Validating galaxy clustering models with Fixed & Paired and Matched-ICs simulations: application to Primordial Non-Gaussianities

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ABSTRACT

The Fix and Pair techniques were designed to generate simulations with reduced variance in the 2-point statistics by modifying the Initial Conditions (ICs). In this paper we show that this technique is also valid when the initial conditions have local Primordial non-Gaussianities (PNG), parametrised by $f_{NL}$, without biasing the 2-point statistics but reducing significantly their variance. We show how to quantitatively use these techniques to test the accuracy of galaxy/halo clustering models down to a much reduced uncertainty and we apply them to test the standard model for halo clustering in the presence of PNG. Additionally, we show that our techniques were designed to generate simulations with reduced variance in the 2-point statistics by modifying the Initial Conditions (ICs) for two different cosmologies (Gaussian and non-Gaussian) we obtain a large correlation between the (2-point) statistics that can explicitly be used to further reduce the uncertainty of the model testing. For our reference analysis ($f_{NL} = 100$, $V = 1 [h^{-1} \text{Gpc}]^3$, $n = 2.5 \times 10^{-4} [h^{-1} \text{Mpc}]^{-3}$, $b = 2.32$), we obtain an uncertainty of $\sigma(f_{NL}) = 60$ with a standard simulation, whereas using Fixed [Fixed-Paired] initial conditions it reduces to $\sigma(f_{NL}) = 12 [\sigma(f_{NL}) = 12]$. When also Matching the ICs we obtain $\sigma(f_{NL}) = 18$ for the standard case, and $\sigma(f_{NL}) = 8 [\sigma(f_{NL}) = 7]$ for Fixed [Fixed-Paired]. The combination of the Fix, Pair and Match techniques can be used in the context of PNG to create simulations with an effective volume incremented by a factor $\approx 70$ at given computational resources.

Key words: cosmology: large-scale structure of the Universe – galaxies: haloes – cosmology: theory – cosmology: inflation

1 INTRODUCTION

Cosmological simulations are routinely used in cosmology, specially in studies of the Large-Scale Structure (for a recent review, see Angulo & Hahn 2022). They can be used to help developing analysis methodology (e.g. Ross et al. 2017; Chan et al. 2022; Avila et al. 2022), validate and compare the performance of different tools (e.g. Avila et al. 2020; Alam et al. 2021; Rossi et al. 2021), understand the impact of observational systematic effects (e.g. Rosell et al. 2022; Spinelli et al. 2022) or to compute covariance matrices (e.g. Manera et al. 2013; Avila et al. 2018; Zhao et al. 2021).

When testing models of galaxy clustering, we are limited by the intrinsic uncertainty associated to the simulation we are using, given by cosmic variance and shot-noise. In order to reduce this, one could increase arbitrarily the simulated volume. However, given that we typically want to focus on the halo mass-range given by a reference galaxy survey, if we keep the mass resolution constant, this process rapidly becomes prohibitively computationally expensive.

In order to alleviate this, the Fix & Pair technique was proposed in Angulo & Pontzen (2016). Fixing consists on setting the amplitude of the overdensity modes in the Initial Conditions (ICs) to its expectation value (without any variance), whereas Pairing consists on running a second simulation with the initial phases Inverted (shifted by $\pi$) with respect to the first one. This technique has extensively studied and was shown to recover unbiased statistics for late-time observables such as the 1-point (halo mass function, luminosity functions, etc.), 2-point (power spectrum and correlation function of dark matter and biased tracers such as halos), 3-point statistics, etc. Additionally, many of those statistic show a decrement of their variance, which is particularly drastic in the 2-point statistics (Angulo & Pontzen 2016; Villaescusa-Navarro et al. 2018; Chuang et al. 2019; Zhang et al. 2021; Maion et al. 2022). This reduction of the variance, which is particularly concentrated at large scales in the power spectrum, can be used to validate models of the Large-Scale Structure (LSS) with increased accuracy for the same computational cost.

Another way to reduce the effective variance when validating models with simulations is to Match the stochastic part of the ICs in simulations with different cosmologies. This induces correlation between the measured clustering, with the cosmic variance partly cancelling when, for example, dividing the clustering of two simulations. This is mentioned in several works like Smith & Angulo (2019), however, the correlation coefficient was not explicitly applied to reduce the uncertainty in the analysis. The correlation between Matched-ICs of simulations has been explicitly used in the CARPool method (Chartier et al. 2021; Ding et al. 2022) but, in that case, between high-fidelity mocks and approximate mocks, in order to retrieve unbiased precise clustering statistics from the approximate mocks. Here, we propose a framework to explicitly use the correlation between simulations with Matched-ICs across different cosmologies to reduce the
expected variance of the summary statistic and to constrain models to an increased accuracy.

