AN ALTERNATIVE TO GRIDS AND GLASSES: QUAQUAVERSAL PRE-INITIAL CONDITIONS FOR N-BODY SIMULATIONS

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Received 2006 June 13; accepted 2006 October 25

Abstract

N-body simulations sample their initial conditions on an initial particle distribution, which for cosmological simulations is usually a glass or grid, while a Poisson distribution is used for galaxy models, spherical collapse, etc. These pre-initial conditions have inherent correlations, noise due to discreteness, and preferential alignments, while the glass distribution is poorly defined and computationally expensive to construct. We present a novel particle distribution that can be useful as a pre-initial condition for N-body simulations, using a simple construction based on a “quaquaaversal” tiling of space. This distribution has little preferred orientation (i.e., is statistically isotropic), has a rapidly vanishing large-scale power spectrum \[ P(k) \sim k^4 \], and is trivial to create. It should be particularly useful for warm dark matter and cold collapse simulations.

Subject heading: methods: n-body simulations

Online material: color figures

1. INTRODUCTION

Numerical simulations have become a very powerful tool for investigating nonlinear gravitational phenomena, such as understanding the evolution and properties of cosmological structures. Since the simulations contain a rapidly increasing number of particles and probe structures on ever smaller scales, it is timely to address some of the fundamental aspects of the initial conditions used in these simulations.

One such aspect is that the standard cosmological model assumes that the early universe is statistically isotropic. This is in contrast with the usual choice of “pre-initial” condition for N-body simulations, most often given by placing particles on a uniform grid, which is intrinsically anisotropic. While it has been shown that this anisotropy can produce nonphysical effects in simulations, such effects are difficult to quantify. For cold dark matter simulations, it is thought that the physically relevant correlations quickly grow and dominate over fluctuations due to discreteness. The same is not true for warm dark matter simulations, for example.

To address this and related questions numerically, it is useful to have alternative pre-initial conditions (PreICs). We construct a novel pre-initial condition by making use of a tiling of three-dimensional space called the quaquaaversal tiling (Conway & Radin 1998). We will show that this new particle distribution, which is statistically isotropic (i.e., has little intrinsic directionality), has mass fluctuations that decay as rapidly as in a grid. At the same time it is a deterministic structure and can be trivially generated. We present a C code for the generation of these structures, which can be downloaded from our Web site.

2. EXISTING PRE-INITIAL CONDITIONS

Let us briefly recall the steps in any cosmological simulation. (1) First one chooses the PreIC, which most often is a regular grid; that is, the particles are placed on a lattice. (2) One then imprints a power spectrum onto these particles by applying an appropriate displacement field specified through the Zel’dovich approximation. (3) Then one runs the cosmological code, taking care of the many numerical issues related to convergence (softening, time stepping, etc.). The present paper focuses solely on the first step, namely, the setting up of the pre-initial condition.

There are three PreICs that are regularly used in the literature. The first, which is the standard choice, places the particles on a regular grid. This is a very well tested method, which most likely produces the correct growth of long-range large-scale fluctuations (Efstathiou et al. 1985). However, it is unknown how much the grid affects small-scale structures. One explicit example in which such effects have been observed to be important is in simulations with warm dark matter (WDM). In the WDM case the thermal motion induces free streaming, which erases structures on small scales. In Bode et al. (2001), it was suggested that WDM might have the novel property of creating structures along a cosmic web, below the cutoff frequency of the power spectrum. Bode et al. (2001) took great care in testing for a large range of known numerical issues and concluded that the effect observed was real and physical. It was later shown that these small-scale structures were spurious. In Götz & Sommer-Larsen (2003), two almost identical simulations were performed, differing only in the pre-initial conditions: one was a grid, and the other was a glass (we will discuss “glass” initial conditions below). It was shown from the results of these simulations (Götz & Sommer-Larsen 2003) that the conclusions reached in Bode et al. (2001) were incorrect precisely because of effects coming from the pre-initial particle distribution: the beadlike structures along the filaments observed were virtually absent in the simulation with a pre-initial glass. We emphasize that this is just an illustration of how difficult WDM simulations can be. Similar difficulties have been discussed in the context of cold dark matter (CDM) simulations; for example, starting from specific configurations (Melott et al. 1997), and at early times (Joyce et al. 2005), it remains unclear how important such effects are in real simulations.

