SAMPLE VARIANCE IN N-BODY SIMULATIONS AND IMPACT ON TOMOGRAPHIC SHEAR PREDICTIONS

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ABSTRACT

We study the effects of sample variance in N-body simulations as a function of the size of the simulation box, namely in connection with predictions on tomographic shear spectra. We make use of a set of eight ΛCDM simulations in boxes of 128, 256, and 512 h⁻¹ Mpc a side, for a total of 24, differing just by the initial seeds. Among the simulations with 128 and 512 h⁻¹ Mpc a side, we suitably select those closest and farthest from average. Numerical and linear spectra P(k, z) are suitably connected at low k to evaluate the effects of sample variance on shear spectra C_ℓ(ℓ) for 5 or 10 tomographic bands. We find that shear spectra obtained by using 128 h⁻¹ Mpc simulations can vary up to ~25%, just because of the seed. The sample variance lowers to ~3.3% when using 512 h⁻¹ Mpc. These percentages could however slightly vary if other sets of the same number of realizations were considered. Accordingly, in order to match the ~1% precision expected for the data, if still using eight boxes, we require a size of ~1300–1700 h⁻¹ Mpc for them.

Key words: gravitational lensing: weak – large-scale structure of universe – methods: numerical

1. INTRODUCTION

The tidal gravitational field of density inhomogeneities distorts the images of distant galaxies in the universe. This effect, dubbed cosmic shear, was first observed in 2000 by correlating distant galaxy ellipticities (Bacon et al. 2000; Kaiser et al. 2000; van Waerbeke et al. 2000; Wittman et al. 2000). In turn, comparing cosmic shear with model prediction is expected to become a critical pattern for model selection, namely if data are suitably shared in redshift bands, to create a sort of cosmic tomography. The key point is that tidal fields allow us a more direct insight into the distribution of masses, independent of light emission mechanisms.

The significance of cosmic shear data, however, goes even beyond that. Being obtained from low-z systems, they are indeed complementary to high-z cosmic microwave background anisotropy measurements. Furthermore, in respect to other low-z observables, as SN 1a redshift distributions, the cosmic shear exhibits a specific dependence on the dynamics of structure growth (e.g., Hu 2002; Albrecht et al. 2006; Peacock et al. 2006; La Vacca & Colombo 2008), enabling us to test the consistency between background and inhomogeneity evolutions.

It is therefore hardly surprising that a number of experiments have been planned, such as BOSS,7 PanStarrs,8 HETDEX,9 DES,10 LSST,11 KIDS,12 WFIRST,13 and Euclid14 (Amendola et al. 2013), that aim to scan a large area of the sky and seek fresh information on weak lensing.

The necessary tools to exploit this information are predictions on the distribution of density inhomogeneities and their evolution, both on linear and nonlinear scales. The former predictions can be obtained through library algorithms, like CAMB (Lewis & Bridle 2002). The latter ones, in contrast, can only be based on simulations and therefore depend on the initial realization of matter distribution through point particles.

Such dependence gradually attenuates when greater cosmic volumes are simulated. Accordingly, the Millennium simulations of a ΛCDM cosmology (Springel et al. 2005) were performed in a box of 500 h⁻¹ Mpc a side. Another, more recent, large (in Russian “Bolshoi”) simulation of ΛCDM (Klypin et al. 2011) was run by using 2048³ particles, although in a 250 h⁻¹ Mpc box. Then, the Deus simulation series (Alimi et al. 2010) of Ratra–Peebles (RP hereafter; Ratra & Peebles 1988) and Supergravity theory (SUGRA for short; Brax & Martin 2000) cosmologies (besides ΛCDM) were run in boxes of quite large sizes, up to 1296 h⁻¹ Mpc. Let us finally mention the significant systematic effort deployed to create the Coyote universe simulation suite (Heitmann et al. 2010, 2014). It yields a prediction scheme for the matter power spectrum (the so-called emulator), accurate at the 1% level, out to k ~ 1 Mpc⁻¹ and redshift z = 1. Their simulations were run in boxes with side lengths up to 1300 Mpc, and they tested a wide set of wCDM cosmologies with constant w between −0.7 and −1.3.

Let us outline that, by using the technique introduced by Casarini et al. (2009), and tested by Casarini (2010), the Coyote universe emulator can also be exploited to find spectra of variable-w cosmologies. Limitations on z are then more severe because, at any z, the technique requires information on a range of constant-w spectra wider than those considered at zero and selected in a nontrivial way (clearly, if a model is characterized by a z-dependent state equation yielding w(z) = w, the simulation better approaching the model at that z is not the one with w = w).
Among large simulations, it is also worth mentioning the recent Millennium-XXL simulation, dealing with a $\Lambda$CDM model only, but using a box of $3\,h^{-1}\text{Gpc}$ a side (Angulo & White 2011).

A basic question that shear experiments will enable us to test, however, is whether one of these classical cosmologies is sufficient to approach the data. In this case we expect full consistency between background and inhomogeneity evolutions. Any doubt on that would be evidence of general relativity (GR) violations (Capozziello et al. 2006; Amendola et al. 2007) or energy exchanges between dark cosmic components (Ellis et al. 1989; Wetterich 1995; Amendola 2000, 2004; Amendola & Toncini-Valentini 2002; Amendola et al. 2003; Klypin et al. 2003; Das et al. 2006), not to mention even more complex options. Although N-body programs were built to tackle a number of these options (Macciò et al. 2004, Baldi et al. 2011, Puchwein et al. 2013), no available simulation set enables us to do immediate tests, while it would also be hard to provide, a priori, a sufficiently wide range of simulations to cover a significant set of alternatives.

