential question of how the relevant parameters introduced by this discretization should be extrapolated in convergence studies if the goal is to recover the Vlasov–Poisson limit. In the second part of the paper, we study numerically, and with analytical methods developed recently by us, the central issue of how finite particle density affects the precision of results above the force-smoothing scale. In particular, we focus on the precision of results for the power spectrum at wavenumbers around and above the Nyquist wavenumber, in simulations in which the force resolution is taken to be smaller than the initial interparticle spacing. Using simulations of identical theoretical initial conditions sampled on four different ‘pre-initial’ configurations (three different Bravais lattices and a glass), we obtain a lower bound on the real discreteness error. With the guidance of our analytical results, which match extremely well this measured dispersion into the weakly non-linear regime, and of further controlled tests for dependences on the relevant discreteness parameters, we establish with confidence that the measured dispersion is not contaminated either by finite box size effects or by subtle numerical effects. Our results notably show that, at wavenumbers below the Nyquist wavenumber, the dispersion increases monotonically in time throughout the simulation, while the same is true above the Nyquist wavenumber once non-linearity sets in. For normalizations typical of cosmological simulations, we find lower bounds on errors at the Nyquist wavenumber of the order of 1 per cent, and larger above this scale. Our main conclusion is that the only way this error may be reduced below these levels at these physical scales, and indeed convergence to the physical limit firmly established, is by extrapolation, at fixed values of the other relevant parameters, to the regime in which the mean comoving interparticle distance becomes less than the force-smoothing scale.

Key words: gravitation – methods: N-body simulations – large scale structure of Universe.

1 INTRODUCTION
Dissipationless cosmological N-body simulations aim to reproduce the clustering of dark matter in the universe, assumed to be in the form of a microscopic particle with extremely weak non-gravitational interactions (for reviews see e.g. Bertschinger 1998; Bagla 2005; Dolag et al. 2008). In the absence of an analytical treatment of the strongly non-linear regime, these simulations have become increasingly central in extrapolating the predictions of the current ‘standard model’ of cosmology to the corresponding scales. Many kinds of observations now probe directly or indirectly the distribution of dark matter at these scales, and will do so with greater precision in the coming years. The resultant need for precision in the theoretical results makes more necessary than ever a better understanding of these simulations. This paper concerns one potentially important source of error which is currently still poorly understood: rather than evolving numerically the theoretical Vlasov–Poisson (VP) equations describing the self-gravitating dark matter, simulations employ the N-body method in which the matter is sampled by ‘macro-particles’. The errors introduced, i.e. the difference between the results of the finite N simulation and

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those in the theoretical model (which corresponds to an appropriate $N \to \infty$ limit), are not understood. This is the discreteness problem in cosmological N-body simulation. It is a problem which has received, given its potential importance, a very modest amount of attention (see references below). Further, the existing literature on the issue is marked by a considerable diversity in its conclusions, both qualitatively and quantitatively. Given the ever more pressing need for robust control on the very considerable precision required of simulations – a goal of 1 per cent precision is now typically considered (see e.g. Huterer & Takada 2005; McDonald, Trac & Contaldi 2006) – it is an issue which deserves attention.

In this paper, we first give a brief review of the problem of discreteness in cosmological N-body simulation. We describe briefly both previous work by other authors on the issue and some recent work by us and our collaborators, in which we have developed new analytical approaches to describe discreteness effects both in the initial conditions of simulations and in their early time evolution. As a starting point, we attempt here to give a precise explicit formulation of the problem of discreteness. This notably distinguishes the problem from strictly numerical issues (e.g. about the agreement of codes using different summation techniques). We emphasize in particular on the necessity to establish, before any discussion about the quantification of errors, precisely how numerical simulations should be extrapolated to approach the desired theoretical limit. Our conclusion is simply that such an appropriate extrapolation is one which takes the interparticle spacing $\ell$ to zero, at fixed values of the other relevant discreteness parameters. Further such extrapolation should be done keeping the initial conditions fixed, which – given that simulations are performed in a finite periodic system – means using the same realization (and modes) of the initial theoretical power spectrum (PS).

After this introductory discussion, we turn to a numerical and analytical study of the issue. The goal of this study is to answer the more practical question of how small the interparticle distance $\ell$ must be to attain convergence of physically relevant quantities to a desired precision. In particular, we focus on the issue, which is at the centre of some controversy in the literature, of the accuracy of results, at scales around and below the initial interparticle distance of simulations which use a force-smoothing scale smaller than this latter scale. To attempt to resolve the question, we use here a simple numerical method to isolate errors which manifestly must arise from discreteness, and which therefore give a lower bound on the discreteness errors. We focus here on the two-point correlation properties of clustering, but the method we use can be extended to any other quantity (e.g. mass function, merger rates). The essential difference between our study and the few previous such attempts is that we do not compare to the application of the perturbations corresponding to the given theoretical initial conditions. The canonical choices in the literature are ‘grid’ [a simple cubic (SC) lattice] or ‘glass’ (White 1993). Here, we consider a wider class of such configurations, employing also two different Bravais lattice configurations [body-centred cubic (BCC) and face-centred cubic (FCC)]. The reason for our choice of these configurations is that they allow us to apply our analytical treatment in a very powerful way. This formalism gives a very accurate description for the early time evolution of simulations starting, in principle, from any perturbed Bravais lattice. The differences in the evolved power spectra, starting from the same realization of the theoretical model discretized on these different distributions, measured in our simulations are in extremely good agreement with these analytical predictions for all wavenumbers at early times, and progressively deteriorates, as anticipated, as we go into the strongly non-linear regime. In this latter regime, we observe that these differences show similar dependences on the discreteness parameters as in the regime where we can fit them analytically. Notably at a given physical scale, they decrease as $\ell$ decreases, and increase monotonically as a function of time at fixed $\ell$.

These tests give us a robust non-trivial lower bound on the size of systematic discreteness errors. For the PS, which is the quantity we focus on, these lower bounds are of the order a few per cent for wavenumbers comparable to and larger than the Nyquist frequency for a starting redshift equal to 2, and then decrease monotonically at smaller wavenumbers. While the precise bounds for any given cosmological model (and the choice of other relevant simulation parameters) will differ, they will be of this order (or larger, as the bounds monotonically increase with the starting redshift). Our results allow us then to draw conclusions about the question of how far $\ell$ must be extrapolated to attain errors smaller than of this order. Specifically, we conclude that the common practice of using results considerably below the scale $\ell$ (or $\pi/\ell$ in reciprocal space) may be justified, but only with a discreteness error bar which is, for the PS, and for normalizations typical of cosmological simulations, of the order of these lower bounds, i.e. several per cent. Precision greater than this for a given wavenumber $k$, e.g. down to below the 1 per cent level for the PS now often cited as necessary, can be achieved only by using particle densities such that $k\ell < 1$. Indeed, results of simulations do not converge to the continuum limit until this parameter range is reached, and thus one cannot have real confidence in results without performing such an extrapolation. While this conclusion has been argued for in several studies by some authors (see references and discussion below), it is a much more stringent requirement than that assumed in much of the literature, and formulates a considerable challenge to simulation.

2 THE PROBLEM OF DISCREteness

The problem of discreteness in cosmological simulation arises from the fact that the numerical simulations are not a direct discretization of the equations of motion of the theoretical model. The latter is (usually) assumed to be described, on the physical scales of relevance, by VP equations (or ‘collisionless Boltzmann equations’) which give the evolution of the (smooth) phase space mass density. N-body simulations, on the other hand, are numerical integrations of the equations of motion of N self-gravitating particles, i.e.

$$\ddot{x}_i + \frac{2}{a} \dot{x}_i = -\frac{Gm}{a^2} \sum_{j \neq i} \frac{x_i - x_j}{|x_i - x_j|^3} W_r(|x_i - x_j|),$$

where dots denote derivatives with respect to time, $m$ is the mass of the particles, $x_i$ is the (comoving) position of the $i$th particle.
and \( W_ε(|x_i - x_j|) \) is a function which regularizes the divergence in the gravitational force at \( |x_i - x_j| = 0 \) below a characteristic scale \( ε \). These unphysical ‘macro-particles’ are artefacts of the \( N \)-body simulation technique, with a mass many orders of magnitude (typically \( \sim 10^{30} \)) larger than those of the theoretical dark matter particles.

As the VP equations may, in principle, be obtained as an appropriate \( N \to \infty \) limit of the particle system, the problem of discreteness is in practice that of determining the discrepancy between the solution of the \( N \)-body equations for some finite \( N \) and their solution for a much larger \( N \), representative of the VP limit. It is therefore evidently essential to precisely specify how to extrapolate cosmological \( N \)-body simulations to this limit. This is the point we first discuss.

### 2.1 Discreteness parameters

In the case of the \( N \)-body method employed to solve the cosmological problem, the unphysical parameters characterizing the numerical solution can be clearly divided into two. First, there are those required, in addition to the parameters of the input theoretical model, to characterize the equations (1) and their initial conditions. Secondly, there are the parameters introduced to then solve these well-posed equations numerically (e.g. time-step, parameters controlling the precision of the calculation of the force). It is only the former, which we will refer to as the **discreteness parameters** and denote by \( \{ D_α \} \), which are the subject of the study here. The latter set of parameters, which we will refer to as the **numerical parameters** of a simulation, control the accuracy with which the set of equations (1), with well-defined initial conditions, are solved. They therefore have no relevance to the problem of discreteness which we are focussing on: we wish to understand the relation between the results of a ‘perfect’ \( N \)-body simulation, i.e. an arbitrarily precise numerical solution of the equations (1) from well-specified initial conditions, and the evolution of the theoretical model from its corresponding initial conditions.\(^1\)

The set of discreteness parameters \( \{ D_α \} \) we consider is as follows.

1. The mass of the macro-particles (referred to as **mass resolution** in the literature), or equivalently (since the mean mass density is specified) their mean (comoving) number density \( n_0 \). We will parametrize this by \( \ell \equiv n_0^{-1/3} \), which we refer to as the **mean inter-particle spacing**.
2. The **smoothing parameter** \( ε \) characterizing the regularization of the force (known as the **force resolution** in the literature\(^2\)).
3. The pre-initial configuration, i.e. choice of grid, glass or other distribution. We will denote this discrete variable as **preIC**.
4. The **initial redshift**, \( z_i \).

\(^1\) The sensitivity of results to this second set is, of course, essential to understand in order to characterize the precision of results of simulations (e.g. using different codes), and indeed considerable effort to improve control has been made in the last few years (see e.g. Heitmann et al. 2008; Lukic et al. 2007). We note that the distinction we make here between the two kinds of parameters is not usually made in the literature on the ‘convergence’ of simulations (see e.g. Power et al. 2003; Lukic et al. 2007).

\(^2\) It is often referred to simply as the ‘spatial resolution’. We will not use this nomenclature here as the central issue we discuss is whether such an identification of the force-smoothing scale with that of the spatial resolution is valid.

Some remarks on this list are appropriate.

(i) Discreteness effects depend on the number of particles \( N \) used in a simulation only through the **density** of these particles. Change in results when \( N \) varies, at fixed \( ε \), is not a discrete effect: to pass from the VP equations to the \( N \)-body equations (1), and their initial conditions, we do not need to introduce the side \( L \) of the cubic box (which, with periodic replicas, is canonically used to approximate the infinite universe) as both sets of equations are well defined in infinite space. The box size \( L \) thus belongs to the second set of parameters, as it is introduced to solve the equations (1) in a (finite) numerical simulation. The dependences on it, i.e. on the variation of \( N \) at a fixed particle density, are finite-size effects. We do not study these effects here, and will always work at fixed \( L \) in our numerical study below. For studies of them, see e.g. Pen (1997), Sirko (2005), Bagla & Prasad (2007) and Bagla, Prasad & Khandai (2009).

