On the problem of initial conditions in cosmological N-body simulations

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Abstract. – Cosmological N-body simulations aim to calculate the non-linear gravitational growth of structures via particle dynamics. A crucial problem concerns the setting-up of the initial particle distribution, as standard theories of galaxy formation predict the properties of the initial continuous density field with small amplitude correlated Gaussian fluctuations. The discretisation of such a field is a complex issue and particle fluctuations are especially relevant at small scales where non-linear dynamics firstly takes place. In general, most of the procedures which may discretise a continuous field, gives rise to Poisson noise, which would then dominate the non-linear small-scales dynamics due to nearest-neighbours interactions. In order to avoid such a noise, and to consider the dynamics as due only to large scale (smooth) fluctuations, an ad-hoc method (lattice or glassy system plus correlated displacements) has been introduced and used in cosmological simulations. We show that such a method gives rise to a particle distribution which does not have any of the correlation properties of the theoretical continuous density field. This is because discreteness effects, different from Poisson noise but nevertheless very important, determine particle fluctuations at any scale, making it completely different from the original continuous field. We conclude that discreteness effects play a central role in the non-linear evolution of N-body simulations.

The purpose of cosmological N-body simulations is to calculate the non-linear growth of structures in the universe by following individual particles trajectories under the action of their mutual gravity [1, 2, 3]. These particles are not galaxies but are meant to represent some sorts of collisionless clouds of elementary dark matter particles. In order to make them move, one must calculate the force acting on each of them due to all the others. In general one may find several algorithms which speed up the \( N^2 \) sum necessary to compute the force on each particle. In this paper we study simulations from the Virgo project [3] which are done

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with an “adaptative P3M” scheme [4, 5]. This scheme is a combination of a PM (i.e. meshed based scheme) and a PP (i.e. particle-particle based scheme). Briefly, this consists of assigning the particle mass on a mesh so as to obtain a density field on the mesh itself. One can then calculate the gravitational potential on that mesh by solving the Poisson equation, and finally the potential at the location of a particle is determined by an interpolation of the values on the mesh. For a better resolution, a true calculation of the force due to nearby particles is done. In highly clustered regions, since this last calculation can be quite long, additional higher resolution meshes are placed. The force used is not a pure $r^{-2}$ one: instead one smooths it at small $r$ by choosing for instance a force proportional to $(r^2 + \epsilon^2)^{-\frac{1}{2}}$ in order to avoid “collisions” between close particles. This brings us to an important hypothesis sometimes made in cosmological N-body simulations: with a softened force and a proper choice of the softening parameter $\epsilon$, the evolution of the N-bodies should be the same as the evolution of a continuous density field (made of a huge number of particles behaving like a fluid) under its own gravity. With this in mind, one interprets collisions, or more correctly strong scattering, between nearby particles in the simulation as due to the discretisation of the density field and therefore artificial [4, 5]. However, it is important to note that, in order to satisfy the above hypothesis, $\epsilon$ should be at least as large as the mean inter-particle distance $\langle \Lambda \rangle$ [6, 7]; this is not always the case as for instance in the Virgo project where $\epsilon = 0.036 Mpc/h$ [3] and $\langle \Lambda \rangle \approx 0.5 Mpc/h$ (see below).

The philosophy behind cosmological N-body simulations is to reproduce galaxy structures that we see today through redshift surveys by choosing some good parameters (cosmological and numerical) for the evolution of the system and especially fine-tuned initial conditions (properly normalised to the primordial fluctuations) given by some theories. This last point is important because one is not interested in some general asymptotic behaviors or quasi stationary states independent of the initial conditions, but in the state of the system after a relatively short time compared with the dynamical time of the simulation.

Initial conditions (hereafter IC) are created from theories typically based on inflation and the subsequent evolution of matter, which are able to predict the properties of a continuous density field with correlated fluctuations [8]. Such a density field is usually Gaussian, and hence all the statistical properties are contained in the two-point correlation function (hereafter CF) or its Fourier transform, the power spectrum (hereafter PS). These two functions depend on the kind of dark matter which is the relevant one on large scales: hot (relativistic), cold (non-relativistic) or warm (a mixture of the two). However the main point for what concerns us is that a continuous and smooth density field with correlated density fluctuations is given as IC. If one wants to study the time evolution of this field with N-body simulations based on particle dynamics, it is then necessary to discretise the field. This means that one has to create a particle distribution which is representative of the continuous density field and to control any finite size effect. Note that a crucial point with respect to structures formation, is that non-linearities firstly develop at small scales where discreteness effects are important. Firstly, we briefly explain the standard way of carrying out the discretisation and then we analyse some of the real space statistical properties of these distributions, restricting ourself to a Virgo Standard Cold Dark Matter (hereafter CDM) simulation with $256^3$ particles [3].