The second PreIC that is often used is the “glass.” The idea is to evolve a set of particles, which are initially randomly distributed in a box, under negative gravity (i.e., Coulomb forces) until one reaches a configuration in which the force on each particle is extremely small (White 1994). While this appears simple at first

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sight, there are a number of well-known practical problems. First, starting from the random configuration, the particles stream toward a lower potential but gain kinetic energy, which makes them oscillate about the minimum of their local potential. To reduce the associated Poisson noise, one needs to damp these velocities. If one does so by reducing the particle velocities at a given time, then a large fraction of the particles will lie far from the minimum of the potential and little is gained. If one applies a more continuous damping of the particle velocities, then either the small-scale fluctuations are erased (if the damping is large) or the glass takes an unreasonably long time to create (if the damping is small).

If one uses the method of simulated annealing, repeatedly heating up and cooling down the system, the creation of the glass becomes computationally very expensive. A major difficulty is that the final configuration is not unique, and indeed, that one does not have a well-defined criterion for determining when an optimal configuration has been reached. We note in this respect (see Gabrielli et al. 2003) that the system that is simulated is just a damped variant of the "one-component plasma" (i.e., point particles interacting through Coulomb forces), which is known (Carr 1961) to undergo a transition to a body-centered cubic lattice configuration at low temperature. The glass is presumably a transient to such a grid-type configuration, but it is not known what the relevant timescales are.

A third possibility, and one that is frequently used to create equilibrium and nonequilibrium halo models, is to simply select random positions for particles. In this case there is Poisson noise at all scales. If one tries to simulate a "cold collapse" using such initial conditions, then the growth of small-scale structures can clearly be seen, which will affect the virialization of the final structure.

In summary, the grid PreIC is trivial to create and has a vanishing power spectrum (below the Nyquist frequency). It has, however, a strong orientation and a power on the scale of the grid spacing. The glass PreIC has, in principle, little preferred orientation, and has a rapidly decreasing power spectrum of density fluctuations, with $P(k) \sim k^4$ (Smith et al. 2003), at large scales. These latter configurations are, however, not clearly defined, and they are computationally expensive to create. Note, however, that the glass PreIC still suffers from large-scale anisotropy as long as periodic boundary conditions are used. Such large-scale anisotropies are evidently also present in the new PreIC to be discussed below.

The random PreIC has no orientation, but it has significant intrinsic power on all scales [$P(k) = \text{constant}$]. We now present a novel PreIC that is clearly defined and easy to generate, has a large-scale power spectrum that vanishes as in the glass configurations [$P(k) \sim k^4$], and has no preferred orientation.

### 3. Constructing a Quaquaversal Tiling

The quaquaversal tiling (Conway & Radin 1998) is a hierarchical tiling of three-dimensional space based on a triangular prism that is repeatedly rotated about orthogonal axes by angles of $2\pi/3$ and $\pi/2$. The principle of our construction of the PreIC is simple. The quaquaversal tiling defines a division of space into equal-volume cells. The particle distribution obtained by assigning a particle of the same mass to each cell is highly uniform: the only source of fluctuations is the redistribution of the mass at the scale of the cell. Indeed, a well-known argument by Zel’dovich (Zel’dovich 1965; Zel’dovich & Novikov 1983) shows that such a local mass conservation constraint should lead to a power spectrum with the behavior $P(k) \sim k^4$ at small $k$. If one adds the further constraint that the center of mass is locally conserved, one expects to obtain $P(k) \sim k^4$ at small $k$. Here we impose this constraint by placing the particle in each tile at its center of mass. Furthermore, the tiling has little preferred orientation, a desirable property that will be inherited by the particle distribution.

Consider a triangular tile made from a 1, $\sqrt{3}$, 2 right triangle, with depth 1/2. This tile can be decomposed into four identical tiles, all with exactly the same angular properties as the original "parent" tile, by placing three lines from the center of the long side (length 2) to the centers of the other two sides (lengths 1 and $\sqrt{3}$) and to the right angle. Then all lines are extended in depth (in the third dimension). One can now choose one of two possibilities, either to rotate the two triangles at the short axis by $2\pi/3$ about an axis in the depth dimension, or to rotate the two triangles touching the right angle by $\pi/2$ about an axis in the $y$-dimension (see Fig. 1). Finally, one places two tiles next to each other, each with their choice of rotation. For further details, see Conway & Radin (1998).