Accordingly, it is quite relevant to test how far sample variance may affect model predictions trying to meet future data. Of course, sample variance is no obstacle to comparing different cosmologies on a theoretical basis: one just needs to start from the same seed for all models. But, when trying to discriminate between models through shear observations, one must make sure that sample variance, within the simulation sample prepared to build angular spectra, stands well below model discrepancies.

This paper is therefore dedicated to testing how sample variance depends on the box size, as well as how much it can be set under control by using a set of simulations in equal boxes, starting from different seeds. More precisely, we aim to test how the sample variance between simulation boxes is transferred into tomographic shear spectra. Being obtainable by integrating through the former ones, their variance can be expected to decrease; how strong this variance damping can be can only be inspected through direct tests. To do all that it is however adequate to work within the context of $\Lambda$CDM models. As the basis of this work, there are therefore sets of eight $\Lambda$CDM simulations, in boxes with $L = 128, 256, 512\,h^{-1}\text{Mpc}$ a side, for a total of 24.

Before these predictions are directly applied to a specific experiment, however, one should apply the related survey window. For instance, nonlinear mode-coupling effects could depend on detailed observational features (see, e.g., Hamilton et al. 2006). Such a detailed study, however, goes beyond the scope of the present analysis.

The observables we shall deduce from our simulations, first of all, are the fluctuation spectra $P(k, z)$. We shall then use them to predict shear spectra $\Sigma_{ij}(f)$, with 5 or 10 tomographic bands, labeled by $i, j$. This will then allow us to test if (and how) the sample variance in shear spectra is related to the number of tomographic bands.

To perform our 24 N-body simulations, we choose model parameters consistent with recent Planck outputs (Planck Collaboration 2013), shown in Table 1, where symbols bear their usual meaning.

The N-body program used is PDKGRAV (Stadel 2001). Initial conditions were produced with GRAPHIC2 (Bertschinger 2001) and, therefore, did not try to account for the impact of wavelength above the box side (the so-called DC modes; see, e.g., Sirko 2005; Li et al. 2014), which, in our case and as will be verified, would yield substantially unappreciable corrections. The particle numbers, proportional to the box volume, are $128^3$, $256^3$, and $512^3$, respectively. In all simulations $k_{\text{Nyq}} = \pi \, h \, \text{Mpc}^{-1}$.

Simulation outputs are then provided for a large number of redshifts $z_i$. Between $z = 0$ and $z = 0.1$, outputs stand at a redshift distance $\Delta z = 0.01$. Then between $z = 0.1$ and $z = 1$, $\Delta z = 0.1$; between $z = 1$ and $z = 3$, $\Delta z = 0.2$; finally, outputs were obtained at a distance $\Delta z = 1$ up to $z = 10$.

The plan of the paper is therefore as follows. In Section 2 we shall discuss the relation between the number of realizations and sample variance spanned. In Section 3 we shall then deepen another essential question: how spectral points deduced from simulations can be interpolated with linear spectra at low $k$, and which pattern shall be followed to use nonlinear results at large $k$, when numerical noise or lack of resolution hides the numerical signal. These problems were often overlooked in the literature; their technical solutions are an original aspect of this analysis. Let us outline, however, that our choices were also aimed at avoiding artificial differences between realizations; for example, at large $k$, one could surely achieve better results if this aim is disregarded. In Section 4 we shall debate the formation of tomographic filters, for both shear and intrinsic spectra. In Sections 5 and 6, we shall give the expressions for shear and intrinsic spectra and exhibit them for one of the relevant cases, both putting in evidence the impact of intrinsic deformations and determining which tomographic spectra are essentially clean from this kind of contamination. The residual contamination will be taken as a meter for the residual sample variance we may allow for. The final section is devoted to a general discussion and to drawing our conclusions.

### Table 1

| $h$    | $\Omega_k$ | $\Omega_m$ | $n_s$ | $\sigma_8$ |
|--------|------------|------------|-------|------------|
| 0.69   | 0.048      | 0.249      | 0.966 | 0.82       |

2. NUMBER OF REALIZATIONS AND SAMPLE VARIANCE

In this work we run $N_R = 8$ simulations of a fixed $\Lambda$CDM model for each box size considered. Such $N_R$ simulations differ just by the pseudorandom number seed (just “seed” in the sequel) used by GRAPHIC2 to create the initial conditions at $z_i = 50$. These differences, magnified at lower redshift, mimic the observational discrepancies between real cosmic volumes of the same size, yielding the so-called sample variance. This section tries to predict how much the sample variance is spanned by an $N_R$ realization.

The estimator used in this paper to derive power spectra from the simulations is described at the beginning of the next section. The averaging procedure described there allows us to assume that, thanks to the central limit theorem, discrepancies, at any given $k$ value, are normally distributed.

So, let us suppose to use the $N_R$ particle distributions to determine the fluctuation spectra $P_n(k, z)$ ($n = 1, 2, \ldots, N_R$) at each $z$. A further ($N_R + 1$)th realization, in general, might yield spectra $P_{N_R+1}(k, z)$ lying among the previous $N_R$ realizations or widening their functional space. For larger $N_R$, of course, the probability of keeping within the space spanned by the $N_R$ initial spectra increases. Once $N_R$ is fixed, however, what is the
probability that \( P_{N_R+1}(k, z) \) lies among the former \( P_n(k, z) \) spectra?