The questions we address are: In which range of scales the initial particle distribution used in the standard cosmological simulations is representative of CDM-like density fluctuations? What drives the non-linear dynamics of structures formation: the discreteness effects due to the short NN interaction or the large scale (continuous) distribution of density fluctuations?

The standard ad-hoc procedure for setting up IC is described in [1, 2, 9, 3]. For galaxy structures formation problems, the IC generation splits into two parts. The first is to set up a “uniform” distribution of particles, which can represent the unperturbed universe. The
second is to impose density fluctuations with the desired characteristics. In this context, one faces the general problem of how to discretise a continuous density field. There are different procedures (e.g. random sampling, threshold sampling, etc.) which can be chosen and they result in different point distributions. Clearly one should have some physical reasons to choose one or another since any procedure introduces some discreteness effects, like Poisson noise, which could then play the main role in the non-linear dynamics of the system. For instance, in a Poisson distribution the dominant part of the gravitational force acting on an average particle is due to its NN \([10, 11, 12]\). If a simulation is run from such IC the fluctuations grow rapidly into non-linear objects at small scales. This happens because a Poisson distribution is \textit{statistically isotropic} only on scales larger than the average distance between NN \([14, 11]\) and the three-point correlation function is non-zero at these small scales: such a situation avoids the perfect cancelation of the net gravitational force due to close particles. Instead, in cosmological N-body simulations, one would like to simulate a system where the main contribution for non-linear structures formation problem, is due to the large scale distribution of the other particles and \textit{not to local NN interactions} \([2]\).

To overcome the fact that a Poisson distribution is only “statistically” isotropic the most widely used solution to this problem has been to represent the \textit{unperturbed universe} by a \textit{regular cubic grid of particles} \([1, 2, 9]\). An infinite lattice, or a lattice with periodic boundary conditions, is “gravitationally stable” because of symmetry reasons. However a lattice is a distribution with fluctuations at all scales and non-trivial correlations. One can show that the unconditional variance in spheres decays as \(\sigma^2(r) \equiv \langle \Delta N(r)^2 \rangle/(\langle N(r) \rangle^2) \sim r^{-4}\) (where \(\langle N(r) \rangle \sim r^3\) is the average number of points in a \textit{randomly chosen} sphere of radius \(r\) \([13]\)) and this is due to the fact that a lattice is a strongly ordered and correlated system at all scales. The two-point CF is such that \(\xi(\vec{r}_1, \vec{r}_2) = \xi(|\vec{r}_1 - \vec{r}_2|) \neq \xi(|\vec{r}_1 - |\vec{r}_2|)|\) because it is not invariant for space rotation \([14]\): A lattice breaks space isotropy. Moreover, the grid-like system has the disadvantage to introduce a strong characteristic length on small scales - the grid spacing - and it leads to strongly preferred directions on all scales.

For the latter reasons, a second way to generate an “uniform background” is by means of the following procedure. One starts from a Poisson distribution and then the N-body integrator is used with a \textit{repulsive} gravitational force in such a way that, after the simulation is evolved for a sufficiently long time, the particles settle down to a \textit{glass-like configuration} in which the force on each particle is very close to zero, i.e. a global stable configuration is found which has no preferred directions \([2]\). The resulting distribution is very isotropic but it is still characterized by long-range order of the same kind of a lattice. As for the lattice the main characteristic of such a distribution is the presence of an \textit{excluded volume}: two particles cannot lie at a distance smaller than a certain fixed length scale \([14]\). In the lattice this scale is the grid space, for a glass such a distance depends on the number of points one has distributed in a given volume. The fact that a lattice is ordered is due to the existence of the deterministic small scale distance. The unconditional variance scales as \(\sigma^2(r) \sim r^{-\alpha}\) where \(3 < \alpha \leq 4\), and it is again a strongly correlated system \([14]\). Its two-point CF depends on the detailed procedures used to generate the glass distribution. However it is possible to show that this class of distribution has \(P(k) \sim k^\alpha\) (with \(a > 0\)) for \(k \rightarrow 0\) and hence \(P(0) = 0\) like the Harrison-Zeldovich PS \([14]\).