Both of those techniques are particularly promising for large-scale clustering. One interesting observable at very large scales is the local Primordial Non-Gaussianities (PNG), parametrised by $f_{\text{NL}}$, which will serve us to illustrate the methods proposed here.

PNG is one of the observables of cosmic inflation: whereas the simplest models predict a level of local-PNG below $O(f_{\text{NL}}) = 1$, more complex models (in particular multi-field inflation), predict larger PNG (Creminelli & Zaldarriaga 2004; Pajer et al. 2013; Byrnes & Choi 2010). Whereas Planck CMB experiment $^1$ constrained local-PNG down to $f_{\text{NL}} = -0.9 \pm 5.1$ (Planck Collaboration et al. 2020b), the precision is near the expected cosmic variance limit, with some room for improvement with polarisation experiments (Baumann et al. 2009). However, future surveys of the LSS (or their combination), such as SKAO$ ^2$ (SKA Cosmology SWG et al. 2020), LSST-Rubin$ ^3$ (LSST Science Collaboration et al. 2009; The LSST Dark Energy Science Collaboration et al. 2018) or SphereX$ ^4$ (Doré et al. 2014, 2018) are expected to break the $\sigma(f_{\text{NL}}) = 1$ barrier (Yamauchi et al. 2014; Alvarez et al. 2014; de Putter & Doré 2017), opening a new window to understand inflation.

One of the most promising ways to constrain PNG is by using the scale-dependent bias that it induces at very large-scales on the power spectrum (Dalal et al. 2008; Slosar et al. 2008; Matarrese & Verde 2008). Over the last decade, measurements of the 2-point functions of the LSS has led to increasingly precise constraints (Slosar et al. 2008; Ross et al. 2012; Giannantonio et al. 2014; Ho et al. 2015; Leistedt et al. 2014; Castorina et al. 2019), with the most precise measurements given by the clustering of eBOSS$ ^5$ quasar clustering: $f_{\text{NL}} = -12 \pm 21$ (Mueller et al. 2022; Rezaie et al. 2021). Recently, Cabass et al. (2022) put similar constraints ($f_{\text{NL}} = -33 \pm 28$) by combining power spectrum and bispectrum using BOSS$ ^6$ galaxies, opening another promising path for more voluminous surveys.

By Fixing the amplitude of the initial conditions, we are actually introducing a type of non-Gaussianity, since we are substituting the Rayleigh distribution of the amplitude of the modes in Normal Gaussian simulations by a Dirac delta. Hence, the first goal of this paper is to demonstrate that the Fix ($&$ Pair, although this part does not pose any a priori issue) technique can be safely used with local Primordial Non-Gaussianities.

The second goal is to demonstrate with a practical example how to validate models of halo clustering (extendable to galaxy clustering) using Fixed & Paired simulations to a reduced uncertainty. Finally, we also show how to explicitly use the correlation of the cluster-istics to validate models of halo clustering (extendable to galaxy clustering).

Inverting the potential can be related by:
\[ \delta(k, z) = \alpha(k, z)\Phi(k), \]
where we have defined
\[ \alpha(k, z) = \frac{2D(z)}{3\Omega_m(z) H_0^2 g(z_{\text{rad}})} \frac{g(0)}{g(\mu)} k^2 T(k), \]
d\[ D(z) \] is the growth factor normalized to $D(z = 0) = 1$ and $T(k)$ the transfer function (with $T(k \rightarrow 0) = 1$, LSS convention). The factor $\frac{g(0)}{g(\mu)} = 1.31$ (for the cosmology described in subsection 3.1) takes into account the difference between the LSS normalization of $D(z)$ with respect the early-time normalisation to $D(z) = 1/(1+z)$ during matter-domination.

Then, ICs can be generated as random realisations of a Gaussian distribution:
\[ \Phi_i(k) \sim N(\Phi_i(k); \mu = 0, \sigma^2 = P(k)/\alpha^2), \]
with $\sim$ denoting its complex nature in Fourier space and $\mu$, $\sigma^2$ and $P(k)/\alpha^2$ are the mean and variance of the Gaussian realisations. The main ingredients of the methodology discussed in the paper stems from choosing the way we generate the ICs that we input to the $N$-Body gravity solver to generate the simulations. Here we discuss how to generate the ICs in a normal Gaussian case, how this gets modified with the Primordial Non-Gaussianities, how to set Fixed and Paired ICs and the role of the stochastic part of the ICs in the matching.