(ii) The smoothing parameter \( ε \), on the other hand, cannot, in modern cosmological simulation, be considered as belonging to the numerical parameters: it is not, in this context, a parameter introduced to facilitate the numerical solution.\(^3\) Rather, as we will discuss further below, it is used with the aim of reducing effects of two-body collisionality, i.e. to try to make the \( N \)-body solution approach better than the theoretical collisionless behaviour corresponding to the VP equations.

(iii) That the initial redshift \( z_i \) is a discreteness parameter in the sense we have defined above has been shown explicitly in Joyce et al. (2005), Marcos et al. (2006) and Joyce & Marcos (2007a) (and is also summarized briefly in Section 2.4). Put simply, the treatment of the evolution of equations (1) in this work shows, analytically, that the initial conditions for the \( N \)-body system derived for a given input PS at a redshift \( z_i \) (using the canonical method based on the Zeldovich approximation) do not evolve exactly under equations (1) to those set up from the same PS at a different redshift \( z_i \). This is true in the limit of arbitrarily small initial relative displacements to the lattice where non-linear (fluid) corrections to the Zeldovich approximation can be neglected.

This list of discreteness parameters is a minimal one, appropriate for, say, a standard \( P^3M \)-type code. Even in this case, it could be elaborated to be more precise. For example, the regularization involves the choice of a function which is not always the same, and \( ε \) can vary in time.\(^4\) Different choices of the sampled modes may also be made in setting up initial conditions. The list is also adequate for a simple \( PM \) code, but evidently it would need to be expanded to describe adaptive codes in which the particle number changes in time and space according to some criteria. We will not consider such complexities here, apart from a few further comments on this point in our conclusions: it is sufficiently ambitious to hope, at least as a first step, to fully control the effects of discreteness for these simpler cases.

### 2.2 Convergence to Vlasov–Poisson limit

Let us now denote by \( \mathcal{Q}(r, z; \{ D_α \}) \) the measured value of any physically relevant quantity in an \( N \)-body simulation, at redshift \( z \), with values of the discreteness parameters \( D_α \), e.g. a two-point

\(^3\) Indeed, the equations (1) may be solved numerically without any such smoothing (and often are in other contexts e.g. galactic dynamics).

\(^4\) We have implicitly assumed it to be fixed in comoving length units, which is usually the case, although many other variants can be found in the literature.
correlation function or a PS (where the variable \(r\) is given the appropriate interpretation, and could equally well represent a set of vector separations for a higher order statistic).

The discreteness problem can be schematically represented then as that of determining an estimate of the difference

\[
\Delta Q(r, z; \{D_n\}) = Q(r, z; \{D_n\}) - Q_{\text{VP}}(r, z),
\]

where \(Q(r, z; \{D_n\})\) is the result of a ‘perfect’ N-body simulation and \(Q_{\text{VP}}(r, z)\) is the result of the same quantity in the VP equations evolved from the same initial conditions.

By construction \(Q_{\text{VP}}(r, z)\) is, in general, unknown. Indeed, it is because we cannot determine it analytically that we turn to N-body simulation. To estimate \(\Delta Q(r, z; \{D_n\})\), the best one can do is thus to study, numerically, the convergence of \(Q(r, z; \{D_n\})\) towards some fixed value as the \(\{D_n\}\) are appropriately extrapolated. If the goal is to approach as closely as possible the evolution of the VP equations, one should evidently extrapolate the relevant parameters in a way which indeed gives convergence to this limit of the N-body system. While it is evident that the interparticle distance \(\ell\) should be decreased, but how the other parameters should be varied (or not) is not. Indeed, as we will discuss further in our conclusions, most of the few convergence studies of cosmological simulations in the literature do not adopt an extrapolation which converges directly to the VP limit.\(^5\)

There is in fact no rigorous treatment in the literature on cosmological N-body simulations, or more broadly in the cosmology literature, establishing the existence of the VP limit: derivations of the VP equations (see e.g. Peebles 1980; Saslaw 1989) are limited to showing that these equations may be obtained by a truncation to the leading term of a BBGKY hierarchy of equations, but do not rigorously establish the conditions under which the required truncation may be made.\(^6\) Formal proofs establishing the validity of the Vlasov mean field approximation for long-range interacting systems can, however, be found in the mathematical physics literature (for a discussion see e.g. Spohn 1991). Notably, Braun & Hepp (1977) have proved that in a finite system of particles interacting through \(1/r^2\) pair forces, regularized so that the potential is bounded below at \(r = 0\), the Vlasov limit corresponds to \(N \to \infty\). In taking this limit, the volume, mass and time of evolution are kept fixed.\(^7\) We will assume, without rigorous proof, the evident extension of this result to the infinite volume case of cosmological simulations: we take the VP limit as \(\ell \to 0\) (i.e. particle number in any finite volume goes to infinity) at a fixed mass density, followed by \(\varepsilon \to 0\).\(^8\)

The convergence at a fixed temporal duration also corresponds to keeping the initial redshift \(z_i\) fixed, and as the limit should clearly not depend on preIC (the choice of pre-initial configuration), we also keep this fixed.

In summary, applied to an N-body simulation, this tells us that an appropriate extrapolation is given by decreasing \(\ell\) (i.e. increasing the particle density) while keeping the other discreteness parameters \(\{D_n\}\) fixed. The limit is taken at fixed \(\varepsilon \neq 0\), which means that the spatial resolution (for unsmoothed gravity) is limited to above this scale. In other words, this extrapolation converges to a smoothed version of the VP equations, which then (we assume) would converge to VP as \(\varepsilon \to 0\). This extrapolation is not necessarily unique – convergence may in principle be obtained while allowing \(z_i\) and/or \(\varepsilon\) to vary in various manners as a function of \(\ell\) – but it is certainly simple. The use of any alternative (if we emphasize, the goal is to obtain direct convergence to the VP limit) should, however, be carefully considered to establish (at least as rigorously as here) that it gives convergence to the VP limit.

It is important to note the specific order of the limits in \(\ell\) and \(\varepsilon\). Beyond the necessity to introduce a regularization in rigorous proofs of the VP limit mentioned above, the reason for this can be understood easily on physical grounds: the scale \(\varepsilon \neq 0\) provides a characteristic scale which is clearly necessary to give physical significance to the limit \(\ell \to 0\). Indeed, taking \(\varepsilon = 0\) and initial conditions specified by a pure power-law input PS, \(\ell\) is the sole characteristic scale of the discrete system (in the limit \(L \to \infty\)), and defines itself the unit of length. Varying \(\ell\) gives, up to a trivial rescaling, a system with exactly the same dynamics, which manifests not that of the VP limit (as it includes explicitly non-mean field effects such as two-body collisionality). When, on the other hand, the same system is treated, but now with \(\varepsilon \neq 0\), the limit \(\ell \to 0\) has a non-trivial meaning if it is taken at constant \(\varepsilon\). Indeed, non-mean-field effects such as two-body scattering, and other ones we will describe below, are explicitly no longer present in the dynamics in this limit.

Finally, we make one important remark about initial conditions. Evidently to establish convergence to the evolution of a given continuum model, one should keep the initial conditions in this limit fixed. While we have explicitly stated that, in extrapolating, the initial redshift \(z_i\) should be held fixed, this does not prescribe unambiguously the initial conditions at any finite \(\ell\): given that simulations are performed in a finite volume, the number of modes in any interval of wavenumber is finite, and thus different realizations of the same initial conditions introduce intrinsic statistical fluctuations in the initial conditions compared to the average theoretical behaviour. For convergence studies of discreteness effects specifically it is simplest to also keep the realization fixed, although of course such effects can in principle be averaged out by a sufficiently large number of realizations.\(^9\)

2.3 How far must one extrapolate?

While the above discussion simply tells us how to extrapolate towards the VP limit, the practical form of the discreteness problem is more detailed: how small do we need \(\ell\) to be, given certain fixed values of other parameters in the set \(\{D_n\}\), to attain a desired precision \(\Delta Q(r, z; \{D_n\})\) on the theoretical quantity \(Q_{\text{VP}}(r, z)\)?

\(^5\) A notable exception is the study reported in Splinter et al. (1998), which we will discuss below, as well as a recent paper by Romeo et al. (2008a).

\(^6\) For an alternative derivation of the VP equations using a coarse-graining of the microscopic equations for the particle system, see Buchert & Domínguez (2005).

\(^7\) Formally, the coupling in the interaction (i.e. \(Gm^2\) for gravity, where \(m\) is the particle mass) scales in proportion to \(1/N^2\).

\(^8\) As noted, the proof of Braun & Hepp (1977) is for finite non-zero smoothing, and the existence of the exact VP limit \(\varepsilon \to 0\) has not in fact been proven. We neglect this mathematical subtlety here, which one would expect to be relevant, at most, to the asymptotically long time behaviour of the system (which does not interest us in this context).

\(^9\) Further, when \(\ell > \varepsilon\), one needs to specify whether power should be added (if present in the theoretical model) in the larger range of wavenumbers which can be sampled in the initial conditions as \(\ell\) decreases. While this is not the source of ambiguity in our extrapolation (as power should evidently not be added in the range that \(\ell < \varepsilon\), for studies in the range \(\ell > \varepsilon\), such as that we will report below, it is relevant. We will use the prescription that the realization of the input displacement field is kept fixed, as this allows us to identify the effects of discreteness most clearly.
Current practice in interpreting the results of cosmological simulations appears to repose on an approximate answer to this question, which we now attempt to summarize (see e.g. Smith et al. 2003; Power et al. 2003). It is supposed that there are essentially two ways in which discreteness can play a significant role in making an N-body simulation deviate from the desired VP evolution:

D1. Through the limits placed on the accurate representation of the initial conditions. Indeed, to avoid aliasing effects, only modes of the input theoretical PS up to the Nyquist frequency \( k_N = \pi / \ell \) should be sampled. Unless \( k_c \ll k_N \), this means that there is ‘missing power’. In simulations of cold dark matter (CDM)-type models, notably, this is always the case. Further, for any initial PS, there is always additional power in the initial conditions, predominantly at \( k > k_N \), generated purely by the discretization.  

D2. Through two-body collisions in the course of the dynamical evolution which cause deviations from the desired mean field behaviour of the VP limit.

The first point is believed not to place, in practice, an important limitation on the accuracy of simulations once they are evolved. The reason is that gravitational clustering, from CDM cosmological initial conditions, is understood to develop essentially by the transfer of power from large to small scales, non-linear structures being formed by the evolution of fluctuations at initially larger scales. The spatial resolution thus improves rapidly as time goes on, essentially following the forming non-linear structures which depend only on the presence of the initial fluctuations which seeded them. Small residual effects are envisaged, arising from the ‘spurious’ power generated by the sampling on a specific pre-initial configuration (grid or glass), but they are usually assumed to be negligible and of no practical importance. An exception is in the case of hot (or warm) dark matter spectra. In this case, one may have \( k_c \ll k_N \) so that all the initial power is well represented, but the small-scale power generated by discreteness can evolve to form structures which may not be ‘wiped out’ sufficiently rapidly by the structures forming at larger scales. Recently, interest in this case has been regenerated in the context of simulation of ‘warm dark matter’ models, and it has been explicitly shown in numerical studies (Gotz & Sommer-Larsen 2003; Wang & White 2007), using different preIC (grid or glass), that such effects may be important, leading to gross discreteness effects in such simulations.