Given a “suitably unperturbed” particle distribution, any desired \textit{linear} fluctuation distribution can be in principle generated using \textit{Zeldovich approximation} \([1]\). Basically, one assumes that the initial background is uniform with average density \(\rho(\vec{r}) = \rho_0\), without fluctuations, and then one applies a displacements field \(\vec{u}(\vec{r})\). Because of the conservation of total mass
after the displacements, one can apply a continuity equation which gives

$$\rho(\vec{r}) - \rho_0 + \nabla \cdot \left( \rho_0 \vec{u}(\vec{r}) \right) = 0 . \tag{1}$$

If statistical homogeneity and isotropy of the displacements field $\vec{u}(\vec{r})$ is assumed, then on going to Fourier space and considering the expectation value of the square modulus of the density fluctuations (the PS), Eq.\ref{eq:cont} leads to $P(k) = \langle \delta_0^2 \rangle = k^2 \langle |\vec{u}(\vec{k})|^2 \rangle = k^2 P_u(k)$. As any PS cannot diverge faster than $k^{-3}$ for $k \to 0$, we have that $\lim_{k \to 0} P(k) \sim k^n$ with $n > -1$. This means that, for instance, one cannot create a density fluctuation field with $P(k)$ which diverges as $k^n$ and $n \leq -1$, or with CF which goes as $r^{-\alpha}$ for $r \to \infty$ and $\alpha \leq 2$ only by applying a displacement field to a uniform background. Moreover one does not start from a continuous field with no fluctuations, but with a particle distribution, which has its own fluctuations and correlations (which in the lattice’s and glass’s cases are long-range). In such a situation one has to ensure that the correlations among density fluctuations implemented by the displacements field are larger than the intrinsic fluctuations of the original particle distribution, and that the large-scale fluctuations dominate the non-linear small scales clustering instead of nearest-particle interactions. Only if one considers very large scales, and/or a displacements field which introduces correlations which are larger than the intrinsic one of the original distribution, one can recover the PS as in Eq.\ref{eq:cont}. Otherwise in a certain range of small enough scales, the point distribution is dominated by discreteness effects, which in this context can be seen as finite-size effects and which are important for what concerns the small-scale non-linear structures formation.

In order to clarify this question, we have checked numerically the kind of correlations introduced in the system with the Zeldovich approximation: We have analysed a CDM simulation with $\Omega_0 = 1$ as an example, but our result are generally valid for any other particular model chosen, as they involve the same method for setting-up initial conditions. Note that we have analysed the statistical quantities for the entire simulation ($N = 256^3$ particles) and not for a sub-sample of it, in order to avoid introducing any kind of sampling noise and we have used periodic boundary conditions. The pre-initial particle distribution (which would represent the “uniform background” as previously discussed) consists of replicas of a $N = 10^6$ particles glass distribution generated by the procedure discussed above. As they are generated with periodic boundary conditions they can be tiled to make larger distributions. After the Zeldovich displacements one obtains the IC which correspond to a redshift $z = 50$. (In general the particles are very little displaced with respect to their initial positions: that is the average distance between NN remains unperturbed.)

It is worth noticing that in general the correlation properties of the initial particle distribution of N-body simulations have been discussed through the analysis of the PS of the density fluctuations. The PS is the Fourier transform of the real space CF $\xi(r)$ and hence it contains the same information, clearly if finite size effects and statistical noise have been properly taken into account. For the comparison with theoretical CDM models, which usually give the PS of density fluctuations $\xi(k)$, we have computed the real space properties:

$$\xi(r) = \frac{1}{2\pi} \int_0^{\infty} P(k) \sin(kr) k^2 dk$$

and

$$\sigma^2(R) = \frac{1}{2\pi} \int_0^{\infty} W(k,R)^2 P(k) d^3k$$

where $W(k,R)$ is the Fourier transform of the sample’s window function (a real space sphere in our case - which is defined to be zero outside the sample and one inside, and its integral over all space is one). In the simulation, the CF is computed by direct pair counting (we have used the estimator introduced by \ref{eq:cont}), and $\sigma^2(r)$ by distributing $N_s$ spheres of varying radius with random centers and computing the number fluctuation. For the latter we have used $N_s = 2 \cdot 10^4$
spheres randomly distributed in the simulation volume and we define our estimator as

\[ \sigma^2_E(r) = \frac{1}{\langle N(r) \rangle^2} \sum_{i=1}^{N_s} \frac{(N_i(r) - \langle N(r) \rangle)^2}{N_s - 1} \]  