This is a hard and somewhat ambiguous question; for example, we should detail when \( P_{n+1}(k, z) \) is considered to lie among the previous \( P_n(k, z) \) \((n = 1, 2, \ldots, N_R)\) spectra and how far the \( P(k, z) \) distribution is from normal.

Here we shall therefore regress to a simpler question. At a given \( z \), let us then take a generic wave number \( k \) and assume that the \( N_R \) values of the power spectrum \( P_n(k) = \phi_n \) are randomly drawn from a normal distribution (see above). Let \( \mu \) then be the mean of such \( N_R \) values \( \phi_n \), and let \( \varepsilon \) be the modulus of the maximum deviation—positive or negative—of \( \phi_n \) from \( \mu \). In this context, we try to evaluate the probability \( P_{N_R}(\varepsilon) \) that a further value \( \phi_{N_R+1} = P_{N_R+1}(k) \) differs from \( \mu \) more than \( \varepsilon \) (let us draw the reader’s attention to the difference between probabilities \( p \) and spectra \( P \), indicated with small and capital letters, respectively). This will be assumed to approach the probability that the \( N_R + 1 \)th spectrum has to lie among the previous \( N_R \).

We can derive a first estimate of the probability of a new \( P(k) \) having a value outside the range of current samples by means of the quantiles of the normal distribution. More in detail, we assume that \( \mu \) coincides with the peak of a suitable normal distribution \( G(s) \) and that the unit area below the Gaussian curve is shared in \( N_R = 8 \) equal parts so that \( N_R/2 = 4 \) values \( \phi_n \) lie at each side of \( \mu \). In the ideal case, the most distant \( \phi_n \) shares then in two equal parts the fourth (most distant) area so that the part of the area beyond the most distant \( \phi_n \) holds \( 1/(2N_R) = 1/16 \) at each side of the distribution. Summing up both sides, the area is 12.5% of the total normalized area.

Let us also outline that, if \( N_R \) is small, \( \mu \) hardly coincides with the peak of the distribution, while each \( \phi_n \) value hardly shares in two equal parts its expected interval. This admittedly rough argument, however, allows us an estimate.

In order to obtain a more reliable estimate of the expected probability

\[
P_{N_R}(\varepsilon) = 1 - G(\mu + \varepsilon) + G(\mu - \varepsilon),
\]

we make a large number (10^5) of random replicas of \( N_R \) values. In the “ideal case” described above, \( P_{N_R} \) is 0.125. After each random replica, however, we can directly measure the value to be taken, instead of 0.125, and our large number of replicas allows us to determine the frequency distribution of each \( s = P_{N_R}(\varepsilon) \) value. In this way we find that such a distribution holds the shape

\[
f(s) \propto (1 - s)^{1/n} \cdot s^m.
\]

The values

\[
n = 0.5 \times (N_R - 2) + 1.8, \quad m = 0.9 \times (N_R - 2)
\]

yield an excellent approximation to the observed distributions for \( N_R > 4 \). They are also shown in Figure 1, normalized to the unit area for \( N_R = 6, 9, 12, 15 \).

Accordingly, the expected probability

\[
\langle P_{N_R}(\varepsilon) \rangle = \frac{\int_0^1 ds \ s (1 - s)^{1/n}s^m}{\int_0^1 ds \ (1 - s)^{1/n}s^m},
\]

while, quite in general, it is

\[
\int_0^1 ds \ s^{\nu-1}(1 - s)^{\mu-1} = B(\mu, \nu) = \frac{\Gamma(\mu)\Gamma(\nu)}{\Gamma(\mu + \nu)};
\]

here \( B \) is the \( \beta \) function, while the \( \Gamma \) functions are the analytic extensions of factorials.\(^{15}\) Owing to the relation \( \Gamma(s + 1) = (s + 1)\Gamma(s) \), it is then immediately obtained that

\[
\langle P_{N_R}(\varepsilon) \rangle = \frac{1/n + 1}{1/n + m + 2}.
\]

For \( N_R = 8 \), we then obtain an expected probability of 15.88%. The complementary probability that \( \phi_{N_R+1} \) falls inside the interval \( \mu \pm \varepsilon \), approximately spanned by the first \( N_R \) values, for \( N_R = 8 \), is then \( \sim 84\% \), approximately corresponding to 1.5 standard deviations.

The conclusion that the spectra obtained from a set of eight equal simulations cover, approximately, 1.5 \( \sigma \)s in the space of

\(^{15}\) I. S. Gradshteyn & I. M. Ryzhik, Academic Press, 1980 edition: 3.191.3, 8.384.1.
possible spectra seems therefore a reasonable estimate. For a generic value of $N_R$, the ratio $\frac{p_{NNR}}{N_R}$ is shown in Figure 2. Even for the largest $N_R$ values considered here, such a ratio still stays significantly above unity.

3. FLUCTUATION SPECTRA

Fluctuation spectra like those considered in the previous section were obtained from simulations by using the algorithm PMpowerM included in the PM package (Klypin & Holtzman 1997). Through a cloud in cell (CiC) procedure, the algorithm assigns the density field on a uniform Cartesian grid starting from the particle distribution.

Here we consider effective values $n = 2^fN$ ($N = 128, 256, 512$), with $f$ from 0 to 3; for example, for $N = 128 (512)$ simulations we arrive at $n = 1024 (4096)$. As is known, such large $n$ are obtainable by considering an $N^3$ grid in a box of side $L/2^f$, where all simulation particles are inset, in points of coordinate $x_{i,f} = x_i - \nu L/2^f$, $\nu$ being the smallest integer number allowing $0 < x_{i,f} < L/2^f$ ($i = 1, 2, 3$ labels spatial coordinates).