The effects of two-body collisionality (D2) are understood to be taken care of by the smoothing \( \varepsilon \). Indeed, it is explicitly for this reason that such a smoothing is introduced, its value being chosen ideally large enough to suppress the related effects, but small enough so that too much spatial resolution is not lost. Since, according to simple estimates (Binney & Tremaine 2004), one expects such effects to be largest in regions of highest density, \( \varepsilon \) is chosen just large enough to suppress them, over the relevant cosmological time-scales, in such regions.

In summary, these physical arguments may be formulated as qualitative answers to the question posed above, as follows. For typical quantities measured in simulations (e.g. two-point correlation function, PS, halo masses and profiles), the errors \( \Delta Q(r, z; \{ D_n \}) \) due to discreteness, for any \( r \) a little larger than \( \varepsilon \), are negligible, i.e. so small as to be of no practical interest (compared to attainable numerical errors, notably), if:

A1. \( \varepsilon \) is sufficiently small so that, at redshift \( z \), the fluctuations at scale \( r \) may be formed by the collapse of fluctuations initially at scales \( k < k_N \).

A2. \( \varepsilon \) is sufficiently small so that the collisional relaxation time-scale in the densest-resolved regions (i.e. the highest density in a region of radius \( \sim \varepsilon \)) is large compared to the age of the universe.

Both of the answers can be converted, by making the use of known phenomenological models describing the results of simulations (notably halo models, or the model of Peacock & Dodds 1996), into approximate criterion for the necessary \( \ell \) (i.e. particle density) expressed in terms of the parameters of the theoretical model, and the scales \( r \) and \( \varepsilon \), and of the redshift \( z \). In Hamana, Yoshida & Suto (2002), one can find, for example, approximate criteria derived using halo models, while Knebe et al. (2000), Power et al. (2003) and Diemand, Moore & Stadel (2004b) present extensive numerical studies. A series of other articles specifically focus on the effects of two-body relaxation in placing limits on the accuracy of density profiles in haloes, mostly using numerical approaches (Binney & Knebe 2001; Diemand et al. 2004a; El-Zant 2006). A recent paper by Bagla & Prasad (2009) concludes, on the basis of some simple numerical tests on different theoretical initial conditions, that discreteness effects may be neglected once the non-linearity scale has evolved to be larger than the mean interparticle separation.

2.3.2 Dissenting views

While these answers may be correct, they are certainly not in any way rigorous. The essential problem is that they assume that the physical effects of discreteness are known, or, at least, that those which play any significant role in simulations are known. While the latter may a posteriori prove to be true, the former certainly is not. Indeed, understanding of the role of discreteness in the highly non-linear evolution of these systems is extremely limited.

One of the surprising aspects, at least at first sight, of the standard criteria just discussed is that they allow the resolution scale of a simulation (at \( z = 0 \)) to be very much smaller than the scale \( \ell \). Indeed, in practice the spatial resolution is usually taken to be fixed by \( \varepsilon \), with \( \varepsilon \ll \ell \). If one considers that this smoothing is introduced to make the ‘macro-particles’ behave like fluid elements, moving under the effect of the mean field, it would appear to be necessary to

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10 Analytical expressions for the full initial conditions are given in Joyce & Marcos (2007b). On a lattice, at linear order in an expansion in the amplitude of the input spectrum, the discrete power is non-zero only for \( k > k_N \). In a glass, there is also a contribution, \( \propto k^2 \) at small \( k \), for \( k < k_N \).

11 A numerical study which nicely illustrates this may be found in Little, Weinberg & Park (1991) (see also Bagla & Padmanabhan 1997 and Bagla & Prasad 2009).

12 Some works (e.g. Smith et al. 2003) attempt to correct for the associated effects by subtracting this power which can be measured in the initial conditions. This procedure assumes that this spurious power does not evolve, an assumption which we have shown analytically to be incorrect in Joyce & Marcos (2007b).

13 In these latter papers, the question of discreteness is not separated from the question of numerical convergence of the N-body equation. Thus, particle density and the smoothing \( \varepsilon \) are considered on the same footing as choice of time-step, and parameters for force precision, etc. The sets of simulations studied do not in fact define a convergence study to the VP limit, as we have discussed above: power is added as the particle density is increased, and the initial redshift also changes. We will return to this point in our conclusions.

14 In the ‘Millenium’ simulation (Springel et al. 2005), for example, \( \varepsilon \approx \ell / 50 \).
have, at least, $\varepsilon \sim \ell$. This point has been forcefully argued by Melott et al. in a series of papers during the nineties (Melott 1990; Kuhlman, Melott & Shandarin 1996; Melott et al. 1997; Splinter et al. 1998), and restated in a recent comment (Melott 2007). In Melott (1990), Kuhlman et al. (1996) and Melott et al. (1997), specific non-Vlasov effects are explicitly shown to be present in numerical experiments, and of much greater importance once the regime $\varepsilon < \ell$ is attained. One of the few controlled studies of the issue of discreteness in the literature in a spirit resembling that advocated above is given in Splinter et al. (1998). The paper focuses on the difference between results of simulation using PM codes and P$^3$M codes at different resolutions. Its conclusion is that results of the latter codes in the regime $\varepsilon < \ell$ do not agree well, most notably for phase-sensitive statistics, with those obtained from higher resolution PM codes (for which $\varepsilon = \ell$). These results, which place a question mark over the reliability of results below the scale $\ell$, have largely been ignored and addressed only very incompletely in subsequent works (see, notably, Knebe et al. 2000; Hamana et al. 2002) which support, broadly, the ‘common wisdom’ which we have outlined above.\footnote{We say ‘incompletely’ because no other published work has, to our knowledge, reported similar precise tests measuring the same quantities. Knebe et al. (2000) ascribe the differences seen in the two-point correlation properties by Splinter et al. (1998) to ‘erroneous evolution in high-resolution (HR) runs’, but without any proof [their own numerical tests, unlike those of Splinter et al. (1998), are not tests for discreteness effects but for the coherence of results produced by different codes.]. The analysis of Hamana et al. (2002), which explicitly calculates how resolution improves with time as foreseen by the ‘common wisdom’ described above, suffers from the weakness, underlined by the authors themselves, that it is based on the use of a halo model description of non-linear clustering, itself drawn from numerical simulations.}

The common wisdom has also been questioned by several other authors (Suisalu & Saar 1995; Baertschiger, Joyce & Sylos Labini 2002; Xiao et al. 2006; Romeo et al. 2008a), all placing in question (like Melott et al.) the use of a smoothing $\varepsilon < \ell$ on the basis of numerical results. In particular, we note that the role played by interactions of particles with their nearest neighbours – which give physical effects clearly not representative of the mean field VP limit – in the evolution of clustering at early times in simulations has been highlighted in cosmological simulations in Baertschiger et al. (2002), and in a simplified class of gravitational N-body simulations in Baertschiger et al. (2007a,b, 2008). In a very recent study, Romeo et al. (2008a) also conclude, on the basis of a study using wavelet techniques to analyse a set of CDM simulations, that results below the scale $\ell$ are unreliable. We also note the discussion of discreteness effects in Binney (2004), which illustrates with a study of a one-dimensional sheet model that discreteness may induce effects prior to virialization (and distinct from two-body effects) by artificially bounding above the growth of the phase space density.

### 2.4 Analytical results

In our recent work and that of our collaborators (Joyce et al. 2005; Marcos et al. 2006; Joyce & Marcos 2007a; Marcos 2008), we have used a perturbative treatment of cosmological N-body simulations to treat discreteness effects analytically. While the method is limited by its range of application (to sufficiently early times), it has the advantage of providing an exact quantification of these effects in that range, as well as an understanding of the physical mechanism at play. In this section, we will briefly review this formalism, which we will employ in the next section in the analysis of our numerical results.

The treatment can be understood as a generalization to discrete distributions of the standard linearization of the equations of a self-gravitating fluid, in the Lagrangian formalism (see e.g. Buchert 1992). At linear order, we thus refer to it as ‘particle linear theory’ (PLT). The full details can be found in these publications, and we will limit ourselves to a short summary of the essential idea, and the salient results. We note that while Joyce & Marcos (2007a) present the details of the use of PLT to quantify discreteness effects in the usual case of a SC lattice as $\textit{preIC}$, Marcos (2008) fully develops its generalization to the cases that $\textit{preIC}$ is a BCC or FCC lattice. We will fully exploit this latter generalization in the next section.

The principle of this approach is very simple: it consists simply in Taylor expanding the force on each particle due to any other in their relative (vector) displacement from the lattice configuration.\footnote{The treatment is analogous to one used standardly in solid-state physics (see e.g. Pines 1963) to treat perturbations about a crystal, for the case of both short range two-body interactions (e.g. Lennard–Jones) and Coulomb interactions (see Marcos et al. 2006 for further discussion).} Since the force is zero in the unperturbed lattice, the force $F(\mathbf{R})$ on a particle originally at lattice site $\mathbf{R}$ can be written, at linear order in the displacements $u(\mathbf{R}, t)$, as

$$F(\mathbf{R}) = -\sum_{\mathbf{R}'} D(\mathbf{R} - \mathbf{R}') u(\mathbf{R}', t),$$

where the sum is over all the lattice sites, and the matrix $D$ is

$$D_{\mu\nu}(\mathbf{R} \neq 0) = Gm \left( \frac{\delta_{\mu\nu}}{R^3} - 3 \frac{R_\mu R_\nu}{R^5} \right),$$

$$D_{\mu\nu}(0) = -\sum_{\mathbf{R} \neq 0} D_{\mu\nu}(\mathbf{R}),$$

where $\delta_{\mu\nu}$ is the Kronecker delta, and the subscripts are the Cartesian indices.\footnote{A sum over the copies, due to the periodic boundary conditions, is left implicit in these expressions.} With this approximation to the force, the equations of motion for the particles (equation 1) may then be written as

$$\ddot{u}(\mathbf{R}, t) + 2H\dot{u}(\mathbf{R}, t) = -\frac{1}{a^3} \sum_{\mathbf{R}'} D(\mathbf{R} - \mathbf{R}') u(\mathbf{R}', t).$$

Defining the discrete Fourier transform (FT) on the lattice and its inverse by

$$\hat{u}(\mathbf{k}, t) = \sum_{\mathbf{R}} e^{-i\mathbf{k} \cdot \mathbf{R}} u(\mathbf{R}, t)$$

$$u(\mathbf{R}, t) = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{R}} \hat{u}(\mathbf{k}, t),$$

where the sum in equation (6b) is over the first Brillouin zone (FBZ) of the lattice, i.e. the set of $N$ non-equivalent reciprocal lattice vectors closest to the origin $\mathbf{k} = 0$,\footnote{For a SC lattice the vectors of the FBZ are thus $\mathbf{k} = n(2\pi/L)$, where $n$ is a vector of integers of which each component $n_i(i = 1, 2, 3)$ takes all integer values in the range $-N^{1/3}/2 < n_i \leq N^{1/3}/2$. See Marcos (2008) for the explicit expressions for the FBZ vectors of a FCC and BCC lattice.} equation (5) can be written in reciprocal space as

$$\ddot{\hat{u}}(\mathbf{k}, t) + 2H(t) \dot{\hat{u}}(\mathbf{k}, t) = -\frac{1}{a^3} \hat{D}(\mathbf{k}) \hat{u}(\mathbf{k}, t),$$

where $\hat{D}(\mathbf{k})$ is a diagonal matrix in the FT domain.