(2)

where \( N_i(r) \) is the number of points contained in the \( i \)th sphere of radius \( r \) and \( \langle N(r) \rangle \) is its average. One may see in Fig.1 that for a CDM model, the \( \sigma^2(r) \) is constant up to a scale \( r_c \approx 0.06 \) (normalized to the simulation box \( L = 239.5 \text{Mpc}/h \)), which is fixed by the turn-over scale of the PS \([13]\), and then it decays as \( r^{-4} \). (The normalization has been performed by requiring that \( \sigma(r = 8\text{Mpc}/h) = 0.51 \) as in \([3]\): we note however that a different normalization does not change our main results which concerns the functional behaviour of the real space properties with scale.) For the glass \( \sigma^2(r) \sim r^{-4} \) at any scale, as expected, while for the IC \( \sigma^2(r) \) decays as \( r^{-4} \) up to \( \langle \Lambda \rangle \) and then it decays slower as \( r^{-1.6} \). This change of slope is the effect of the displacements field. In Fig.2 we show the results for the two-point CF. For the CDM model used here \([8]\) \( \xi(r) \sim \text{const.} \) up to \( r_c \) and then after crossing zero, it goes as \( \xi(r) \sim -r^{-4} \) \([4]\). We find instead that \( \xi(r) \) for the IC and the glass are rather similar at small scales and they oscillate around zero; the peaks due to the first, second and third NN are clearly visible. Note that the average distance between NN is \( \langle \Lambda \rangle = 0.003 \) (in normalized units) for both the glass-like distribution and the IC and it corresponds to the first peak of the conditional average density \( \sim \langle n \rangle(1 + \xi(r)) \) (see Insert Panel of Fig.2). At large scales there is a slight difference between the two, which changes the behaviour of \( \sigma^2(r) \). However in any range of scales there is no agreement between the \( \xi(r) \) and \( \sigma^2(r) \) of CDM and IC. This is especially relevant for the nature of fluctuations in IC and CDM: for the latter one should see an over-density up to a scale \( r_c \) followed by a peculiar under-density (with \( \xi(r) \sim -r^{-4} \)) while for the first we find that they are a sequence of over-densities and under-densities which results in an oscillating \( \xi(r) \).

Let us now discuss the second point of this paper. A lattice or a glass are gravitationally unstable with respect to small perturbations of their configuration. For this reason an interesting question concerns what drives the non-linear dynamics in these simulations. Once the Zeldovich displacements have been implemented, the new configuration does not have the perfect symmetry of the pre-initial distribution. Hence the question concerns: are discreteness effects dominant for the small-scales non-linear dynamics with respect to the force due to large scales smooth fluctuations? In order to study this point, we have computed (see Fig.3) the behaviour of the mean gravitational force on a particle due to all the particles contained in the sphere of radius \( r \) around, as a function of \( r \). Firstly, we note that the force increases of a factor 10 approximately between the glass and the IC. In the case of the latter, one can see that the force due to the first shell is almost compensated by the second one and starts to grow at least until the sphere reaches the size of the box. Furthermore the force due to the first shells is one third of the force at large distance and fluctuations are of the same order than the average. One can therefore say that the contribution from the NN is not as important as in the Poisson case because the force doesn’t reach its asymptotic value at scales \( \sim 2\langle \Lambda \rangle \) \([11]\). The average force increases with scale up to the box’s size; however the fluctuations at all scales are large enough to conclude that small-scales discreteness effects are not negligible with respect to the large scale contribution.

This last analysis would be totally useless without taking into account the initial velocity of the particles. Indeed if the particles were too fast they would not be trapped by nearby particles and discreteness would only make particles trajectories less regular. However, we expect the particles to be slow since we study CDM. In order to make this more quantitative, we did the following test: calculate the force on a particle due to particles in a sphere around, calculate the velocity of the particle in a direction perpendicular to the force and finally compare the
time needed to travel a certain distance with this velocity but without any force ($t_v$) and the time to travel the same distance with the force but without any initial velocity ($t_f$). Our result is that the velocities are indeed small. For instance if we take $\langle \Lambda \rangle /10$ for the distance to travel, one has that $t_v$ goes from $\sim 3 t_f$ to $\sim 10 t_f$ when the radius of the sphere for the force goes from 0.004 to 0.4. This shows that structures should be able to form even at the smallest scales $r \sim \langle \Lambda \rangle$ in the simulation. Indeed, at a distance $\langle \Lambda \rangle /10$ from its initial position, the force from its NN could be already driving a particle, instead of its initial velocity. Discreteness effects are therefore important for what concerns the non-linear growth of structures at small scales and this is the relevant range of scales where one wants to study strongly or weakly ($\xi(r) \gtrsim 0.1$) non-linear regimes [3]. (see [16] for a more complete discussion of this point and of the whole time evolution of the simulations).