In what follows we shall mostly report results obtained from simulations in 128 and 512 $h^{-1}$ Mpc boxes, with $n = 1024$ and 4096, respectively. Some results from the 256 $h^{-1}$ Mpc box with $n = 2048$ will only be cited in the final section.

At low $k$, the spectral values obtained from the simulations still exhibit a significant dependence on the seed yielding the initial conditions (IC). This is clearly visible in Figure 3, referring to the 128 $h^{-1}$ Mpc box. Here we make use of the spectra arising from the different seeds, dubbed $\pi, \phi, \zeta(3), \sqrt{2}, e, \gamma, \ln(2), k$; these symbols are preceded by the related box side in $h^{-1}$ Mpc. For instance, for the box with 128 $h^{-1}$ Mpc a side, the simulations 128 $\pi$ and 128 $\gamma$ (512 $h^{-1}$ Mpc) will be used. (When needed for graphic reasons, these names are shortened, e.g., by omitting the box side or even by replacing $\zeta(3)$ or $\sqrt{2}$ by $\zeta$ or $\sqrt{.}$)

In Figure 3 we considered $P(k, z)$ up to $k \approx 0.32$ $h$ Mpc$^{-1}$, or approximately up to where spectral discreteness is visible on a logarithmic plot, when plotting $\frac{P(k)}{\langle P(k) \rangle}$, the denominator being an average among different realization spectra. This then allows us to appreciate that deviations from such average, due to the seed, are persistent at all subsequent $z$, starting from initial conditions.

Little use of $\langle P(k) \rangle$ will however be made in our spectral analysis. Instead of using it, we shall instead refer to the actual realization closest to it. Then the sample variance is estimated by comparing its spectra with those of the realizations most distant from $\langle P(k) \rangle$ itself. According to the discussion in the previous section, we shall neglect the discrepancy between a full ensemble average and the eight-average considered, as well as the discrepancies between the spectra closest to $\langle P(k) \rangle$ and $\langle P(k) \rangle$ itself. Neglecting these will, however, allow us to treat the two simulations on the same footing.

![Figure 3](https://example.com/figure3.png)

Figure 3. Simulation spectra of different realizations (dubbed $\pi, \phi, \zeta(3), \sqrt{2}, e, \gamma, \ln(2), k$) in a 128 box vs. their averages at eight different redshifts: $z = 3.00$ (red), 2.20 (orange), 1.5 (yellow), 1.00 (green), 0.7 (blue), 0.35 (indigo), 0.00 (violet).
The relevance of this approximation can be better appreciated by averaging among simulation octets and comparing spectra from different box sizes, as is done in Figure 4. More precisely, in this figure we consider the ratio \( P(k, z)/P_{\text{lin}}(k, z) \) between the spectrum of simulations and the linear spectrum; we subtract from it the same ratio at \( z_{\text{IC}} \), where the IC were set; finally we average among the eight realizations obtained from different seeds for the three box sizes. This operation aims to minimize the discreteness jumps that, as seen in Figure 3, persist through redshifts, further smoothing the result by averaging among seeds. The error bars yield the sample variance at \( 1 - \sigma \).

The figure allows us to confirm that the DC term we omitted in the initial conditions implies a correction to variance substantially smaller than the expected discrepancy between estimated and actual sample variance. In fact, in the low-\( k \) almost-linear range, although some lack of power of smaller boxes seems appreciable by eye, the sample variance at all \( k \) comfortably includes the zero point; furthermore, as soon as we enter the nonlinear regime, the figure shows the lack of any apparent trend indicating that smaller box spectra have less power than larger ones. On the contrary, in the initial mildly nonlinear regime, the greatest fluctuation amplitudes are those obtained from the smallest box, while, along the whole scale range shown, the greatest box-average spectra never are the top ones (for an example of greater statistics making the DC term significant, see, e.g., the plot in Figure 6 of Heitmann et al. 2010, analogous to Figure 4).

Let us now turn to the main aim of this work: detecting the impact of variance on shear spectra \( C_{\ell}(\ell) \). To do so, we must treat each realization separately, ignoring other ones, by devising a recipe that enables us to use the spectra \( P(k, z) \), obtained from each single realization, separately.

Each single spectrum, as derived from the simulations, exhibits problems at small \( k \), as we just appreciated, as well as large \( k \) problems. The latter may be due either to lack of resolution—due to mass discreteness—or to numerical noise. In fact, the signal due to the initial lattice can cover the \( P(k) \) signal at high \( \tilde{z} \) if, as usual, the initial conditions are given on a grid rather than on a glass. The recipe to deal with this problem will be detailed in the next subsection.

Figure 4. Average of spectra after subtracting initial conditions from each of them, compared with linear growth.

Figure 5. Low-\( k \) interpolation between CAMB and numerical spectra for a box side \( L = 128 \ h^{-1} \) Mpc at \( z = 0 \). The interpolatory curve in the upper frame is obtained by displacing the CAMB spectrum upward as soon as the linear interpolation of the ratio \( R(k_z) \) (see text) exceeds unity. In the bottom plot, the \( R(k_z) \) values and its linear interpolation are shown. All units are suitable \( h^{-1} \) Mpc.