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where $\mathcal{D}(k)$, the FT of $\mathcal{D}(R)$, is a symmetric $3 \times 3$ matrix for each $k$.

The solution of the dynamical problem now reduces simply to the diagonalization of the $\mathcal{D}(k)$, which is straightforward (and inexpensive) numerically. For each $k$, this gives three orthonormal eigenvectors $e_i(k)$ and their eigenvalues $\omega_i^2(k)$ ($n = 1, 2, 3$). The evolved displacements from any initial perturbed lattice configuration, specified at a time $t_0$, may then be written as

$$u(R, t) = \frac{1}{N} \sum_k \left[ \mathcal{P}(k, t) \tilde{u}(k, t_0) + \mathcal{Q}(k, t) \tilde{u}(k, t_0) \right] e^{i k \cdot R},$$

where the matrix elements of the ‘evolution operator’ $\mathcal{P}$ and $\mathcal{Q}$ are

$$\mathcal{P}_{\mu\nu}(k, t) = \sum_{n=1}^{3} U_n(k, t) (e_n(k))_{\mu} (e_n(k))_{\nu},$$

$$\mathcal{Q}_{\mu\nu}(k, t) = \sum_{n=1}^{3} V_n(k, t) (e_n(k))_{\mu} (e_n(k))_{\nu}. $$

The functions $U_n(k, t)$ and $V_n(k, t)$ are linearly independent solutions of the mode equations

$$\ddot{\tilde{f}} + 2H \dot{\tilde{f}} = -\frac{\omega_i^2(k)}{a^2} \tilde{f},$$

chosen such that $U_n(k, t_0) = 1, U_n(k, t_0) = 0, V_n(k, t_0) = 0$ and $V_n(k, t_0) = 1$.

The expression equation (8) for the evolution is, up to the validity of the linearized approximation to the force, exact for the discrete system. To use it to determine discreteness effects we must, as we have discussed at length in the previous sections, identify first unambiguously the correct continuum limit, and how it is obtained by extrapolation of the discreteness parameters. We have shown in Joyce & Marcos (2005) and Marcos et al. (2006) that this may be done directly from equation (8): taking the limit $\ell \to 0$, this expression for the evolution converges exactly to that obtained (Buchert 1992) by linearizing the equations for a self-gravitating fluid in the Lagrangian formalism, which reduces asymptotically to the Zeldovich approximation. The latter represents the appropriate analogous treatment of the VP limit. Note again that the limit $\ell \to 0$ in equation (8) is taken at fixed $t_0$ (i.e. fixed initial redshift $z_i$) and for a fixed input spectrum of displacements $\tilde{u}(k)$ (and velocities $\dot{\tilde{u}}(k)$).

The differences between the evolution given by equation (8) and this continuum evolution may then be computed exactly for any given initial conditions, yielding the discreteness effects, in the regime of validity of the PLT approximation. In Marcos et al. (2006), we have numerically studied the domain of validity of PLT for a range of different initial conditions, and conclude that, for some simple statistical quantities, it describes the evolution up to the time when many particles approach their nearest neighbours, which corresponds approximately to shell crossing in the corresponding fluid limit.\(^{20}\) In Joyce & Marcos (2007a), we have presented a quantitative analysis of the discreteness effects in this corresponding regime, for some basic quantities in typical cosmological simulations. Some of the essential results are as follows.

(i) The modification at shell crossing (up to which the PLT treatment described fully the discreteness effects) of the evolution of any given mode of the displacement field grows monotonically with time. Indeed, taking the limit $z_i \to \infty$ at a fixed particle density (i.e. fixed $\ell$) the evolution of the N-body system diverges from the continuum VP limit.

(ii) The modification due to discreteness at shell crossing, for a fixed $z_i$, depends approximately on the ratio $k\ell$, increasing as $k\ell$ does. This is physically very reasonable: the longer the wavelength of a mode compared to the interparticle scale, the less affected is the evolution by discreteness. For the typical values of $z_i$ in cosmological simulations, the effect is typically to reduce the power in modes, by up to about 50 per cent at the Nyquist frequency, and by about 10 per cent at half this value.

Given this treatment of discreteness effects – exhaustive and analytical, but with a limited domain of validity in time – what can we conclude about the questions raised in the previous sections? Concerning the formal extrapolation to the VP limit, we have already noted that PLT indeed converges to the theoretical VP behaviour when the parameters are extrapolated as prescribed above. With respect to the question of how far we must extrapolate in $\ell$ in order to converge with some required precision to the VP evolution, the treatment also gives a clear answer, at shell crossing. The answer depends, of course, on the quantity considered, and then also on $z_i$ and on the cosmological model (which determined the redshift of shell crossing given $\ell$). In Joyce & Marcos (2007a), we have shown, for example, that for $z_i$ a factor of 5 larger than the redshift of shell crossing, errors of 5 per cent in the PS are achieved only for $k < k_0/4$. Thus if we want, at shell crossing, an accuracy of less than this on the power, we can use only results in this range.

This second conclusion is strikingly different from what one might expect given the ‘common wisdom’: the evolution of the simulation makes the range of scale over which the continuum model is accurately represented (to some given precision) decrease, rather than increase. It in fact suggests that the view that $\ell$ should be a lower limit for spatial resolution may even be too optimistic. These findings, however, only apply at shell crossing, and the ‘common wisdom’ above may still apply later on. Indeed, as we described, the justification for this common wisdom is that when the transfer of power, characteristic of gravitational clustering in these systems, sets in, differences at smaller scales are wiped out. These results at shell-crossing show, however, that between $z_i$ and shell crossing, errors develop in the long-wavelength modes (below $k_0$) which were not present in the initial conditions. As a result, modes at later time which depend on this power will necessarily inherit this error.

An important point which we emphasize is that the fundamental reason why the discreteness errors determined using PLT do not behave as expected by the common wisdom is that they arise from physical effects of discreteness which are not usually envisaged. Indeed, the physical effects described by PLT compared with the...
VP limit are different from the two effects envisaged usually which we
listed above. First, they are dynamical effects which modify the
evolution of any given mode in a way which is independent
of the initial conditions. Secondly, they are clearly not two-body
collisional effects.21 The effect they describe can be characterized
physically as a dynamical sparse sampling effect: PLT compared
with its VP limit tells us how the evolution of a fluctuation de-
pendson the spatial density of the sampling particles. An important
question is then evidently to understand how this physical effect –
which there is no reason to believe should go away when we pass
to the non-linear regime – quantitatively affects results in the latter
regime. We will return to this point in our conclusions.

3 A CALIBRATED NUMERICAL STUDY
OF DISCRETENESS EFFECTS

We return now to the practical question of how small \( \ell \) needs to be
for a measured quantity to have converged to a desired precision.
Since the force smoothing \( \varepsilon \) places a lower bound on the spatial
resolution, a simplified, more specific, form of the question is: how
small does \( \ell \) have to be in order that, at any given redshift, the
effects of discreteness are negligible down to scales of order \( \ell \varepsilon \)?
The answer provided by the ‘common wisdom’ above is that \( \ell \) is
sufficiently small, in typical simulations, if \( \ell \varepsilon \ll \ell \). This is indeed the strategy advocated
in Splinter et al. (1998), which reports a study of this type down to a
resolution \( \ell_2 = \varepsilon \). It concludes, as noted above, that there are signif-
ificant differences in results, i.e. no evidence for convergence, in the
range \( \ell_1 > \varepsilon > \ell_2 \). Other authors (Knebe et al. 2000) argue, however,
that these differences are ascribable to ‘erroneous evolution in HR
runs’. The difficulty in reaching a convincing conclusion is that the
questions of discreteness effects are intertwined with numerical and
finite size effects. While such differences should be resolvable by
further numerical tests, this would require considerable investment
of resources which, apparently because of the wide acceptance of
the ‘common wisdom’, has not been made.22

Instead of undertaking such a numerical study – which, given the
modest numerical resources at our disposition, would not in any
case likely to be any more conclusive than that reported by Splinter
et al. (1998) – we focus in the rest of this paper on another kind
of test. We will see that this will allow us to reach conclusions,
with modest-sized (but very well numerically converged) simula-
tions, about the central issue: the validity/precision of results in the
range of scales around or below \( \ell \), in simulations with \( \ell \gg \varepsilon \). The
aim is to provide a method which gives a non-trivial lower bound
on discreteness error in such simulations. To do so, we simply
compare the results of simulations from identical theoretical initial
conditions, changing only the choice of the discreteness parameter
\( preIC \), i.e. the pre-initial configuration. We can then study how this
error depends on time and scale. Although the measured effects
are quite small – at the most of the order of 5 per cent in the PS
for the times and scales relevant to cosmological simulations – we
can clearly establish, using the analytical PLT formalism combined
with numerical tests of their dependence on \( \ell \) and \( \varepsilon \), that they are
indeed discreteness effects. We can then address in a controlled way
the question of how far \( \ell \) needs to be extrapolated so that one can
be confident that the true systematic errors due to discreteness have
converged to significantly less than this lower bound (e.g. to less than
1 per cent).

Rather than considering a specific cosmological model, we con-
sider a simple power-law PS with exponent \( n = -2 \), evolved in an
EdS universe. This choice is both suitable for our study as it is simple
– introducing no characteristic scale in the input model – and close
to the currently favoured CDM-like cosmological model, which has
an initial PS with effective exponent ranging between \( n \approx -1 \) and
\( \approx -3 \) over the relevant range of scales. In particular, we note that
this PS is, like these cosmological models, long-wavelength domi-
nated so that the very efficient transfer of power from long to short
wavelengths which, as we have discussed above, is believed to play
a role in wiping out discreteness effects, should be well represented.
We will comment further in our conclusions on the generalization
to other initial conditions, and specifically to those of currently
favoured cosmological models.

All our simulations have been performed using the publically
available parallel tree-mesh code \textsc{gadget2} (Springel, Yoshida &
White 2001). We use this single (widely used and highly tested) code
for our study for the reasons we discussed above: the discreteness
effects we are trying to understand and control for are distinct
from differences arising between different codes, and indeed distinct
from any dependence of results on the numerical parameters of a
given code. The ‘calibration’ of our results with our analytic
tools here provides in fact a robust check that \textsc{gadget2}’s code’s
integration of the N-body equations of motion is sufficiently precise
that this is indeed the case. Comparison with other codes would
be, in the relevant regime, a check on the accuracy of these codes,
rather than a check on our results. In the regime where our analytic
results do not apply, we can have, of course, less confidence in
the identification of our measured effects as physical discreteness
effects, and a comparison with other codes could be instructive. We
will address this issue below, where we give details of the detailed
checks of numerical convergence of our results which we have
performed using \textsc{gadget2}.

3.1 Initial conditions

We use the standard method, based on the Zeldovich approximation,
to set up initial conditions by applying appropriate displacements
to four different \textit{preIC}: a SC lattice, a BCC lattice, a FCC lattice
and a glass configuration, shown in Fig. 1.