### 2.1 Gaussian Initial Conditions

In the standard simulations, the initial conditions are generated from Gaussian realisations of the overdensity field $\delta(k)$ whose variance is given by the power spectrum $P(k)$. Equivalently, one can express these initial conditions in terms of the primordial gravitational potential $\Phi$. For clarity when introducing later the PNG and the Fix technique, we will express the ICs in terms of the latter.

The time late linear overdensity and the primordial gravitational potential can be related by:
\[ \delta(k, z) = \alpha(k, z)\Phi(k), \]
are sampled from a probability distribution function (right). Alternatively, $\Phi$ can be decomposed into modulus and phases $|\Phi|$, $\varphi$. The modulus, then, follows a Rayleigh distribution:

$$|\Phi(k)| \sim \mathcal{P}_{\text{Rayleigh}}(|\Phi(k)|) = \frac{\Phi(k) |\alpha|^2}{P(k)} \exp \left(\frac{-|\Phi(k)|^2 |\alpha|^2}{2 P(k)}\right),$$

and the phases $\varphi$, a uniform distribution between 0 and $2\pi$

$$\varphi_i \sim \frac{1}{2\pi} \Theta_{[0, 2\pi]}(\varphi).$$

The $i$ denotes that it is a random realisation, given by a seed in our code. This seed is changed for different realisations of the simulations. If we Match the random seed for different cosmologies ($f_{\text{NL}} = 0$ and $f_{\text{NL}} = 100$ in our case), we will be using the same phases $\varphi_i$ and the same relative excess/decrement in amplitude of modes with respect to their expectation value: $|\Phi(k)| \sim |\alpha|/\sqrt{P(k) \cdot \pi/2}$. Hence, sharing great part of the noise realisation.

Finally, these perturbations of the Newtonian potential $\Phi$ (or equivalently in the overdensity field) are used to compute the displacements and velocities of the dark matter particles through the second-order Lagrangian Perturbation Theory (2LPT, Bouchet et al. 1995). For that, we use the public code 2LPTic (Crocce et al. 2006, 2012) to generate the initial conditions.

### 2.2 Local Primordial Non-Gaussianities

For a Gaussian random field, all the information is contained in the 2-point statistics, with the higher order ones vanishing. For most models of inflation, the primordial field $\Phi$ follows a nearly Gaussian distribution. Then, small Primordial Non-Gaussianities are parametrised by $f_{\text{NL}}$, which quantifies the level of non-Gaussianity associated to the primordial bispectrum. Other higher contributions are quantified by other parameters such as $g_{\text{NL}}$ or $\tau_{\text{NL}}$ which we do not explore here.

The primordial bispectrum can take different shapes, depending on the ratios of the different modes considered. The simplest configuration to study is the local PNG, which modifies the primordial potential perturbations as (Komatsu & Spergel 2001; Salopek & Bond 1990):

$$\Phi(x) = \Phi_G(x) + f_{\text{NL}} \Phi_G(x)^2 - \Phi_G^2,$$

where $\Phi_G$ represents a Gaussian gravitational field, as described in the previous subsection, and $\Phi$ now represents the Non-Gaussian gravitational field, which can be related to the non-Gaussian linear overdensity by Equation 1. We will drop the $\text{loc}$ label for most cases in this paper, as we will be referring by default to local PNG. We remark that Equation 6 describes a modification in configuration space, whereas most of the equations described earlier refer to Fourier space. It has been shown (Komatsu & Spergel 2001) that this type of non-Gaussianities leads to a primordial bispectrum given by

$$B(k_1, k_2, k_3) = f_{\text{NL}} 2 (P(k_1) P(k_2) + P(k_2) P(k_3) + P(k_3) P(k_1)).$$

The local PNG (and other types of PNG) are already implemented in 2LPTic as described in Scoccimarro et al. (2012).

### 2.3 Fix and Pair techniques

Angulo & Pontzen (2016) proposed to Fix the amplitude of the initial perturbations to their expectation value in the ICs in order to reduce the variance associated to simulations. Mathematically, this means substituting the Rayleigh PDF (Equation 4) by a Dirac delta:

$$|\Phi(k)| \sim \frac{1}{2\pi} \delta_D(|\Phi(k)| - \sqrt{P(k) \cdot \pi/2}/|\alpha|).$$

From now on, we will refer to these simulations as Fixed, whereas the simulations whose ICs follow a Rayleigh distribution will be tagged as Normal. We note that, whereas there is not any stochasticity left in the amplitude of the ICs modes, the phases $\varphi_i$ will still be random realisations (Equation 5).

By describing the ICs in terms of $\Phi$, Equation 8 can be directly applied to the Gaussian and local-PNG cases. In the local-PNG case we apply Equation 8 to the Gaussian component and subsequently we apply the quadratic correction in Equation 6.