After this first tiling, we are left with eight triangles, each identical to the original parent triangle, but a factor of 8 smaller in volume. (The angles of the individual triangles are the same, but the sides are smaller by a factor of 2). We can now repeat this process again for each triangle, giving us 64 identical triangles. After $N$ such iterations, we will have $8^N$ identical triangles with the same angular properties as the original parent triangle.

To obtain our configuration, we then place a particle in the center of the volume of each tile. Finally, we place two parent tiles on top of each other to form a rectangular box with sides of length 1, 1, and $\sqrt{3}$. This final distribution, which is our new PreIC to be used in simulations, thus contains $2 \times 8^N$ particles. From now on, we will refer to this kind of particle distribution as a "Q-set." For simulations in which periodic boundary conditions are needed, one can only make Q-sets with 16, 128, $\ldots$, 4.2M, 33.6M, $\ldots$ particles, where the multiplier "M" stands for "millions." It is proved in Conway & Radin (1998) that, in the limit of an infinite number of iterations, the orientations of the tiles are essentially random [uniform in SO(3)]. We infer that our distribution (with finite but large $N$) will have little directionality (see discussion in § 4.4).

Naturally, one can imagine similar constructions based on other tilings. In this paper, however, we will focus on this simple quaquaversal structure.

#### 3.1. Computer Code

We briefly describe the idea behind this code. Each tile is uniquely defined through the definition of the spatial position (in three-dimensional space) of four corners (three corners would
suffice, of course). Thus, the original parent tile is defined through four different 3-vectors. This is expressed through one 12-vector, \( V \).

The eight subtiles in the next level of tiling, \( n+1 \), are defined through a constant matrix, \( M \), that is applied to each vector at level \( n \) such that

\[
V_i(n+1) = MV(n),
\]

where \( i = 1, \ldots, 8 \) define the eight new subtiles. Thus the constant matrix \( M \) has 128 entries, and it uniquely defines each tiling step.

The code recursively applies \( M \) to the vectors (it recursively tiles each subtile) until the desired level, \( N \), has been reached. Then a particle is placed in the center of the volume of that tile, and that point is written to a file. Constructed in this way, the code is very fast and requires very little memory.

In our implementation the matrix \( M \) is constant. This implies that the specific rotations by fractions of \( \pi \) are identical at each level of refinement. It would be possible to generalize the procedure by allowing the rotations to differ at each level; for example, sometimes rotating by \( 4\pi/3 \) instead of \( 2\pi/3 \). In that way one could achieve a slightly higher level of isotropization.

We now consider the properties of the particle distribution in this rectangular box, in terms of mass variance and power spectrum.

4. Statistical Properties

4.1. Mass Variance \( \sigma_M^2(R) \)

Let us first analyze the amplitude of mass fluctuations in a sphere of radius \( R \) with respect to the average mass. If \( M(R) \) is the mass (for a discrete distribution, the number of particles) inside a sphere of radius \( R \), the normalized mass variance is defined as

\[
\sigma_M^2(R) = \frac{\langle M(R)^2 \rangle - \langle M(R) \rangle^2}{\langle M(R) \rangle^2},
\]

where the brackets indicate an ensemble average. For a distribution like ours (or, e.g., a grid), one can define the ensemble average as the average over random positions of the initial box. Such an ensemble average definition is equivalent to a spatial average, with the mass variance then given as the infinite volume limit of the estimator defined below.

For our mass variance calculations we have used the simple estimator

\[
\sigma_{M, \text{est}}^2(R) = \frac{1}{\langle N_r \rangle^2} \sum_{i=1}^{N_r} \frac{|N_i(R) - \langle N_r \rangle|^2}{N_r - 1},
\]

where \( N_i(R) \) is the number of particles in the \( i \)-th of \( N_r \) randomly thrown spheres constrained to be inside the sample volume. The quantity \( \langle N_r \rangle \) is the mean number of particles in such a sphere, given exactly by \( \langle N_r \rangle = 4\pi r^3/3 \). \( v \) is the volume per particle (i.e., the volume of a single tile in the Q-set).