Our reference set of simulations, which we denote as S1, have the
number of particles shown in Table 1. The numbers for the BCC and

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{From left- to right-hand side: unit cell of the SC, BCC and FCC lattices.}
\end{figure}

21 To make this very explicit, we have shown in Joyce & Marcos (2007a) that
the inclusion of a simple Plummer smoothing in the force actually increases
the difference between PLT and the VP limit for unsmoothed gravity.

22 See, however, the recent paper by Romeo et al. (2008a), which we will
comment on in our conclusions.

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The PS of the pre-initial glass. The dashed line indicates the behaviour $\propto k^4$.

Discreteness error in N-body simulations

\begin{align}
\bar{u}(x) &= \sum_k [a_k \sin(k \cdot x) k - b_k \cos(k \cdot x) k], \\
&= R_1 \frac{P_{a0}(k)}{k^2}, \quad b_k = R_2 \frac{\sqrt{P_a(k)}}{k^2},
\end{align}

where $R_1$ and $R_2$ are two independent Gaussian random numbers with dispersion equal to unity. In writing the displacement field as a Fourier sum, we use the fact that the preIC are set up on a periodic cube, and the sum over the vectors $k$ extends then over the appropriate reciprocal lattice. Further, if the input PS itself does not have a cut-off at a wavenumber significantly smaller than the Nyquist wavenumber of the sampling preIC distribution, such a cut-off must be imposed to avoid aliasing effects. Here, where we consider a simple power-law PS without a cut-off, we will take the sum in $k$ to extend over the FBZ of the SC lattice, i.e. the reciprocal vectors $k = n(2\pi/L)$ with each integer component $n_i \in [-N/2, N/2]$. As we will discuss further below, this is the choice which minimizes aliasing effects for the SC lattice, but not for the other preIC configurations. We will measure the associated, very small aliasing effects in the initial conditions and keep track of their role in generating differences in the evolved distributions.

The only other parameter which needs to be fixed is the normalization of the input PS $P_a(k)$ (which is equivalent to the choice of the initial redshift $z_i$). In the set S1 we have taken, for all preIC,

\begin{equation}
k_N^3 P(k_N) = 0.6,
\end{equation}

where, in our units, $k_N = 64\pi$. We have made this choice for our reference simulations because it is close to that chosen for such initial conditions, on a SC lattice, by the widely used graphics package (Bertschinger 1995). We will discuss below the effect of modifying this choice.

Before turning to the evolution from this set of initial conditions, let us consider more precisely their correlation properties, and in particular the effects of aliasing we have mentioned above. To do so, we make use of the detailed analysis of initial conditions of N-body simulations reported in Joyce & Marcos (2007b). The PS of the perturbed preIC distribution can be written conveniently in the form

\begin{equation}
P(k) = P_c(k) + P_d(k),
\end{equation}

where $P_c(k)$ is the ‘continuous’ part, independent of the preIC distribution, and $P_d(k)$ is a ‘discrete’ term which depends on the latter. The full analytic expression for both these quantities can be expanded order by order in the amplitude of the input theoretical PS $P_a(k)$. At leading order, one obtains

\begin{align}
P_c(k) &= P_a(k), \\
P_d(k) &= P_{a0}(k) + P_{a}(k),
\end{align}

where $P_{a0}(k)$ is the PS of the unperturbed preIC configuration (i.e. lattice or glass) and

\begin{equation}
P_{a0}(k) = \frac{k^2}{(2\pi)^3} \int d^3q (\hat{q} \cdot \hat{k})^2 \frac{P_a(q)}{q^2} [P_{a0}(q + k) - P_{a0}(k)].
\end{equation}

This package determines the starting redshift $z_i$ by normalizing so that the maximum value of the density fluctuation field at any point of the lattice is unity. This gives a mass variance at this scale considerably less than unity, sufficiently small that non-linear corrections to the Zeldovich approximation should be small.
is a contribution to the PS which, if non-zero at small $k$, describes an aliasing of the input PS. If the \textit{preIC} is a perfect lattice, $P_{\text{IC}}(k)$ is given by equation (11) and therefore, for $k \neq K$, we have

$$P_{\text{IC}}(k) = k^3 \sum_{k \neq 0} \frac{\left| (K - k) \cdot \hat{k} \right|^2}{(K - k)^4} P_0(K - k),$$

(18)

where $K$ are the appropriate subset of reciprocal lattice vectors for each lattice. For the SC lattice, the vectors $K$ are given by $K = \frac{2\pi}{a} n \equiv 2k_\perp n$, where $n$ is any non-zero vector of integers. It can then be verified easily\(^{26}\) from the expression in equation (18) that $P_{\text{IC}}(k)$ is zero inside the FBZ of this lattice, i.e. for all $k$ with each component $k_\parallel, k_\perp \in [-k_\parallel, k_\parallel]$, if we impose a cut-off by making $P_{\text{IC}}(k)$ zero outside the same region. This choice, which is the one we have used (and which is that standardly used in this context; Bertschinger 1995; Couchman 1991) is optimal, in the sense that it maximizes the size of the region about $k = 0$ in reciprocal space where the representation of the input power is exact, at linear order in the amplitude of the input PS.

For other lattices, an analogous, but different, optimal choice can be made, taking the input PS non-zero only inside the given lattice’s FBZ. Here, we have not done so as such a procedure would require sampling the input PS at different wavevectors, which is incompatible with the requirement that we use an identical realization of the theoretical initial conditions. As a result we will have for the non-SC lattices a small contribution coming from the aliasing term as given in equation (18). For the glass, on the other hand, a more significant contribution from this term (as given in equation 17) is expected, as it is always non-zero and proportional to $k^3$ at sufficiently small $k$ (see Joyce & Marcos 2007b for further detail). In what follows, we will carefully study in simulations the evolution of these residual differences at small $k$ power in the initial conditions, showing that they can in fact be neglected in understanding the differences in the evolved power which emerge at these scales.

### 3.2 Numerical evolution of S1

We evolve\(^{27}\) these four initial conditions in an EdS cosmology, from a scale factor $a = 1$ to $2^7$. At this final time, as we will see below, the scale of non-linearity has reached the box size, and finite size effects dominate. \textsc{gadget} implements a smoothing which modifies the force from exactly Newtonian only below a scale $\epsilon$. We take here $\epsilon = \ell_{\text{sc}}/15$, where $\ell_{\text{sc}}$ is the interparticle spacing of the SC lattice. This is, according to the ‘common wisdom’, a conservative choice for the final resolution scale.\(^ {28}\)

### 3.3 Snapshot inspection

In Figs 3 and 4, we show snapshots, for each of the four initial conditions, of a slice of depth 0.3L of the simulation box. The four snapshots correspond to $a = 1$, $a = 2^4$, $a = 2^5$ and $a = 2^7$. In the initial conditions, at $a = 1$, the distributions look very different, reflecting the different small-scale properties, and long-range order, of the \textit{preIC} configurations. Blurring slightly one’s vision, however, one can make out clearly in the lattice configurations the very similar superimposed fluctuations at larger scales. The glass looks very different because it does not have the deterministic long range order of the lattice, which makes the projection appear considerably denser.\(^{29}\) In the second slice, at $a = 2^4$, the first non-linear structures have formed, and already now the visual impression is of a very strong resemblance in the clustering. Distinct differences are, however, still evident. In particular alignments inherited from the lattice configurations are clearly visible, most evidently in the SC lattice. In the next slice at $a = 2^5$ (which, as we will see below, is about the time at which the largest modes included in the box go non-linear), the first visual impression is of an even greater resemblance of the configurations, but again closer inspection reveals differences at smaller scales. Likewise, in the last slice, when almost all the mass is in just a few haloes, the broad features at large scales are impressively similar, while the spatial organization of smaller structures reveals evident differences.

Some of the differences observed visually in the earlier time snapshots are manifestly related to the subtle differences in the initial conditions, and are therefore clearly discreteness effects. The differences in the more evolved snapshots are, however, not necessarily indicative of anything other than the intrinsically chaotic dynamics of the non-linear regime of the evolution.\(^ {30}\) What we are interested in, and will now examine, are differences in the \textit{statistical} properties of these distributions, which are what we use them to infer in cosmology.

### 3.4 Power spectrum and correlation function

Let us consider more quantitatively the differences in the two-point properties of these distributions. In Figs 5 and 6, we plot the reduced two-point correlation function $\xi(r)$ and the PS $P(k)$, for a series of four different time slices.\(^ {31}\) Also shown, in an inset panel in each case, are the normalized residuals of each quantity with respect to the average, i.e. for a quantity $C^i(i)$ in the $i$th bin (of $k$ or $r$) in the simulation of initial conditions $I$ ($I = \text{SC, BCC, FCC, glass}$) the residual is

$$bC^i(i) = \frac{4C^i(i) - \sum_j C^i(i)}{\sum_j C^i(i)}.$$

(19)

Also shown in each case is the ‘linear theory’ (LT) prediction for the evolution of the theoretical PS, i.e. the initial theoretical PS multiplied by $a^3$.

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26 See Joyce & Marcos (2007a) for a more detailed discussion.
27 The details on the numerical parameters we have used for the results reported are given in Appendix A.
28 For comparison we note that, if our comoving particle density is assumed equal to that in the Millenium simulation (Springel et al. 2005), the comoving size of our box is then approximately $15h^{-1}$ Mpc. The ratio $\ell_{\text{sc}}/\epsilon$ in Springel et al. (2005) is approximately 50.
29 In passing we underline that, contrary to what is sometimes stated (e.g. Wang & White 2007), the glass is a long-range ordered distribution. In fact, it has the property that $P(k = 0) = 0$, which imposes the \textit{global} constraint that the integral of the two-point correlation function is zero. Discussion of the very particular stochastic long-range order of such ‘superhomogeneous’ (or ‘hyperuniform’) distributions, with $P(k = 0) = 0$, may be found in Gabrielli, Joyce & Sylos Labini (2002), Gabrielli et al. (2003) and Torquato & Stillinger (2003). To generate them starting from a Poisson distribution, as here, one requires long-range correlation in the displacements of the particles, provided here by the dynamics under the Coulomb force (which rearranges the points so that the fluctuations in any volume are proportional to the surface i.e. sub-Poissonian).
30 For a discussion of chaos in $N$-body self-gravitating systems see e.g. Sideris & Kandrup (2002).
31 Details of how these quantities have been estimated are given in Appendix B. Note that we write the two-point correlation function and the PS as functions only of the modulus of their arguments as an average over spherical shells in real and reciprocal space, respectively, is performed.
Figure 3. Snapshots of a slice of the system for the different ICs (BCC, top left; FCC, top right; SC, bottom right; glass, bottom left) at $a = 1$ (upper four panels) and $a = 2^3$ (bottom four panels).
These results broadly reflect the impression gained by visual inspection above. In particular, the inspection of the correlation function shows four distributions which are apparently very different at the initial time evolve to closely resemble one another already at $a = 2^5$. Note indeed that, at this time and the subsequent ones, the correlation functions are so similar as to be indistinguishable in the main plot down to about $r = 10^{-3}$, which coincides with our chosen $\epsilon$. In reciprocal space, the resemblance of the initial conditions – the
Thus, the expectation that non-linear structures grow monotonically with $a$ agrees in all cases and the final plot, $\xi$, we see differences in the PS which appear and grow monotonically with $a$, i.e. the gravitational evolution appears to produce some small differences at large scales which were not present initially. While such an effect is predicted by PLT, as documented in detail in Joyce & Marcos (2007a) and described briefly above, this is valid only at sufficiently early times. This first view of these results thus very strongly supports the ‘common wisdom’: there is very efficient transfer of power from larger scales to smaller ones at early times when the non-linear structures first develop at smaller scales. Indeed, between $a = 2^1$ and the final plot, at $a = 2^3$, there appears to be little evidence for any further washing out of the residuals in the power. On the contrary, they appear to grow, giving a dispersion of the order of several per cent at the final time.