Large \( k \) problems, however, are not so essential as those found at low \( k \), which, in turn, are quite different from those faced in building an “average” nonlinear spectrum at a given approximation level, as done, for example, within the Coyote simulation suite (Heitmann et al. 2010). In fact, here we need to preserve the peculiarities derived from each specific model realization in the assigned box, which are the essential features whose impact on shear spectra we wish to gauge. In turn, at low \( k \), with each spectral point being derived by averaging over quite a limited number of realizations allowed inside the box size, significant jumps upward and downward, like those shown in Figure 3, are unavoidable.

The recipe to be used at low \( k \) will also be discussed here and detailed in the next subsections. Let us also outline that no use of perturbative expressions of mild spectral nonlinearity will be made.

As a matter of fact, a great deal of work on this subject has been carried out over the more than three decades since the Peebles (1980) book and the Bernadeu et al. (2002) review. Recent work (Crocce & Scoccimarro 2006; Anselmi & Pietroni 2012; Anselmi et al. 2012) shows that corrections to the linear spectrum approaching 1% may be present up to \( k \sim 0.003 \ h \) Mpc\(^{-1}\), that is, over scales about four times greater than those inspected by our greatest simulation box. More significantly, they extend perturbative techniques to \( k \) values well beyond the baryon acoustic oscillation (BAO) range, where nonlinearity apparently dominates.

However, apart from the difficulty of extracting from these results a handable parametric expression, such summation techniques apply to full ensemble averages. Possibly, their use could be effective in improving results obtained from averaging.
among a significant number of simulations. On the contrary, they are unlikely to apply to the results of single simulations.

Accordingly, we shall stay on the phenomenological side and make use of an expression bearing a purely analytical significance. Incidentally, when using our 512 $h^{-1}$ Mpc box, they unequivocally find that convergence on the linear results is attained for $\log(k/h\text{Mpc}$) $\sim -1.2$, in agreement with Matsubara (2008) and Carlson et al. (2009).

The basic steps of our technique are as follows. We first interpolate the linear spectra to obtain their values $P_L(k_i)$ at the very $k_i$ where the simulation spectrum $P_S(k_i)$ is calculated. We then fit the ratio

$$R(k_i) = \log[P_S(k_i)]/\log[P_L(k_i)]$$

with a curve growing linearly with $k$ for the first few points, allowing for a more detailed correction after a few of them. To do so we neglect the first point $k_1$ and refer to different numbers of $k_i$ values for the different box sizes, although selecting them through fixed rules. In order to be more precise, let us now distinguish between different box sizes.

3.1. Simulations in the 128 $h^{-1}$ Mpc Box

The hardest case is the $128^3$ particle simulations, for which we provide some more details. In this case we start from the $k_i$ values with $i$ from 2 to 6 (five values) and determine the $P$ and $Q$ coefficient minimizing the expression

$$\text{diff} = \sum_i [(P + Qk_i)/R(k_i) - 1]^2,$$

adding a specific condition, specified below. We then fit the simulation spectrum with the expression

$$\log[P_S(k)] = \log[P_L(k)] \times (P + Qk)$$

for all $k$ values where it exceeds $\log[P_L]$. The specific condition outlined above is that the spectrum must however meet the linear spectrum at any $k$ smaller than a suitable $\bar{k}$. The point is not only that nonlinear effects are surely (almost) absent below such a suitable $k$ value, but that simulations cannot provide information on possible (residual) nonlinearities for length scales $2\pi/k$ too close to the box side. For our box side of $L_{\text{box}} = 128$ $h^{-1}$ Mpc, we then take $\bar{k} = 0.1$ $h$ Mpc$^{-1}$ (yielding a length scale $\sim L_{\text{box}}/2$).

Figure 5 gives more details and shows the results of this operation. In the upper panel we show the overall interpolation (magenta curve). In the lower panel we show the ratios $R(k_i)$ and their linear interpolation $P + Qk$, to be used where it exceeds unity (the magenta line). This technique is meant to preserve the BAO structure outlined by the linear algorithm, just suitably shifting it upward, according to the requirements coming from the first $k_i$ values in the simulation.

We then consider six more points and allow for a correction to $P + Qk$ by a term $R(k - k_6)^2$, $R$ and $\alpha$ being again determined through a least-squares fit. This is meant to allow a progressive rise of the spectral steepness, following the gradual incoming on nonlinear dynamics. Accordingly, this approach must be gradually modified at higher $z$, when nonlinear dynamics does not yet affect smaller $k_i$ values. As a matter of fact, at fairly large $z$ values, not only may the $P$ and $Q$ coefficients turn out to be quite small, but there may be no need for power-law corrections. Then, if $P_{fi}(k)$ exceeds $P_S(k)$ in two —or more— $k$ points ($7 \leq i \leq 12$), we shall deal with these points as we do with those above the 12th, as described below.

In Figure 6 we show the limits on the $k$ axis of the two above intervals, both in this case and for the forthcoming 512 $h^{-1}$ Mpc box.

Starting from $k_n$ with $n \geq 13$, we then perform a Savitski–Golay (SG) interpolation. More precisely, we consider 2$p$ values $k_{n\pm j}$ ($j = 1,...,p$), plus $k_n$ itself, and interpolate them to obtain $2p + 1$ equispaced points on a log $k$ scale, with extremes in $k_{n \pm p}$. In this way we work out a spectral value for $k_i = 10^{[\log(k_{n-r}) + \log(k_{n+r})]/2}$, a point quite close to $k_n$ but not coinciding with it. The values of $p$ go from 4 to 8, suitably increasing toward larger $k_n$ values.

