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IMPLEMENTING THE DC MODE IN COSMOLOGICAL SIMULATIONS WITH SUPERCOMOVING VARIABLES

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ABSTRACT

As emphasized by previous studies, proper treatment of the density fluctuation on the fundamental scale of a cosmological simulation volume – the "DC mode" – is critical for accurate modeling of spatial correlations on scales $\gtrsim 10\%$ of simulation box size. We provide further illustration of the effects of the DC mode on the abundance of halos in small boxes and show that it is straightforward to incorporate this mode in cosmological codes that use the "supercomoving" variables. The equations governing evolution of dark matter and baryons recast with these variables are particularly simple and include the expansion factor, and hence the effect of the DC mode, explicitly only in the Poisson equation.

Subject headings: cosmology: theory – methods: numerical

1. INTRODUCTION

Cosmological simulations have become the main theoretical tool for studying the evolution of cosmic structures. Their applications range from modeling the subparsec scale environments of first stars and supermassive black holes to the large-scale distribution of matter and galaxies. Correspondingly, sizes of simulated regions range from hundreds of kiloparsecs to gigaparsecs.

Many modern simulations use small simulation volumes, focusing limited computational resources on resolving important small-scale dynamics of galaxies or dark matter substructure. In order for such a simulation to remain a fair realization of a region of the universe, it must properly account for the time evolution of the non-vanishing fluctuation of the cosmic density at the scale of the simulation box. Following Sirko (2005), we call this fluctuation the "DC mode,"[7] $\delta_{\rm DC}$, to reflect the fact that it is constant in space over the simulation volume.

While any simulation of a finite volume has a non-vanishing DC mode, it is not easy to compute for a volume of arbitrary geometry. Therefore, in the following we assume that the simulation volume is a cubic box of size L, and that periodic boundary conditions are imposed along each box dimension. This is indeed the most common setup for cosmological simulations.

Throughout this paper we use a cosmological model consistent with the third year WMAP results ($\Omega_m = 0.24$, $h_{100} = 0.73$, $\sigma_8 = 0.75$, and $n_S = 0.95$), as this is the model used in our reference $80h^{-1}$ Mpc simulation that we adopt as an approximation to a representative volume of the universe. None of our conclusions, however, are dependent on the specific values of cosmological parameters.

2. EFFECTS OF THE DC MODE IN COSMOLOGICAL SIMULATIONS

In the infinite universe the power spectrum of density fluctuations, $P(k)$, and their correlation function, $\xi(r)$, are the Fourier transforms of each other. In a cubic periodic simulation box of finite size this is no longer true. Since the real space quantities are directly related to observables, one can argue that it is more important to maintain correct $\xi(r)$ than $P(k)$ within the simulation volume (Pen 1997). In this case the power spectrum of the density fluctuations inside the simulation box of size L becomes a convolution of the true cosmic power spectrum $P(k)$ and the window function of the simulation volume $W_L(\vec{k})$,

$$P_{\rm grid}(\vec{k}) = \int P(k')W_L(\vec{k}-\vec{k}')d^Dk', \qquad (1)$$

where

$$W_L(\vec{k}) = \prod_{j=1}^{D} \frac{\sin(k_jL/2)}{\pi k_jL}$$

and D is the dimension of space. Even if $P(0) = 0$, $P_{\rm grid}(\vec{0})$ is not, in general, equal to zero because rms value of density fluctuation at the box scale is not zero. Simulations aiming to model density fluctuations on scales comparable to box size correctly must therefore incorporate a non-zero DC mode.

In order to illustrate the effect of using $P_{\rm grid}$ instead of the true linear $P(k)$ while generating the cosmological initial conditions, we create a large number of realizations of the linear density field for each value of the simulation box size L and measure the linear mass variance on the scale of $8h^{-1}$ Mpc, σ_8, as the average over the whole ensemble[8]. Figure 1 shows σ_8 as a function of

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[7] By analogy with the constant electric Direct Current.

[8] The specific number of realizations, N, for each value of L is determined by the requirement that the average σ_8 is measured to 1% precision.