These results are clearly illustrated in Fig. 7, which shows the square root of the variance of PS calculated at each $k$, and each of the four times as indicated, over the four realizations, i.e.

$$
\sigma_P(k, a) = \left\{ \frac{1}{m-1} \sum_{l=1}^{m} \left[ P_l(k) - \overline{P}(k) \right]^2 \right\}^{1/2}
$$

Figure 5. PS (left-hand column) and correlation function in real space (right-hand column) for $a = 1$ (top row) and $a = 2^3$ (bottom row).
where $l$ labels the $m = 4$ different preIC, and we have defined

$$P(k) = \frac{1}{m} \sum_{j=1}^{m} P_l(k).$$

Given that the amplitude of the effects is so small – at small $k$ and early times in particular – we evidently need to be careful in interpreting these differences as resulting from the physical discreteness effect we set out to measure. We could envisage that such a time- and space-dependent dispersion could be produced, in particular, by numerical effects in the evolution or by statistical effects in the estimators. For example, it is conceivable that there is an interplay between the numerical errors relating to the calculation of the force and each particular initial condition, or that the variance measured is simply a statistical variance which would decrease if we took more particles (i.e. a larger box at the same particle density). In the rest of this section, we examine this question carefully, establishing – we believe very convincingly – that, at least up to the slice at $a = 2^5$, this measured dispersion is a discreteness effect.

3.5 Numerical convergence

Let us first consider the stability of the results with respect to variation of the numerical parameters, i.e. those controlling the accuracy of the numerical integration of the $N$-body equations at given values of the discreteness parameters $D_\alpha$. In the GADGET2 $N$-body code, there are two sets of such parameters: a first set controlling the time-stepping and a second one the resolution in the calculation of the force. In Appendix A, we give the full details of two sets of parameter choices for which we now compare results: a ‘low-resolution’ (LR) simulation, corresponding to the values used in obtaining the results given above and subsequently in the paper, and a ‘HR’ simulation. As we discuss in further details in Appendix A, the LR are typical choices for large cosmological simulations in the literature (e.g. those of the VIRGO consortium, as described in Jenkins et al. 1998), while our HR values are even more stringent choices than...
Figure 8. Normalized differences of the PS for the BCC and SC preIC configuration, for HR simulations (thick lines) and LR simulations (thin lines) at $a = 2^3$, $a = 2^5$ and $a = 2^7$.

Figure 9. Normalized differences of the PS of HR and LR runs, at $a = 2^3$, $a = 2^5$ and $a = 2^7$. In each panel, the thick lines correspond to the BCC preIC configuration and the thin one to the SC one.

This means simply that the numerical errors associated with these changes in parameters are correlated strongly with the full PS, which is very close to the same in the two cases, and so cancel out when we take the difference. This suggests that, generally, it may be easier to place this kind of lower bound on discreteness effects than to attain a comparable level of numerical convergence on other quantities (such as the full PS).

3.6 Comparison with PLT

The PLT formalism for the evolution of the displacements off the lattice, developed explicitly in Joyce et al. (2005) and Marcos et al. (2006) for the SC lattice, has been generalized in Marcos (2008) to both BCC and FCC lattices. We exploit these analytical results here, for the case of the SC and BCC lattice, as a control on the accuracy of our numerical simulations at sufficiently early times when PLT...
is a valid approximation. Conversely, this comparison can be seen –
given the results just shown above on the numerical convergence of
our results – as a check on the range of applicability of PLT. We
will see that this range turns out to be considerably greater than
that which was established in the studies in Marcos et al. (2006),
making PLT a very useful tool for calibrating numerical results.

To compare our numerical results with PLT we simply generate,
for each set of BCC and SC initial conditions, the configurations
given by PLT evolution of equation (8), where the eigenvalues and
eigenvectors are those for the corresponding lattice. The details of
these latter calculations may be found in Marcos (2008).

In Fig. 10 are shown, for the GADGET2 simulations and the PLT-
evolved configurations, the normalized differences between the PS
for the BCC and SC, i.e.

$$\frac{P_{\text{bcc}}(k, a) - P_{\text{al}}(k, a)}{\frac{1}{2} \left[ P_{\text{bcc}}(k, a) + P_{\text{al}}(k, a) \right]},$$  \hspace{1cm} (22)

where the subscript indicates the preIC. We also show for com-
parison in Fig. 11 the same quantities, except that the PLT-evolved
configurations are replaced by those evolved with its fluid limit
(which we will denote by FLT, for ‘fluid LT’). For initial condi-
tions set up, as done here, with the Zeldovich evolution, this is
simply the extrapolated evolution in this same approximation.

The agreement with PLT at $a = 2^3$ is extremely good for all the
measured $k$, while at $a = 2^5$ it is restricted only to the very longest
wavelength modes in the box. FLT, on the other hand, traces the
observed differences well until $a = 2^3$, but only the $k$ larger than $k_N$.

These different ranges of agreement for PLT and FLT are simple
to understand, using the results quoted above in equations (15–
17). These formulae relate, at sufficiently early times and small $k$,
the theoretical PS of density fluctuations $P_{\text{al}}(k)$ to the full PS of
density fluctuations in the generated point distributions. FLT gives
a linear amplification of the displacement fields, independent of $k$,
and therefore a linear amplification of the terms $P_{\text{al}}(k)$ and $P_{\text{al}}(k)$. Outside the range of $k$ where $P_{\text{al}}(k)$ contributes, i.e. inside the FBZ,
FLT thus simply describes a linear amplification of the full initial
PS, which leaves the normalized quantity in equation (22) strictly
invariant. Outside the FBZ, on the other hand, the term $P_{\text{al}}(k)$
becomes important. When this is the case, the full evolution is well
approximated by the FLT evolution because (see Joyce & Marcos
2007a) the evolving term, $P_{\text{al}}(k)$, is in fact dominated by initial
power at small $k$ for which the evolution is very well approximated
by FLT.

The regime in which PLT traces the differences very well, but
FLT does not, corresponds to the $k$ inside the FBZ which are, in
PLT, amplified linearly in slightly different ways on each lattice.
In this case, the physical discreteness effect arises thus from the
modification with respect to FLT of the dynamical evolution
of the same initial power. In the regime in which FLT gives a good
approximation, on the other hand, the corresponding discreteness
effects arise from the power associated with the slightly different
initial samplings on the different lattices of modes which evolve
approximately in the same way.

Let us further consider the range of validity of PLT in these plots.
The perturbative expansion underlying PLT as developed in Marcos
et al. (2006) and Marcos (2008) is strictly valid, as we have discussed
above, only when the relative separation of all particles is small
compared to their initial separation. In Marcos et al. (2006), it has
been shown that it gives a very good approximation to the evolution
of the PS (and significantly better than FLT) at least until the time
when a significant fraction of the particles have come close to
another particle for the first time (which corresponds approximately

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Discreteness error in N-body simulations

Figure 11. Normalized variance of the PS of the BCC and SC PI, computed from FG simulations (continuous lines) and from simulations using PLT (dashed lines) for, from top to bottom and left- to right-hand side, $a = 2^3$, $a = 2^5$, $a = 2^7$ and $a = 2^7$. All the curves are normalized with the PS obtained with FG.

Figure 12. Normalized difference between the PS computed with FG and PLT for the BCC (thick lines) and SC (thin lines) configurations.

Figure 13. Real deviation normalized by the estimated deviation computed using equation (24).

Range in which PLT correctly describes the differences between the SC and BCC simulations extends in fact to when the plotted quantity is of the order of 2, i.e. into a regime in which PLT no longer follows well the full power in each PS accurately. This is evidently possible only if the deviation from the PLT-evolved initial conditions is essentially the same for both preIC, i.e. this additional non-linear power itself has smaller discreteness corrections than those given by PLT. We note that this is very coherent with our observations above concerning the numerical integration: we observed in that case much better numerical convergence of the measured differences than in each of the PS individually. Thus these numerical residuals are strongly correlated with the non-linear power which is the same in both simulations, and so cancel out when we take the difference.
We will discuss briefly in our conclusions these observations about the regime of validity of PLT.

It is instructive also to examine, in the range in which PLT traces accurately the differences in the evolution, what the relation is between this measured difference, and the true discreteness error, which can also be calculated in PLT. Indeed, in the FBZ, it is simply the difference between the PLT- and FLT-evolved power. A simple qualitative measure plotted in Fig. 13 is thus

\[
\text{Dev}(k, a) = \left[ \frac{(P_{\text{bcc}}(k) - P_{\text{PLT}}(k))^2 + \left( P_{\text{pl}(k)} - P_{\text{sc}}(k) \right)^2}{(P_{\text{bcc}}(k) - P_{\text{pl}(k)})^2} \right]^{1/2},
\]

where the \(a\)-dependence on the right-hand side is left implicit. Limiting ourselves to the modes for which PLT furnishes a good approximation to the full evolution of the individual PS, i.e. to the regime in which the quantity plotted in Fig. 12 is less than or of the order of 1, we see that Dev \((k, a)\) shows a clear tendency to increase with \(a\), particularly for smaller \(k\). Indeed, at \(a = 2^3\), for the very smallest \(k\) for which PLT is still approximately valid, our lower bound on the discreteness error is one order of magnitude smaller than the real discreteness error. The reason is simply that the difference in the exponents characterizing, in PLT, the growth of the displacement fields in these two different lattices at these values of \(k\) is considerably smaller than the difference between these exponents and the FLT behaviour (giving growth in proportion to \(a^6\)). Even if, taking this factor into account, we arrive at a real discreteness error of the order of 1 per cent, this result shows that, for all our results here, we should bear in mind that the measured differences provide only lower bounds on the discreteness error which may be very different from the full discreteness error.

33 As described in Section 3.1, the number of particles in the non-SC configurations is chosen as close as possible to these numbers (Table 1).

34 More precisely, as described in Section 3.1, we sample exactly the modes in the FBZ of the SC lattice.

3.7 Variation of particle number \(N\)

A further direct numerical check on our interpretation of the differences we have identified as discreteness errors may be given by looking at their dependence on particle number \(N\) (i.e. effectively, given that we work at a fixed box size, on the particle density parametrized by \(\ell\)). We thus consider varying \(N\) while keeping all other discreteness parameters fixed (and, again, checking also the stability of results considered to the variation of numerical parameters). Shown in Fig. 14 are the results for the normalized variance \(\sigma_n(k)\) (as defined in equation 20) on a set of four simulations of identical initial conditions (i.e. identical modes of the displacement fields on the four \(\text{preIC}\) for \(N = 32^3\) and \(64^3\) particles). Note that, to have identical displacement fields in the two cases, we have cut the initial PS at the Nyquist frequency of the \(N = 64^3\) distribution.