Before moving on to briefly describing the large-$k$ treatment, let us still outline that the same treatments are reserved to all seeds. In particular, when $P_{fi}(k)$ exceeds $P_S(k)$ for almost two $k$ points ($7 \leq i \leq 12$) in one simulation, we start operating an SG interpolation for all of them.

As far as large $k$ and low $z$ are concerned, resolution problems begin to damp the spectrum at $k/h$ Mpc$^{-1} \sim 3$. In contrast, at large $z$, numerical noise cancels spectral features; for example, at $z = 2.8$, this occurs at $k \sim 5$.

The problems we meet, therefore, concern a range where a physical signal cannot be predicted by using gravitation only. Accordingly, our treatment is meant just to test the sample information on possible (residual) nonlinearities for length scales $2\pi/k$ too close to the box side. For our box side of $L_{\text{box}} = 128$ $h^{-1}$ Mpc, we then take $\bar{k} = 0.1$ $h$ Mpc$^{-1}$ (yielding a length scale $\sim L_{\text{box}}/2$).

Figure 5 gives more details and shows the results of this operation. In the upper panel we show the overall interpolation (magenta curve). In the lower panel we show the ratios $R(k_i)$ and their linear interpolation $P + Qk$, to be used where it exceeds unity (the magenta line). This technique is meant to preserve the BAO structure outlined by the linear algorithm, just suitably shifting it upward, according to the requirements coming from the first $k_i$ values in the simulation.

We then consider six more points and allow for a correction to $P + Qk$ by a term $R(k - k_6)^2$, $R$ and $\alpha$ being again determined through a least-squares fit. This is meant to allow a progressive rise of the spectral steepness, following the gradual incoming on nonlinear dynamics. Accordingly, this approach must be gradually modified at higher $z$, when nonlinear dynamics does not yet affect smaller $k_i$ values. As a matter of fact, at fairly large $z$ values, not only may the $P$ and $Q$ coefficients turn out to be quite small, but there may be no need for power-law corrections. Then, if $P_{fi}(k)$ exceeds $P_S(k)$ in two

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**Figure 6.** Points indicate the $k_i$ for which $P_S$ spectra are obtainable, when using a 128 or 512 $h^{-1}$ Mpc box. Vertical lines indicate the limits of the three intervals where $P_S$ is interpolated with $P_L$, according to procedures outlined in the text. For the 128 (512) $h^{-1}$ Mpc box, the number of points in the two intervals is 6 (11).

16 Numerical Recipes, Cambridge U. Press 1986, 1992; Section 14.8.
3. Simulations in the $h\text{Mpc}^{-1}$ Box

The same technique used for the smaller box is now extended to this wider box to allow for a linear/nonlinear connection. In Figure 6 we compare the range of $k$ values used in the two cases. The number of “points” used in the low-$k$ intervals is now 11. Attempts performed with close numbers of points (e.g., 10 or 12) yield greater fitting residuals.

Figure 9 is then analogous to Figure 7, although spectral “points” here extend down to smaller $k$ values, just marginally nonlinear. These points are indeed obtained by averaging over a limited number of realizations, so the sample variance is large and partially hides nonlinearity itself. In the inner box this scale range is magnified, also showing the smoothness of the linear/nonlinear interpolated red and green curves, although crossing a few times.

The overall situation is more clearly outlined by Figure 10, analogous to Figure 8; notice, however, the reduced range of the ordinates. Here we clearly distinguish the effects due to the limited number of realizations at low $k$, which persist through all $z$ without an appreciable amplitude growth, from the actual sample variance between the two seeds, in the $k$ interval $(-0.6 \sim +0.7)$, steadily growing because of nonlinearity: at $z = 2.6$ the spectral ratio is still $\sim 1\%$; at $z = 0$ it finally reaches $5.32\%$ (evaluated with the same criterion as in Figure 8).

4. TOMOGRAPHIC WINDOWS

Let us now investigate how these variance effects transfer from fluctuation to shear spectra. To do so, let us build the needed tomographic windows, by starting from the expression of the background metric reading

$$ds^2 = a^2(\tau)\left[d\tau^2 - d\mathbf{\xi}^2\right].$$

Figure 7. Spectra obtained from simulations in a box with $L = 128 \text{ h}^{-1} \text{ Mpc}$ a side, interpolated with linear CAMB outputs. The main feature shown in this figure is the significant discrepancy between the two seeds, dubbed $128\gamma$ (closest to average) and $128\epsilon$ (farthest from average and smaller than it). Magenta and black points, respectively, yield the resulting simulation outputs. From CAMB and them we derive the green and red spectra (also respectively), as explained in the text.

Figure 8. Ratio between the spectra derived from the seeds $128\epsilon$ and $128\gamma$ at the redshifts indicated in the frames. The top discrepancy shown, at $z = 0$ and $k/(h \text{ Mpc}^{-1}) \sim 0.65$, is $\approx 57.4\%$.