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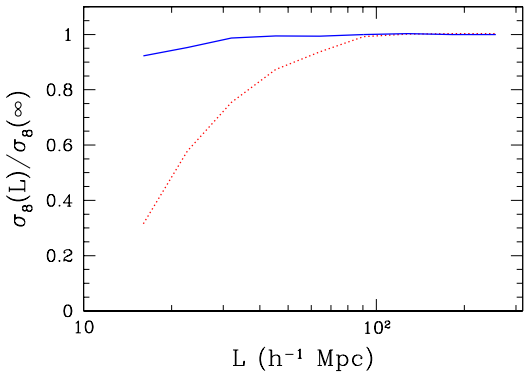

FIG. 1.— The linear mass variance in spheres of radius $8h^{-1}$ Mpc (σ_8) at $z = 0$ as a function of the simulation box size L, as measured from a large number of realizations. Red dotted line shows the standard method, where the true linear $P(k)$ is used to generate the cosmic density field, while the blue solid line shows the method that uses $P_{\rm grid}$ for setting the density amplitude on the grid.

simulation box size L at $z = 0$ for two sets of realizations - one that uses $P_{\rm grid}$ and another one that uses true linear $P(k)$. In the former method the linear mass variance in spheres is preserved to at least 90% at scales as small as half the box size, while in the standard method (e.g., Bertschinger 2001; Prunet et al. 2008) the mass variance is only accurate in spheres that are less than 10% of the box size in radius. The same is true for many other real-space clustering measures, as is amply demonstrated by Pen (1997) and Sirko (2005).

Using $P_{\rm grid}$ to set up initial conditions clearly increases the fidelity of a small-box cosmological simulation. However, how important is it to have a non-zero DC mode? After all, the non-zero value of $P_{\rm grid}(0)$ only implies a non-vanishing *rms* of a Gaussian-distributed DC mode. A single simulation can always impose the constraint of $\delta_{\rm DC} = 0$ without violating the statistical properties of the initial conditions, although, strictly speaking, such initial conditions will not be a true random realization of the universe. Hence, if an ensemble of simulations is performed, then proper sampling of the DC mode is crucial, even if the ensemble only contains just two simulations.

To illustrate this point, we show in Figure 2 the rms variation in the number of dark matter halos as a function of their maximum circular velocity or the virial mass. To compute the rms, we generate two sets of five different random realizations of initial conditions, in a $L = 20h^{-1}$ Mpc box. In the first set of initial conditions the DC mode is forced to be zero, while in the second set the DC mode is computed properly as a Gaussian distributed random number with the rms value of $P_{\rm grid}(0)L^3$. Each of the ten realizations of initial conditions is then evolved to $z = 0$ with the N-body part of the Adaptive Refinement Tree (ART) code (Kravtsov et al. 1997; Kravtsov 1999) with 128^3 particles and 2^{12} dynamic range.

As a control sample, we use a halo population from a single simulation of $L = 80h^{-1}$ Mpc with zero DC mode. The simulation followed 512^3 particles with a dynamic spatial range of 2^{15}. Simulation results of this larger box at $z = 0$ are used to compute the rms number density fluctuations of dark matter halos in cubic boxes of $20h^{-1}$ Mpc on a side. In both simulations halos were identified using a variant of the Bound Density Maxima algorithm, as described in Kravtsov et al. (2004).

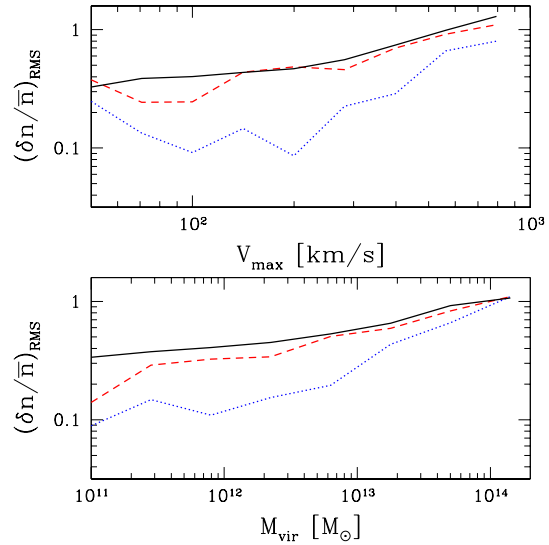

FIG. 2.— The rms fluctuations in the numbers of dark matter halos as a function of halo maximum circular velocity (top) or the virial mass (bottom) in cells of $L = 20h^{-1}$ Mpc. Dotted blue and dashed red lines show the average over two ensembles of 5 simulations each, with the DC mode forced to zero and the properly computed DC mode respectively. Simulations followed evolution in a box of $L = 20h^{-1}$ Mpc; each of the ten simulations used different random realizations of initial conditions. Solid black lines show the rms computed from a single simulation of the same cosmology of $L = 80h^{-1}$ Mpc box size.