We apply this estimator to a grid, a Poisson distribution, a typical \( \Lambda \)CDM initial condition (\( z = 70 \)), and a Q-set. We have used 128\(^3\) particles in a cube of side unity for the first three, while the Q-set employed seven tiling levels, which gives \( 2 \times 8^7 = 2 \times 128^3 \) particles in a rectangular box. The dimension of the Q-set box is chosen so that the mean density is equal to that of the other distributions. This is a convenient choice for comparison of the results, as it is the mean particle density \( n_0 \) that fixes the asymptotic level of the Poisson variance at small scales in any point distribution, with \( \sigma_M^2(R \to 0) = 1/\langle n_0 V_s(R) \rangle \), where \( V_s = 4\pi R^3/3 \) (see, e.g., Gabrielli et al. 2002). Several tests confirm that our estimator calculates the correct spatial properties (see further discussion below). We see (Fig. 2) that the mass variance of a Q-set has the same behavior as that of a grid with \( \sigma_M^2 \sim R^{-4} \) above the interparticle distance. The mean interparticle distance, \( \Lambda = 1/128 \), for the structures with 128\(^3\) particles is also shown in the figure. Note that this is exactly the length of the shortest side of a tile in the level 7 quaquaversal tiling used for the Q-set considered here.

4.2. Power Spectrum \( P(k) \)

The power spectrum is the primary statistical tool used to characterize fluctuations in cosmology. It is defined as

\[
P(k) = \lim_{r \to \infty} \frac{1}{V} \langle |\delta(k)|^2 \rangle,
\]

where \( \delta(k) \) is the Fourier transform of the density fluctuation field \( \delta(x) = \langle \rho(x) - \rho_0 \rangle/\rho_0 \). In the case of a discrete distribution (i.e., of point particles), these quantities simply become

\[
\delta(x) = \frac{V}{N_p} \sum_{x_p} \delta_D(x - x_p) - 1, \quad (5a)
\]

\[
\delta(k) = \frac{V}{N_p} \sum_{x_p} e^{-i k \cdot x_p} \quad (k \neq 0), \quad (5b)
\]

where \( x_p \) is the location of each particle and \( \delta_D \) is the Dirac delta function.

To estimate the power spectrum, we have used the “brute force” method; that is, we calculate it directly from the formula one obtains by substituting equation (5b) into equation (4), without the
infinite volume limit and the ensemble average. Our finite volume \( V \) is thus a rectangular box with sides \( L_x \), and we assume periodic boundary conditions so that the \( k \) in the Fourier sums take the values \( k = 2\pi (n_x/L_x, n_y/L_y, n_z/L_z) \), where \( n_i \) are integers. We obtain \( P(k) = P(|k|) \) by averaging over a bin of finite width around \( k = |k| \) (Sirko 2005). It is important to take care in the interpretation of the large-scale (i.e., small \( k \)) modes, which will be both affected by undersampling and contaminated by the boundary conditions (which systematically suppress power at small \( k \)). With this simple estimator, however, we do not have to worry about the effect of assignment function, which typically causes problems in fast Fourier transform (FFT) methods (Jing 2005).

As for the mass variance, we calculate the power spectrum for a grid, a Poisson distribution, a typical ΛCDM initial condition, and a Q-set. This time we use a smaller number of particles in order to facilitate the more computationally demanding procedure of calculating \( P(k) \): they all have 32\(^3\) particles, except for the Q-set, which has \( N = 5 \) and therefore again has twice as many points (32\(^3\) = 8\(^3\)). Like that for the mass variance, this makes the Poisson level \( (V/N_p) \) the same for all the distributions considered.

We see in Figure 3 that the Q-set has the anticipated \( k^4 \) behavior up to the wavenumber \( k_s \), where it flattens, on average, to the Poisson level. We have used a very fine binning in order to capture this characteristic slope, as well as the peaks arising from typical interparticle distances. We note that peaks appear at frequencies of \( 2^{-n}k \), where \( n \) has integer values. It can be shown (see Radin 1999) that in hierarchical structures, a feature in real space between two radii, \( r_1 \) and \( r_2 \), also must appear between the radii \( \kappa r_1 \) and \( \kappa r_2 \), where \( \kappa = 2 \) for a quaquaversal structure. Consistent with this interpretation, we note that adding random perturbations to the particles, hence creating a shuffled Q-set, gives \( P(k) \sim k^2 \) with peaks of diminished amplitude.

A comparison between the different distributions can be seen in Figure 4. Note that the grid has zero power up to \( k_s \), where it is strongly peaked, and that all distributions, on average, reach the Poisson level at this wavenumber.