Figure 9. Spectra obtained from simulations in a box with $L = 512 \text{ h}^{-1} \text{ Mpc}$ a side, interpolated with linear CAMB outputs. The seeds closest and farthest from (mostly greater than) average are those dubbed $512\sqrt{2}$ and $512\gamma(3)$. Here again, the spectra in black are CAMB outputs. Black and magenta points yield actual simulation outputs. From CAMB and them we derive the red and green spectra (respectively), as explained in the text. Notice also the significant spectral discrepancy occurring at small $k$ values, magnified in the inner box; for a significant $k$ interval, its sign is opposite that of the main trend, as the very “points” of spectrum A, which lay above the “points” of spectrum E.
the filters
\[
\Pi_r(z) = \int_{z_r}^{z_{r+1}} dz' \frac{\exp \left[ -\frac{(z - z')^2}{2 \sigma^2(z)} \right]}{\sqrt{2\pi} \sigma(z)}
\]

\[
= \frac{1}{2} \left[ \text{Erf} \left( \frac{z_{r+1} - z}{\sqrt{2 \sigma(z)}} \right) - \text{Erf} \left( \frac{z_r - z}{\sqrt{2 \sigma(z)}} \right) \right]
\]

to \(n(z)\). In this way we obtain the distributions

\[
D_r(z) = n(z) \Pi_r(z)
\]

whose integrals are \(\approx 1/\mathcal{N}\). In this work we shall take \(\sigma(z) = 0.05 (1 + z)\), coherently with EUCLID expectations (Amendola et al. 2013; see also Casarini et al. 2011); the distributions \(D_r\), when normalized to unity, are then dubbed \(\delta_r\).

They are used to define the window functions

\[
w_r(u) = \frac{3}{2} [1 + z(u)] \int_u^\infty du' \delta_r(u') \frac{u' - u}{u'}
\]

also shown in Figure 11.

5. SHEAR SPECTRA

Shear spectra are then related to the power spectra \(P_{\delta}(k, u) \equiv P[k, (z(u))]\), through the relation

\[
C_\psi(\ell) = \left( H_0^2 \Omega_0 \right)^2 \int_0^\infty du w_r(u) w_r(u) P_\delta(\ell/\ell, u)
\]

Integrals are performed by using a modified Riemann algorithm with 10,000 equispaced integration points \(u_0\) up to \(u_{\text{top}} \approx 9000\) (instead of \(\tau_0\)). Integration results are visually indistinguishable from those obtained with just 400 points, and, for this case, in Figure 12 we show the points selected on the log \(k\)--log \(\ell\) plane for a subsample of \(\ell\) values, lying along tilted straight lines.

Integration therefore requires interpolation of \(w_r(u)\) at \(u_0\), and of \(P_\delta\), first along \(k\) and then again along \(u\). A number of cases are then considered: for 5 and 10 tomographic bands; for simulations in 128 (256) and 512 \(h^{-1}\) Mpc boxes, with the resolution pushed up to 1024 (2048) and 4096 points, respectively; and for those two seeds, selected for each box size, for being closest to and farthest from average.

5.1. Shear Spectra from Simulations in the 128 \(h^{-1}\) Mpc Box

In Figure 13 we plot the shear spectra obtained from the fluctuation spectra arising from the seed 128\(g\), in the case of a 5-band tomography. Beside them we also show (black dotted curves) the spectra obtainable from 128e. In Figure 14 we then show the spectra for a 10-band tomography obtained from 128e.

The discrepancy between seeds is better visible in Figures 15 and 16, for the 5- and 10-band cases, respectively. These plots allow us two comments: (1) the shear spectra discrepancy is substantially independent from the number of bands and reaches 24.7% for \(C_{11}\) for a 5-band tomography; this top discrepancy is estimated similarly to \(P_\delta\) spectra, by averaging over \(\ell\) with \(\mathcal{N} = 10\); (2) if we remember that shear spectra are obtained by integrating over redshift, thus including contributions from \(P_\delta\) up to \(z \approx 2\), we appreciate that no substantial decrement of spectral discrepancy occurs when passing from fluctuation to shear spectra.
5.2. Shear Spectra from Simulations in the $512\, h^{-1}\, \text{Mpc}$ Box

Discrepancies, as expected, are significantly smaller when a larger simulation box is used. In Figure 17 we plot the shear spectra obtained from the $512\zeta (3)$ seed, in the case of a 5-band tomography. As in the smaller box case, we overlap these spectra with those obtainable from the $512\sqrt{2}$ seed, which is the most distant from average and, in this case, exceeds the average. Discrepancies, however, are quite hard to perceive in this way.

Figure 11. Expected distributions on redshift of galaxies belonging to different bands (lhs) and related filters (rhs). Upper (lower) panel refers to the 5 (10) band case.

Figure 12. Integration patterns for a number of \( \ell \) values between 5 and 3300. The points indicated are those used in the case of Riemann integration with 400 points (yielding results visually indistinguishable from those with more points). The red dashed line is the limit beyond which (just a few) integrand values are to be obtained by interpolation. In the right frame we show the patterns of window functions \( w_{i}(u) \) in the case of five bands.

Figure 13. Solid lines yield the shear spectra $C_{ij}(\ell)$ for the $128\gamma$ seed, in the case of a 5-band tomography. The colors account for $i,j$ indices. Almost overlapped with them, we also plot the spectra obtained from the $128e$ seed (black dotted curves), thus outlining the significant discrepancies between the two seeds.
In Figure 18 we then plot shear spectra $C_{ij}(\ell)$ in the case of a 10-band tomography, as obtainable from the $512\sqrt{2}$ seed. In Figures 19 and 20, we finally plot the ratios between the shear spectra obtained from the simulations $512\zeta(3)$ and $512\sqrt{2}$ in the cases of 5 and 10 bands.

Tiny oscillations in the curve arise from residual oscillations of $P_3$, visible here because of the reduced amplitude of the overall ratio; when comparing Figures 19 and 20 with Figures 15 and 16, also take notice of the reduced range of the ordinates.