Let us briefly summarize the discussion. The idea of the standard procedure to set-up IC in cosmological N-body simulations, is that one starts with a “uniform distribution” which, once discretised, can be a lattice or a glassy system. Then one gives correlated displacements to the particles in such a way that one gets a system which should behave like a continuous fluid with correlated density fluctuations which have the desired (i.e. representative of the continuous field) correlation properties. However, that one considers point distributions which introduce discreteness effects due to their intrinsic fluctuations and correlations. We have addressed the problem whether these discreteness effects due the imprint of the (correlated) fluctuations of the pre-initial point distribution are strong enough to super-seed the given correlations. Indeed, we have shown that this is the case and we have pointed out that the standard ad-hoc procedure used to create N-body IC does not give rise to the desired CDM-like correlation of density fluctuations. This implies that the small-scales non-linear dynamical evolution of the system is driven by fluctuations which arise from the particular ad-hoc procedure used to discretise the field. In this context, these fluctuations can be seen as finite size effects, and are completely different from CDM-like fluctuations. Moreover we have studied the behaviour of the gravitational force acting on an average particle with the result that the force due to the nearest particles is highly fluctuating and gives a contribution of the order of the large scale one. For this reason we conclude that discreteness effects can be significant relative to the smooth distribution and that they therefore play an important role in the small-scales non-linear evolution of cosmological N-body simulations. Finally we stress that most of procedures used to discretise a continuous field (e.g. threshold or random sampling) unavoidably introduces Poisson noise. In such a situation, due to the strong NN interactions, the large scale fluctuations play an even smaller role in the non-linear dynamics which would be dominated mainly by particle-particle interactions.

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Fig. 1. – Behaviour of $\sigma^2(r)$ for the pre-initial glass distribution, for the initial condition of the simulation ($z = 50$) and for the theoretical expectation for a CDM model. For the glass configuration $\sigma^2(r) \sim r^{-4}$, while for the IC it deviates from this behavior at $r \sim \langle \Lambda \rangle$ beyond which it behaves as $r^{-1}$. For the CDM model instead $\sigma^2(r) \sim \text{const.}$ up to $r \sim r_c \sim 0.1$ and then it decays as $r^{-4}$. (For the x-axis we have used normalized units to the box size $L = 239.5 Mpc/h$). Note that there is no agreement at any scale, between IC and CDM.

Fig. 2. – The behaviour of $\xi(r)$ for the same distributions of the previous figure (for the x-axis we have used normalized units to the box size $L = 239.5 Mpc/h$). For the glass and IC $\xi(r)$ is oscillating around zero. For the theoretical expectation for a CDM one should find $\xi(r) \sim \text{const.} > 0$ for $r \leq r_c \sim 0.1$ and then $\xi(r) \sim -r^{-4}$ at larger scales. Note that the nature of the fluctuations in the IC and CDM distribution is rather different: for the first one has a sequence of over-densities and under-densities (i.e. an oscillating $\xi(r)$) while in the second case one would expect an over-density $\xi(r) > 0$ followed by an under-density $\xi(r) < 0$. In the insert panel it is shown the behaviour of the conditional density $\sim [\xi(r) + 1]$ which makes clear the oscillatory nature of $\xi(r)$.

Fig. 3. – The behaviour of the average total force and its variance as a function of distance (for the x-axis we have used normalized units to the box size $L = 239.5 Mpc/h$) for the pre-initial (glass) and initial particle distribution. For the glass configuration the force is very small and almost zero. For the IC, one may note that the NN gives a very fluctuating contribution to the total force of the order of the asymptotic one. Finally, note that the force does not converge at the box size.
$\sigma^2(r)$ vs. $r$

- Glass
- ICS
- CDM
- $r^{-4}$
- $r^{-1.6}$
- $r^{-4}$
$|\xi(r)|$ vs. $r$

Glass
ICS
CDM

$\langle n(\xi(r)+1) \rangle$ vs. $r$