We clearly see the explicit \(N\) (and \(\ell\)) dependence of the results in all but the very strongly non-linear regime. In the PLT regime, the difference in power depends parametrically on \(N\) as \(N^{-2/3}\) (see equation 26). Interestingly, one can observe between \(a = 2^3\) and \(a = 2^7\) an apparent ‘spreading’ of this explicit dependence to larger \(k\), a behaviour which is naturally interpreted as the transfer of the discreteness effects accumulated at \(a = 2^3\) in the linear regime to larger \(k\) modes as the corresponding scales go non-linear. On the other hand, we see no clear evidence for a dependence on \(N\) at the strongly non-linear scales – and most notably over the entire range at the final time, \(a = 2^7\) – and so we will not assume...
Here we would like to discuss the implications for the two-body potential. The differences even at $a = 2^3$ may quite consistently be, and indeed are, naturally, ascribed to those at the previous time, $a = 2^3$, without the latter having to show the same explicit dependence on $\ell$. Indeed, in the strongly non-linear regime we do not expect a simple dependence of the final power on the amplitude of the power in the preceding weakly non-linear phase, and therefore the dependence on $\ell$ inherited from this phase could quite possibly be much weaker than that observed in the preceding phase.

### 3.8 Variation of $\varepsilon$

Another check on our results is given by considering the effect of varying $\varepsilon$, keeping all the other discreteness parameters fixed. In Fig. 15, we again show the normalized variance $\sigma_\Pi(k)$, now again for four different simulations with $N = 64^3$, for three different values of $\varepsilon$: the same one as used in the results reported until now ($\varepsilon = \ell/15$), and now also for simulations (from exactly the same initial conditions) with $\varepsilon = \ell$ and $\varepsilon = 2\ell$. We show only the range of $k$ below the Nyquist frequency as this is the regime of physical interest, i.e. in which results are expected to converge to those for (unsmoothed) gravity, fixed approximately by the mode inverse to the largest value of $\varepsilon$. (We do not show results for smaller $\varepsilon$ as they are negligibly different in this range from those at $\varepsilon = \ell/15$.) The behaviour observed at $a = 2^3$ is completely consistent with what is expected given that we have seen that PLT provides an excellent description of these differences at this time: the exponents

![Figure 15. Normalized variance of the PS for $\varepsilon = 1/15$, $\varepsilon = 1$ and $\varepsilon = 2$ at, from top to bottom, $a = 1$, $a = 2^3$ and $a = 2^7$.](image_url)

for growth of the modes of the displacement field calculated in PLT (which may be calculated for any two-body potential) only begin to change significantly when $\varepsilon \sim \ell$, simply because PLT is an expansion about the particles placed at their lattice sites. As $\varepsilon$ increases the deviation from the fluid evolution becomes in fact more and more significant (see Joyce & Marcos 2007a), but this deviation does not manifest itself as a difference between evolution on the different lattices as the smallest scales on which they differ are then smoothed over. Thus, the differences we measure decrease (in the FBZ, where they are due to the difference in the exponents relative to their FLT values). At $a = 2^7$, we essentially see the same behaviour for the modes for which PLT was valid, while for the larger modes there is also some more marked decrease already for $\varepsilon = \ell$. At $a = 2^7$, we see a larger spread, with an apparent tendency for the largest $\varepsilon$ to lead to the smallest differences, which would certainly be consistent with the hypothesis that these errors could also be interpreted as due to discreteness. It is important to note that, in all these figures, the reduction of the differences measured as $\varepsilon$ is increased does not imply a convergence of the simulations towards the physical (VP) limit, but at the most towards a smoothed version of it, which may be further from the physical limit than the results obtained with the smallest $\ell$. Indeed, in the PLT regime we have shown in Joyce & Marcos (2007a) that increasing $\varepsilon$ at fixed $\ell$ does indeed increase the deviation of the growth exponents of modes from their fluid value.

### 3.9 Variation of initial redshift

The initial redshift $z_i$ is the remaining parameter in the list of discreteness parameters $\mathcal{D}$, we gave in our discussion in Section 2. As the dependence of varying it while keeping the other parameters fixed can be understood analytically using PLT, in the regime
in which we know it to be valid (of small relative displacements), here we do not report numerical results.\textsuperscript{36} Quite simply we note that, in the EdS cosmology, the evolution of the PS in PLT can be written (Marcos et al. 2006) to a very good approximation as
\[
P(P, a) = a^2 v^2 \ell^2 \epsilon^2 P(P, a = 1),
\]
where \(\delta_i(\hat{k})\) is a function of the orientation of the vector which depends on the \textit{preIC}. It follows that the normalized difference in the power, averaged in a bin of wavenumbers centred at \(\hat{k}\), scales approximately as
\[
\sim \left[\delta_{\epsilon}(\hat{k}) - \delta_{\epsilon}(\hat{k})\right] k^2 \ell^2 \log a,
\]
where \(\delta_i(\hat{k})\) are appropriate effective values of the parameter \(\delta_i(\hat{k})\) over the bins of wavenumbers. The differences we have measured thus increase without limit as \(\zeta\) does, with a logarithmic dependence on the latter.

4 DISCUSSION AND CONCLUSIONS

We now summarize our main findings and conclusions, as well as indicating some directions for further study to clarify these issues.

(i) Cosmological simulations should evidently be tested for discreteness effects by an appropriate, and well-controlled, extrapolation of the relevant parameters. To recover the continuum VP limit, we have noted that the simplest such extrapolation is to increase the particle density (i.e. \(\ell \rightarrow 0\)) keeping the other relevant parameters introduced by the discreteness fixed -- specifically the force smoothing \(\epsilon\), initial redshift \(\zeta\) and \textit{preIC}. While this may seem rather evident, this kind of procedure is not systematically applied in the literature, apart from the few isolated studies we have mentioned (notably those of Melott and collaborators). More specifically, many of the (relatively few) convergence studies in the literature adopt a different approach, typically decreasing \(\epsilon\) in proportion to \(\ell\), keeping always \(\epsilon \ll \ell\). While such an extrapolation is not necessarily wrong, i.e. it may allow one to arrive at conclusions which are correct concerning discreteness effects, it has the intrinsic problem that it does not converge to the VP limit. Physically, this means that such an extrapolation \textit{does not remove the non-VP effects} in the dynamics (e.g. two-body collisionality, or the effects described by PLT) but simply moves them to smaller scales. Given that the interplay of different scales in the fully non-linear regime of gravity is not understood, this is not a solid procedure. In this respect, we also note that in this approach, additional power in the initial conditions -- corresponding to the extra modes which may be sampled as \(\ell\) is decreased -- is usually added. This means that structures do indeed form first at the smallest scales, where discreteness is manifestly important. Further such modification of the initial conditions makes it difficult to identify with precision, as in the present study, variations which are due to discreteness. We note, however, that using wavelet techniques, Romeo et al. (2008a) have recently claimed to numerically detect discreteness effects embedded in the scatter of a set of cosmological simulations using different realizations of the initial conditions (and extrapolated power).

(ii) There has been some controversy in the literature about the widely used practice of taking results to be physical (i.e. representative of the VP limit) at scales below \(\ell\), in simulations with \(\epsilon < \ell\). We have addressed this issue with a controlled numerical study of such a simulation (with \(\epsilon = \ell/15\)). Our conclusion is that such a procedure appears to be reasonable, to a \textit{first approximation}: efficient transfer of power from large to small scales does indeed tend to make the results on scales below \(\ell\) converge, ‘wiping out’ the significant differences on these scales in the initial conditions (see e.g. Little et al. 1991; Bagla & Prasad 2009). However, this mechanism is by no means perfect and we have demonstrated with our study beyond doubt that there are indeed \textit{measurable} residual effects of discreteness \textit{at all scales}, at a level relevant to the precision (of the order of 1 per cent) now set as a target for such simulations. Considering, very conservatively, only our results up to \(a = 2^5\) in Fig. 7 as indicative of what one would find in a typical cosmological simulation (i.e. starting at an initial redshift \(\zeta = 32\)), one infers a lower bound on discreteness effects which reach about 1 per cent at the Nyquist frequency. We emphasize that these measures are only \textit{lower bounds}, which may be very much below the full discreteness error. Indeed, we have seen that in the regime (of validity of PLT) in which we can calculate this full error, the lower bound is (at small \(\ell\), at \(a = 2^5\)) one order of magnitude larger than the estimated error (i.e. about 1 per cent rather than the measured lower bound of a tenth of a per cent at these scales). Most importantly, the only way to attain greater precision, and indeed the \textit{only way to firmly establish the convergence to the physical limit}, is to extrapolate to \(\ell \ll \epsilon\). Thus, while the ‘common wisdom’ is probably reasonable for the modest precision required for many uses of the results of these simulations, the criticisms formulated by some groups (notably Melott and collaborators) are fundamentally correct and, further, relevant for the levels of precision required for some applications (e.g. future weak lensing observations). In this respect, we also note that we have analysed here solely two-point properties (essentially the PS), while Melott has emphasized that the numerically measured effects of discreteness are more important in other (phase-sensitive) quantities. The methods used here to establish ‘calibrated’ lower bounds on discreteness error can easily be generalized to study such quantities. Such a study, as well as more extended numerical studies of controlled extrapolations to the regime \(\ell \ll \epsilon\) like those of Splinter et al. (1998), using possibly also the methods of analysis employed in Romeo et al. (2008a), would provide further insight into these issues.

(iii) An important element in our numerical study is the use of the PLT formalism. It allows us to analytically fit the measured dispersion in results for the PS (or, in principle, any quantity) due to discreteness, at sufficiently early times. This not only allows us to ‘calibrate’ our numerical results, establishing that the method does really indeed measure discreteness effects (rather than other numerical or finite-size effects), but also gives us an understanding of the physical origin of these effects: a finite sampling of a fluctuation modifies its evolution with respect to the smooth limit. This is a physical effect of discreteness which has not been previously envisaged, and it very clearly illustrates that the widely made assumption that the effects of discreteness are solely those which arise from (i) missing initial power and (ii) two-body collisionality is indeed just an assumption, which can at best be approximately correct. Indeed, PLT explicitly describes the effect of small scales on larger scales which, albeit not the dominant one in the evolution of the gravitational clustering, is not zero when the ratio of these

\textsuperscript{36} See also Joyce & Marcos (2007a) for quantitative results. Some numerical results for the effect of varying \(\zeta\) are only given in McDonald et al. (2006), but only for very specific quantities (ratios of PS for different dark energy models).
scales is finite. Such effects at large scales (i.e. significantly larger than $\ell$) have until now escaped detection in cosmological N-body simulations, even in studies which looked for them.\textsuperscript{37} Further, we have noted that our results indicate that, apart from the very early non-linear evolution which 'fills in' the missing power at large $k$, the discreteness errors at any scale continue to grow monotonically in time, as in PLT, throughout the simulation. Such behaviour would naturally be explained if the physical effects of PLT continue to act in the non-linear regime, and indeed it is very plausible that this should be the case: one would expect that the evolution at any scale will be affected by the discreteness of the sampling, as in PLT, even if this sampling is not uniform in space as in PLT. We underline, however, that understanding of discreteness effects in the fully non-linear regime is completely lacking, and it is quite possible that other effects also come into play. For this reason alone, it is important that carefully controlled extrapolations are systematically undertaken.

(iv) We have also seen in our numerical study that PLT provides an excellent fit to the evolved power at a wavenumber $k$, until the time that this wavenumber goes non-linear, and indeed describes the differences between simulations on different preIC for even slightly longer. This extends its validity considerably beyond that established by the numerical study in Marcos et al. (2006), which showed that it extended only to the time when the typical relative displacement of nearest neighbour particles becomes of the order of the interparticle distance $\ell$. While this is what is expected from a naive analysis of the validity of PLT – requiring that the linearization in the relative displacements of the force be valid – it is not in fact surprising that its regime of validity extends to the non-linearity of any given mode: to obtain a good approximation to the evolution of the displacement fields at a given scale the breakdown of PLT in describing the force due to particles at smaller scales is not relevant.