4.3. Relations between \( \sigma_M^2(R) \) and \( P(k) \)

The quantities \( \sigma_M^2(R) \) and \( P(k) \) are related by the standard expression

\[
\sigma_M^2(R) = \frac{1}{2\pi^2} \int_0^{\infty} P(k) \hat{W}^2(kr) k^2 \, dk,
\]

where \( \hat{W}^2(kr) \) is the Fourier transform of the spherical top-hat window function.

By studying equation (6) for a power spectrum of the form \( P(k \to 0) \sim k^n \), one finds (Gabrielli et al. 2002) that for \( R \to \infty \),

\[
\sigma_M^2(R) \sim \begin{cases} 
1/R^{3+n} & \text{if } n < 1, \\
\log(R)/R^4 & \text{if } n = 1, \\
1/R^4 & \text{if } n > 1.
\end{cases}
\]

Two particular and simple examples that are useful reference points against which to gauge new distributions are the following:

1. Poisson: \( \sigma_M^2(R) \sim R^{-3} \), \( P(k) \sim V/N_p \sim \text{constant} \).
2. Shuffled lattice: \( \sigma_M^2(R) \sim R^{-4} \), \( P(k) \sim k^2 \).

The numerical results for the mass variance and power spectrum in §§ 4.1 and 4.2 are all in line with these analytic results; notably, our new Q-set has \( \sigma_M^2(R) \sim R^{-4} \) and \( P(k) \sim k^4 \). This (large scale) behavior makes the Q-set a member of a group of systems that have been termed “superhomogeneous” (Gabrielli et al. 2002, 2003) or “hyperuniform” (Torquato & Stillinger 2003). Such distributions, defined by the property \( P(k \to 0) = 0 \), are characterized in real space (cf. eq. [7] above) by the asymptotic behavior of their variance, \( \sigma_M^2(R) \sim 1/R^n \), with \( d < m < d + 1 \), where \( d \) is the spatial dimension. This quantity thus decays faster than in a Poisson point process \( (m = d) \), and, in the cases we have considered, attains the same behavior as other superhomogeneous distributions \( (m = d + 1) \). This is in fact the fastest possible decay...
of this quantity for either point- (Beck 1987) or continuous (Gabrielli et al. 2002) mass distributions. We note that the glass PreIC also belongs to this class, as it shares the same behavior of the variance and power spectrum as that of the Q-set that we have introduced and analyzed.

4.4. Isotropy

One of the nice features of the Q-set is, as we have underlined, that it is isotropic. This result applies, however, in the limit of an infinite number of iterations of the algorithm we have described. It is interesting to quantify the degree of isotropy of a finite level of tiling. To do so we show in Figure 5 a plot giving (triangles) the distinct directions defined by the tiles of the quaquaversal tiling used to construct the Q-set with $N = 7$. The directions are those of the shortest axis of each tile with respect to the orientation of the mother tile. Also shown (open circles) is an analogous characterization of a grid, which gives just the six orientations of the vectors pointing to the nearest neighbor sites.

Figure 6 shows, on the other hand, the dependence of the number of distinct orientations, in the $(\theta, \phi)$-plane, on the level of the tiling. The degree of isotropy grows very rapidly with increasing $N$.

5. CONCLUSIONS

We have studied an alternative to the standard pre-initial conditions for $N$-body simulations of cosmological structures. The standard grid has strong orientations, and the glass is poorly defined and computationally expensive to create. We have therefore considered a particle distribution created starting from an equal-volume tiling of space, which we have called the quaquaversal tiling. The particle distribution is trivial to create, has virtually no orientation (is statistically isotropic), and has a rapidly vanishing large-scale power spectrum. We provide a C code for the generation of these structures at our Web site.\(^5\)

S. H. H. is supported by the Swiss National Foundation. M. J. is indebted to J. Lebowitz for the essential references on tilings and to C. Radin for subsequent useful exchanges. O. A. would like to thank A. B. Romeo for valuable discussions. We also thank T. Baertschiger, A. Gabrielli, B. Jancovici, A. Knebe, A. Maccio`, B. Marcos, J. Peacock, F. Sylos Labini, and S. Torquato for many useful discussions on related issues. We thank the anonymous referee for very useful remarks and suggestions.

5 Available at http://krone.physik.unizh.ch/~hansen/qua.

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