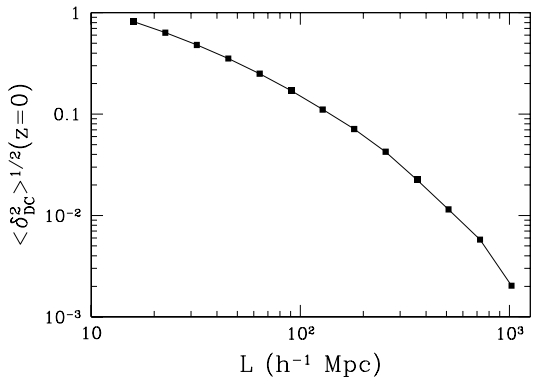

FIG. 3.— The rms amplitude of the DC mode at $z = 0$ as a function of the simulation box size L.

As Figure 2 illustrates, the ensemble of simulations with the DC mode (red dashed lines) properly accounts for the fluctuations on the box size scale. Setting the DC mode to zero (blue dotted lines) results instead in a factor of $\sim 2 - 3$ underestimate of the true variance.

3. INCORPORATING THE DC MODE IN A COSMOLOGICAL CODE

The DC mode is substantial for many of the commonly used simulation box sizes. For example, Figure 3 shows the rms DC mode as a function of the simulation box size. The rms DC mode falls below 1% only for box sizes $L > 500h^{-1}$ Mpc. While 1% may seem like a small number, many studies use such boxes to calibrate statistics, such as power spectrum and abundance and clustering of halos, to accuracy of $< 5\%$. Therefore, effect of the DC mode may need to be evaluated even for boxes of

hundreds of megaparsecs in size.

The DC mode thus cannot be "approximately neglected," at least not in any study aiming at obtaining correct statistics on the scale of the simulation box size. How easy it is to incorporate the DC mode depends on the nature of a cosmological simulation code and could be a non-trivial task.

Cosmological simulations most commonly employ periodic boundary conditions and simulation box can be considered as a separate universe that expands at a different rate than the target model universe. Following Sirko (2005), we define two expansion factors: the scale factor of the simulation box, $a_{\rm box}$, and the true, global expansion factor of the universeas, $a_{\rm uni}$. As mass is conserved, the average mass density in the simulation box should be equal to the density of a region with the overdensity $\delta_{\rm DC}$ in the target model universe,

$$\frac{\Omega_M}{a_{\rm box}^3} = \frac{\Omega_M}{a_{\rm uni}^3}\left[1+\delta_{\rm DC}(a_{\rm uni})\right], \tag{2}$$

or

$$a_{\rm box} = \frac{a_{\rm uni}}{\left[1+\Delta_{\rm DC}D_+(a_{\rm uni})\right]^{1/3}}, \tag{3}$$

where we explicitly spelled out the dependence of the DC mode on the universal expansion factor $a_{\rm uni}$, $\delta_{\rm DC}(a_{\rm uni}) \equiv \Delta_{\rm DC}D_+(a_{\rm uni})$. Here D_+ is the linear growth factor of density perturbations; it is one (namely, growing) of the two independent solutions of the linear perturbation equation for dust-like matter in the Newtonian approximation[9] (e.g., Bonnor 1957; Peebles 1980):

$$\ddot{\delta} + 2\frac{\dot{a}}{a}\dot{\delta} = 4\pi G\bar{\rho}\delta, \tag{4}$$

where $\delta \equiv (\rho-\bar{\rho})/\bar{\rho}$ is the matter overdensity with respect to the mean density of the universe $\bar{\rho}$, $a(t)$ is the expansion factor, and derivatives are taken with respect to the physical time t.

We adopt a normalization for D_+ such that in a universe filled with matter and radiation only (i.e., at sufficiently early times),

$$D_+(a) = a + \frac{2}{3}a_{\rm eq} + \frac{a_{\rm eq}}{2\ln(2)-3}\times \left[2\sqrt{1+x} + \left(\frac{2}{3}+x\right)\ln\frac{\sqrt{1+x}-1}{\sqrt{1+x}+1}\right], \tag{5}$$