Once again we appreciate that discrepancies are almost independent of the number of tomographic bands, and their top value is $\sim 3.32\%$.

Let us finally outline the peculiar feature that ratios exhibit at low $\ell$, where they become less than unity. As a matter of fact, at low $k$, the very ratio between $P_3$ spectra exhibits significant oscillations about unity (see Figure 10), smeared out by the integrals (16), yielding the prevailing contribution, in a direction opposite the main trend at greater $k$.

These kinds of peculiarities become more and more significant as we go to larger boxes and, consequently, also to smaller bulk discrepancies. If making use of different seeds, for which such bulk discrepancy is however smaller, we find similar anomalies. The essential point is that they fall in a region necessarily separate from that, allowing us the basic estimate of top discrepancies.
6. DISCUSSION AND CONCLUSIONS

This paper makes use of sets of $\Lambda$CDM $N$-body simulations to investigate sample variance, in view of the possible use of ad hoc simulations to fit data exhibiting evident deviation from GR or other peculiar effects due to the nature of the dark components.

Such evidence could be derived from the analysis of weak lensing data. Accordingly, the effects of sample variance on tomographic shear spectra are also inspected.

Our analysis is based on eight $N$-body simulations in boxes of increasing side $L$. According to simple probabilistic arguments, the spread between their results approaches $\sim 1.5 \sigma$. Experiments in progress plan to achieve a precision of $\sim 1\%$; accordingly, the size of the simulation box and the related resolution should enable us to reach the same precision, at least.

In Figure 21 we then plot the maximum discrepancies between the “most distant” realizations considered as a function of the box size. The $k$ values where they arise lie in the spectral region where $k$ discreteness is still relevant. This is so, in spite of their being damped by our procedure, using sets of simulation points to “bend” linear spectra to account for the rise of nonlinearity. More precisely, in Figure 21, we consider the ratios $R = \log(P^{(3)}(z=0)/P^{(0)}(z=0))$ (in blue) or $\log(C^{(1)}_{ij}/C^{(2)}_{ij})$ (in black); the apices refer to the two seeds considered (closest and farthest from average) for each box size. Such ratios overcome unity by an amount which,
multiplied by 100, yields the percent discrepancy. This surely yields values greater than an estimate referring to spectral covariance, based on averaging among discrepancies, as was done by previous authors (see, in particular, Takahashi et al. 2009). In Figure 21 we show that the percent discrepancy between the most distant realizations decreases almost linearly with the box side, being cut by a factor of \(~0.35\sim0.45\) when the side doubles. This is true both for \(P_i(k)\) and \(C_{ij}(\ell)\).

The decrease is surely expected, as the number of realizations considered within each box increases with the box size. An analogous decrease is shown, for example, in Figure 12 of Takahashi et al. (2009), although they plot spectral covariance, and their increase in the realization number arises from increasing the number of equal-size boxes taken, within a very large number of independent simulation boxes.

Being wider, however, the size of our dependence on the box side is safer, with respect to varying the IC in a set of eight simulation boxes. An estimate of such residual dependence is obtainable from the apparent deviation of the \(L\) dependence from linear. In Figure 21 and for the \(C_{ij}\) discrepancies, two dashed lines frame the expected interval for a linear behavior. If we assume that the uncertainty of each estimate is set by the width of such interval, we find \(~13\%)%. Similarly, for \(P(k)\), we find \(~15\%).

If we extrapolate the linear behavior to seek where realization discrepancies within an eight-box set, defined according to our criterion, are expected to lie below \(1\%\), we find a box side in the range \(1300\sim1700\ h^{-1}\) Mpc, within the allowed range of slopes. It is also clear that discrepancy estimates do not depend just on box size, but also on mass and force resolution. Our choice is however a typical one, meant to optimize the results of the numerical effort.

This leads us to conclude that a set of eight simulations in a box with \(512\ h^{-1}\) Mpc a side is still insufficient to provide a unbiased test for any model. If the desired precision level ranges around \(1\%\), such an aim might, however, be approached with a box side \(~3\sim4\) times greater, staying at the same resolution level and, therefore, accordingly increasing the dynamical range.

As many researchers previously did, for example, to provide spectral estimators (see, e.g., Lawrence et al. 2009, 2010; Heitmann et al. 2010, 2014), one could prefer to run a large number of simulations in smaller boxes, aiming to examine the same number of realizations without expanding so far the required dynamical range. For instance, one could replace the eight boxes \(~1700\ h^{-1}\) Mpc a side, with \(~300\) boxes with \(~500\ h^{-1}\) Mpc a side or \(~60\sim70\) realizations in boxes with \(~800\ h^{-1}\) Mpc a side.

A first point to outline is then that including the impact of DC modes, that is, of wavelength wider than the simulation box, marginally irrelevant when the statistics is limited to eight boxes, would then become indispensable.

Changing the box size, however, bears a further consequence, as the density of values along the \(k\) axis is bound to vary. Changing the discrete mode set in the simulation will then affect the covariance of the three-dimensional mass density. In turn, this affects the covariance of the mass density power spectrum. These mode-coupling effects were first outlined by Hamilton et al. (2006) (see also recent results by Takada & Hu 2013 and Li et al. 2014).

Sample variance is directly connected to that, so we cannot restrict ourselves to barely counting the number of realizations as a function of the overall volume. This point is to be borne in mind and carefully weighed when a further effort to attain a \(C_{ij}\) prediction at precision level \(\Delta(1\%)\) is deployed.

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