The regime of validity observed is what results if one assumes that one needs the PLT linearization of the force on a particle to be valid only for particles at separations of order $k^{-1}$ or larger. The fact that PLT does even better in tracing the differences between evolution from identical initial conditions sampled on different preIC than in following the full evolution on an individual preIC indicates that the leading non-linear corrections have discreteness corrections which are smaller than those in PLT at linear order. A full study of the extension of PLT to next order (i.e. to second order in the Taylor expansion of the forces) should be able to explain this behaviour in detail. More generally, we underline that the success of PLT in analytically fitting the quantities we have measured shows that it can be a very useful instrument for controlling analytically the results of numerical simulations. Indeed, to our knowledge, the data in Fig. 10 are by far the most stringent analytic controls which have been placed on an N-body code, showing that GADGET can trace correctly, to a precision of as great as one in a thousand, differences in the PS from slightly different initial conditions. Thus, interestingly, the measurement of discreteness effects in simulations can be seen as a way of controlling the numerical accuracy of codes. Indeed, in cosmological N-body simulation, a reasonable goal for the numerical accuracy of any code is that it should measure such effects, as it is not of physical interest to do better than reach this level of systematic error.

(v) The numerical study presented was for the case of an initial power-law PS $P(k) \propto k^n$ with exponent $n = -2$. We have also fully analysed the cases $n = 0$ and 2, for which, starting from similar amplitudes of fluctuations at the scale $\ell$ with the same number of particles, the range of $a$ prior to that at which the box goes non-linear is much greater. We have qualitatively observed the same behaviours and, in particular, the monotonic growth of the measured lower bounds on discreteness as a function of $a$. The method can, of course, be used for any initial conditions, and in particular for the current standard $\Lambda$CDM model. The precise results for this case will depend, of course, in particular, on what physical scale is identified with $\ell$. The use of PLT as a 'calibrator' in this case would require its generalization to this cosmology, which, as noted in Joyce & Marcos (2007a), should be straightforward. We note that the recent study by Romeo et al. (2008a) of this case reaches very consistent conclusions with those found here (and those of Melott et al. over a decade ago): using a wavelet analysis of a set of simulations, a positive detection of discreteness errors is made for spatial scales smaller than the order of the interparticle spacing. It would be interesting to combine in future studies these methods of numerical analysis with the analytical and numerical methods used here.

(vi) We have considered only numerical simulations with fixed $\ell$ and $\epsilon$, and our conclusions are valid, of course, therefore only for this case (i.e. PM or $P^3M$ simulations). One possibility, discussed by Romeo et al. (2008a) in their conclusions, and briefly by Melott in a comment (Melott 2008, see also the reply of Romeo et al. 2008b) on this paper, is that the intrinsic limitations on accuracy imposed by discreteness might be addressed with numerical efficiency using AMR-type codes, with the mesh defining the resolution of the force (i.e. effectively $\epsilon$) being adapted in higher density regions so that the condition that the number of particles per cell is always significantly larger than unity. Therefore, the idea is, one would have always a local interparticle distance smaller than the effective force resolution scale, thus satisfying locally the condition apparently necessary to control discreteness effects ($\ell \ll \epsilon$) while allowing a greater spatial resolution, in denser regions, than that fixed by the interparticle distance $\ell$ of the initial grid. While such an approach would be expected to greatly reduce certain physical effects of discreteness – specifically any effects due to deviations from the mean field force acting on particles due to particles in their immediate neighbourhood (e.g. by two-body collisions) – our findings here lead us to be very cautious about this conclusion about AMR: we have emphasized that the discreteness effects which we have been able to understand physically and quantify here (using the PLT formalism) are dynamical effects induced at any scale by the coupling to smaller scales at which particle sampling noise becomes dominant. When the smoothing scale is changed, one does not undo these effects, but simply modifies them by modifying the evolution of the fluctuations at small scales. Indeed in PLT, as has been shown explicitly in Joyce & Marcos (2007a), increasing the force resolution scale $\epsilon$ at fixed $\ell$ does not make the evolution of the N-body system approximate better than the physical limit. Put simply, the only way to reduce these kinds of effects of discreteness at any given scale is to increase the particle density. Thus, we do not consider that it is clear, in general, that an AMR-type code can give a more accurate result (i.e. closer to the physical model) than a standard $P^3M$ code (with $\epsilon \ll \ell$) when both codes use the same particle number. On the other hand, we would expect that an AMR code may indeed do better for many quantities than a simple PM code (with an effective $\epsilon \geq \ell$) at the same particle density. In any case, as remarked by Melott (2008), careful tests of this or any alternative strategy to reduce discreteness effects should themselves, of course, be subjected to controlled tests for convergence.

\textsuperscript{37} See e.g. Little et al. (1991) and both the recent studies of Bagla & Prasad (2009) and Romeo et al. (2008a).
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APPENDIX A: DETAILS OF NUMERICAL INTEGRATIONS

Listed in Tables A1 and A2 are the parameter values in GADGET2 we have used in our ‘LR’ and ‘HR’ runs.

GADGET2 uses adaptive time-steps, which are chosen, for each particle, using the formula:

\[ \Delta t = \min \left( \Delta t_{\text{max}}, \left( \frac{2\eta}{|a|} \right)^{1/2} \right), \]  

(A1)

where \( \Delta t_{\text{max}} = \text{MaxSizeTimestep} \) is the maximum time-step and \( \eta = \text{ErrTolIntAccuracy} \) is the error tolerance of the force calculation. \( |a| \) is the acceleration of the particle in the previous time-step (\( \epsilon \) is the softening length). Our runs have chosen the parameter \( \text{MaxSizeTimestep} \) sufficiently large compared to \( \text{ErrTolIntAccuracy} \) so that in practice only the latter parameter is relevant. GADGET2 computes the gravitational force using a tree-mesh technique. At large scales, the force is computed with a PM algorithm on a grid with \( 128^3 \) cells. At small scales, the force is computed using a tree algorithm. A node is opened (i.e. the force between a particle and a node of the tree is computed using the monopole moment of the gravitational force) if

\[ Ml^2 > |a|r^4, \]  

(A2)

where \( M \) is the mass of the node of extension \( l \) at a distance \( r \) of the particle of which the force is computed, \( a \) is the total acceleration in the last time-step and \( \alpha = \text{ErrTolForceAcc} \). We set the option \( \text{TypeOfOpeningCriterion} = 1 \) and therefore the parameter \( \text{ErrTolTheta} \) is used only in the first force computation, and is therefore irrelevant.

Our LR simulations use the same range of parameters usually used in the literature. For example, for the VIRGO consortium.

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the parameter which controls the time accuracy taken as ErrToIn-
Accuracy = 0.01 and the one which controls the calculation of the for-
ce as ErrToForceAcc = 0.005 are considered the fiducial ones (Jen-
skins et al. 1998), and are the ones which are effectively used (e.g.
Stoehr et al. 2003; Stoehr 2006), for a softening length \( \varepsilon \) =
[0.002, 0.02]\( \varepsilon \). Other works (e.g. Crocce et al. 2006) divide
their runs like us in 'LR' and 'HR' ones. Their 'LR' runs have
similar resolution than our 'LR' ones (ErrToIn-
Accuracy = 0.025 and ErrToForceAcc = 0.005), but our 'HR'
ones take more stringent parameters (ErrToIn-
Accuracy = 0.01 and ErrToForceAcc = 0.002), for a value of the
softening length \( \varepsilon \) \in [0.02, 0.4]\( \varepsilon \).

| Table A1. Numerical parameters for our 'LR' runs. |
|-----------------------------------------------|
| Accuracy of time integration                  |
| ErrToInAccuracy                               | 0.025 |
| MaxRMSDisplacementFac                         | 0.2   |
| CourantFac                                    | 0.15  |
| MaxSizeTimestep                               | 0.025 |
| MinSizeTimestep                               | 0.0   |
| Tree algorithm and force accuracy             |
| ErrToTheta                                    | 0.7   |
| TypeOfOpeningCriterion                        | 1     |
| ErrToForceAcc                                 | 0.005 |
| TreeDomainUpdateFrequency                    | 0.1   |
| Softening length                              |
| SofteningHalo                                 | 0.000 372 023 809 523 81 |

| Table A2. Numerical parameters for our 'HR' runs. |
|-----------------------------------------------|
| Accuracy of time integration                  |
| ErrToInAccuracy                               | 0.001 |
| MaxRMSDisplacementFac                         | 0.2   |
| CourantFac                                    | 0.15  |
| MaxSizeTimestep                               | 0.025 |
| MinSizeTimestep                               | 0.0   |
| Tree algorithm and force accuracy             |
| ErrToTheta                                    | 0.7   |
| TypeOfOpeningCriterion                        | 1     |
| ErrToForceAcc                                 | 0.0001|
| TreeDomainUpdateFrequency                    | 0.1   |
| Softening length                              |
| SofteningHalo                                 | 0.000 372 023 809 523 81 |

APPENDIX B: DEFINITION AND ESTIMATION OF TWO-POINT STATISTICS

B1 Real space

The reduced two-point correlation function \( \xi(r) \) is defined (see e.g. Gabrieli et al. 2004) as
\[
\xi(r) = \langle \delta(r + x) \delta(x) \rangle, \tag{B1}
\]
where \( \langle ... \rangle \) means ensemble average over all the possible realizations of the system. For particle distributions, \( \xi(r) \) has a singularity at \( r = 0 \), and it is therefore convenient to divide it as
\[
\xi(r) = \frac{1}{n_0} \delta_p(r) + \xi(r), \tag{B2}
\]
where \( n_0 \) is the mean number density. The quantity we give results for in the paper, and denote by \( \xi(r) \), is a direct real space angle-
averaged estimator of \( \xi(r) \):
\[
\xi(r) + 1 = \frac{1}{n_0 V(r, \delta r) N_c} \sum_{i=1}^{N_c} N_i(r), \tag{B3}
\]
where \( N_i(r) \) is the number of particles in the spherical shell of radii \( r, r + \delta r \), volume \( V(r, \delta r) \), centred on the \( i \) th particle of a subset of \( N_c \leq N \) particles randomly chosen from the \( N \) particles of the system.

B2 Reciprocal space

Because we consider distributions with periodic boundary conditions, we can write the density contrast as a Fourier series:
\[
\delta(x) = \frac{1}{V} \sum_k \exp(i k \cdot x) \tilde{\delta}(k) \tag{B4}
\]
with \( k \in \{(2\pi/L)n | n \in \mathbb{Z}^3\} \). The coefficients \( \tilde{\delta}(k) \) are given by
\[
\tilde{\delta}(k) = \int_V \delta(x) \exp(-i k \cdot x) \, dx. \tag{B5}
\]
The PS is defined as
\[
P(k) = \frac{1}{V} |\tilde{\delta}(k)|^2, \tag{B6}
\]
which we estimate with
\[
P(k) = \frac{1}{N(k)} \sum_{k' \leq k + \delta k} |\tilde{\delta}(k')|^2, \tag{B7}
\]
where \( N(k) \) is the number of vectors \( k' \) considered in the sum. To speed up the computation, we perform a sampling at larger \( k \) on the vectors \( k' \). We have checked that our results are robust to this choice.

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