[9] One may question the validity of the Newtonian approximation on large scales in simulations of large box sizes, $L = O(c/H_0)$, given that evolution of large-scale modes should be governed by fully relativistic equations. However, we note that equation (4) is identical to the corresponding fully relativistic linear perturbation growth equation in the synchronous gauge or, more generally, in the comoving "total matter gauge". The equations governing evolution of perturbations in the synchronous gauge are presented, for example, in Ma & Bertschinger (1995). We can derive equation identical to eq. (4) above by 1) substituting their eq. 21a into 21c, 2) considering the case of universe with energy density dominated by non-relativistic matter ($\delta T_0^0 = \bar{\rho}\delta$, $\delta T_i^i = 0$), for which $dh/d\tau = -2\delta$ (their eq. 42), and 3) by making appropriate transformations from conformal time τ to physical time t using $d\tau = dt/a(\tau)$. This means that linear evolution of perturbations is treated correctly in the Newtonian approximation of cosmological codes at any scale, provided one interprets results of simulations in the appropriate gauge (see, e.g., Wands & Slosar 2009; Chisari & Zaldarriaga 2011).

where $x \equiv a/a_{\rm eq}$ and $a_{\rm eq} \equiv \Omega_R/\Omega_M$ is the scale factor of matter-radiaton equality. The last two terms can often be neglected, the third one falls below 1% for $z \lesssim 1{,}100$ and the second one is below 1% for $z \lesssim 35$.

Sirko (2005) also presents a different form for the $a_{\rm box}-a_{\rm uni}$ relation, which he calls a "Lagrangian viewpoint" as opposite to the "Elurian viewpoint" of equation (3), but in essence is just a first order expansion of Equation (3) in $\Delta_{\rm DC}$,

$$a_{\rm box} \approx a_{\rm uni}\left[1-\frac{1}{3}\Delta_{\rm DC}D_+(a_{\rm uni})\right]. \tag{6}$$

When we use this to compute the rms variation in the number of dark matter halos shown in Figure 2, we find a result which is virtually indistinguishable from the "Eulerian viewpoint" shown with red dashed lines. We choose to use the "Eulerian viewpoint" as our primary method for accounting for the DC mode, because it explicitly conserves mass to all orders in the perturbation theory.

The parameter $\Delta_{\rm DC}$ is constant in a given simulation and describes the amplitude of the DC mode in a given realization of initial conditions. In principle, equation (3) is also valid in the non-linear regime, if we treat D_+ as a specific non-linear growth mode in a given simulation box that properly accounts for the coupling of the DC mode to other modes (including modes with wavelengths larger than L). In practice, however, there exists no way to compute the non-linear growth rate besides the numerical simulation itself, so hereafter we assume that the DC mode remains with sufficient precision in the linear regime throughout the whole time-span of the numerical simulation. Of course, the term "sufficient precision" depends on the required precision of the simulation results. For example, for our ensembles of $20h^{-1}$ Mpc boxes the rms value of $\delta_{\rm DC}(1)$ is almost 0.7; never-the-less, the linear approximation for the DC mode is sufficient to achieve about 20% agreement between an ensemble of $20h^{-1}$ Mpc simulations and a single $80h^{-1}$ Mpc run in Figure 2.

Historically, the DC mode was sometimes incorporated into a simulation by appropriately rescaling the values of cosmological parameters. An example of such rescaling is also given in the appendix of Sirko (2005). Effectively, in a spatially flat cosmology such a rescaling introduces non-zero spatial curvature (or additional curvature if the universe is assumed to be spatially non-flat) with the extra curvature parameter $\Delta\Omega_K \approx -(5/3)\Omega_M\Delta_{\rm DC}$.

However, such approach does not work in more general cosmological models. For example, one *cannot* consider simulation with a DC mode as a separate universe in models with non-negligible amount of relativistic matter, general dark energy component, decaying dark matter, or modified gravity.

We, therefore, advocate an alternative approach that can be used to include the DC mode in simulation codes exactly. This can be done by following both $a_{\rm box}$ and $a_{\rm uni}$ as a function of cosmic time and incorporating this difference in simulation equations explicitly. A disadvantage of this approach is that some of the equations become unnecessarily complicated. For example, the evolution equation for the peculiar velocity of a dark matter particle in the expanding coordinate system commonly used

in cosmological codes is

$$\frac{d\vec{v}}{dt} = -2\frac{\dot{a}_{\rm box}}{a_{\rm box}}\vec{v} - \frac{1}{a_{\rm box}^2}\nabla_x\phi,$$

where dot symbolizes the time derivative, ϕ is the peculiar gravitational potential, and spatial derivatives are taken with respect to the comoving coordinates $\vec{x}$, which is emphasized by the subscript x under the gradient symbol. Computing $\dot{a}_{\rm box}$ requires a differentiation of equation (3) and leads to uncouth and inelegant (but fully tractable) formulae.

A much more elegant way to incorporate the DC mode in a cosmological code is via the so-called *supercomoving variables*, first introduced by Doroshkevich et al. (1980), and then used in several numerical codes (Shandarin 1980; Gnedin 1995; Martel & Shapiro 1998; Kravtsov et al. 2002; Teyssier 2002). Specifically, the proper coordinates $\vec{r}$, velocity $\vec{u}$, density ρ, and gravitational potential Φ are replaced with comoving coordinates $\vec{x}$, supercomoving peculiar velocities $\vec{v}$, comoving density ϱ, and peculiar supercomoving gravitational potential φ according to the following transformations:

$$\vec{r} = a\vec{x}, \tag{7}$$

$$\vec{u} = aH\vec{x} + \frac{1}{a}\vec{v}, \tag{8}$$

$$\rho = \frac{\varrho}{a^3}, \tag{9}$$

$$\Phi = -\frac{a\ddot{a}}{2}x^2 + \frac{1}{a^2}\varphi. \tag{10}$$

In addition, the cosmic time t is replaced with the supercomoving time, τ, defined such that

$$d\tau = a^2 dt. \tag{11}$$

In variables $\tau, \vec{x}, \vec{v}, \varrho, \varphi$ the equations of motion of dark matter particles assume the form identical to that in the proper, non-expanding reference frame, without any explicit cosmological terms,

$$\frac{d\vec{x}}{d\tau} = \vec{v},$$
$$\frac{d\vec{v}}{d\tau} = -\nabla_x\varphi.$$

Similarly, the Euler equations for monatomic gas (polytropic index $\gamma = 5/3$) include no explicit cosmological terms either. The only equation, in which the cosmic scale factor a appears explicitly, is the Poisson equation,

$$\nabla_x^2\varphi = 4\pi G a(\varrho - \bar{\varrho}) \equiv 4\pi G a\bar{\varrho}\delta, \tag{12}$$

where $\bar{\varrho}$ is the mean comoving matter density of the universe. Note that $\bar{\varrho} =$ const in cosmological models in which the dark matter does not decay into radiation.

Incorporating the DC mode into a simulation code using the supercomoving variables is straightforward: all that is required is to identify the scale factor a in equation (12) with the box scale factor $a_{\rm box}$,

$$\nabla_x^2\varphi = 4\pi G a_{\rm box}\bar{\varrho}\delta, \tag{13}$$

and compute both $a_{\rm box}$ and $a_{\rm uni}$ as a function of the supercomoving time τ.

For simulations including gas and other physics, $a_{\rm box}$ should be used anywhere a code would use the scale factor internally. For example, in unit conversions, in cooling functions and star formation and feedback recipes, for checking energy conservation, in the radiative transfer solver, etc. For some physical processes, for example redshift-dependent cosmic backgrounds (radiation, cosmic rays, etc), the proper choice of scaling is model dependent. If a hydrodynamic simulation uses cooling rates that account for the cosmic ultraviolet background in a tabulated form (e.g., Kravtsov 2003; Wiersma et al. 2009), the table should typically be evaluated at $a_{\rm uni}$. If the sources of the radiation are inhomogeneous on the scale of the simulation, however, evaluating at $a_{\rm box}$ would more accurately capture the large-scale density dependence. The only remaining use for $a_{\rm uni}$ is in identifying the snapshot epoch and the final epoch (if a simulation is evolved to $z = 0$, the stopping criterion is $a_{\rm uni} = 1$, not $a_{\rm box} = 1$).

4. CONCLUSIONS

In this short note we illustrated a known but not widely appreciated fact that taking the DC mode into account in small box cosmological simulations is a requirement for the simulation to serve as a representative volume of the universe and to model density fluctuations correctly. The DC mode must be included in simulations if more than a single realization of the initial conditions is used.

While approximate methods for including the DC mode have been proposed, here we advocate the use of the supercomoving variables in cosmological simulations with which the effect of the DC mode is limited to a simple multiplicative term in the Poisson equation (13) and can be incorporated simply and exactly.

An efficient and reliable cosmology module that computes several important quantities ($a_{\rm box}$, $a_{\rm uni}$, supercomoving time τ, the linear growth rate D_+, etc.) via lookup tables in the linear regime is available from the authors upon request.

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