Both Equation 6 and Equation 8 represent a modification to the Gaussian ICs. Hence, it is one of the goals of this paper to demonstrate that these two techniques can be safely used together and that the Fixed technique does not introduce any significant spurious PNG signal.

### 3 THE HALO CLUSTERING WITH FIXED & PAIRED PNG SIMULATIONS

#### 3.1 The Goliat-PNG simulation suite

The GOLIAT-PNG simulation suite builds on previous existing runs used for Avila et al. (2015) and Wang et al. (2020). For this reason, we take for reference the cosmology of WMAP-7 (Komatsu et al. 2011) shown Table 1 and a resolution of $512^3$ particles in a $V = 11 h^{-1} \text{Gpc}^3$ box. We run the initial conditions with the 2LPTic (see also section 2). Then, we evolve those ICs with the public gravity solver GADGET2 down to $z = 1$. Finally, we identify halos with the Amiga Halo Finder and use halos with a minimum of 10 particles, which gives us a number density of $n = 2.5 \cdot 10^{-4} \text{Mpc}^{-3} h^3$.

7 cosmo.nyu.edu/roman/2LPT (Crocce et al. 2006; Scoccimarro et al. 2012; Crocce et al. 2012)
8 https://wwwmpa.mpa-garching.mpg.de/gadget/ (Springel 2005)
9 http://popia.ft.uam.es/AlF/ (Knollmann & Knebe 2009)
We focus on the redshift $z = 1$ snapshot, as running the simulations down to $z = 1$ requires about half of the time of that required to run them to $z = 0$. Additionally, large observational surveys with promising forecasts on PNG will focus on the $z \geq 1$ Universe in order to probe larger volumes. We note that, even though the used cosmology is ruled out by current observational constraints (Planck Collaboration et al. 2020a,b) and the limited resolution could have an effect on derived parameters such as $p$ (PNG response, see subsection 4.1), the focus of this work is on the methodology to increase the resolution of the derived constraints by using the Fix, Pair & Match techniques, and to verify that the Fixing can be applied to PNG simulations in the same way as we do for the Normal ones.

We run 41 different realisations for the $f_{\text{NL}} = 0$ and $f_{\text{NL}} = 100$ cosmologies for 4 cases:

- **Normal-Original**.
- **Normal-Inverted**.
- **Fixed-Original**.
- **Fixed-Inverted**.

### 3.2 Mean halo power spectrum with the Goliat-PNG simulations

Here, we will validate the usage of Fixed PNG simulations in order to study the halo power spectrum. We leave a more detailed validation, considering other statistics, to Appendix A.

We compute the power spectrum of the Goliat-PNG halo catalogues with NBodykit. In Figure 1, we represent the halo power spectrum of the Goliat-PNG simulations for $f_{\text{NL}} = 0$ and $f_{\text{NL}} = 100$. We find that, for both cases, the average power spectrum is consistent between the Normal simulations and the Fixed simulations. Whereas this has already been extensively studied for the case of $f_{\text{NL}} = 0$ (Chuang et al. 2019; Villaescusa-Navarro et al. 2018; Maion et al. 2022), this is the first time this is shown for the local PNG case with $f_{\text{NL}} \neq 0$. This is important since the Fixed technique itself introduces a type of non-Gaussianity in the initial conditions. Nevertheless, Figure 1 shows that the ratios of the Normal to Fixed results (within the noise level) are found very similar for the $f_{\text{NL}} = 0$ and $f_{\text{NL}} = 100$ cases. Hence, we find no evidence that the Fix technique for local PNG needs any special consideration. Additionally, it is worth noting that the goal of the paper focuses on the power of a single realisation to constrain cosmological parameters. Hence, our reference scatter is the light-shaded region.

The **Normal-Original** and the **Normal-Inverted** simulations are statistically equivalent by construction, hence, they have the same expectation values for any statistics. It is only when combining both that we expect modifications on the variance of, for example, the power spectrum. The same happens with the **Fixed-Original** and the **Fixed-Inverted** cases. To verify this, we also show in the bottom panels of Figure 1 the comparison between the **Original** and the **Inverted** simulations, finding negligible statistical differences. For the rest of the paper, we will always consider the average of all the **Normal** (Original+Inverted) or Fixed (Original+Inverted) simulations, when referring to the average statistics. The next subsection will describe how we deal with the variance.

### 3.3 Halo power spectrum variance of the Goliat-PNG simulations

For the case of a Gaussian density field with a given power spectrum $P(k)$ and discretised with a Poisson-law to a number density $n$, the expected variance over a volume $V$ is given by (Feldman et al. 1994; Blake 2019)

\[
\sigma_{\text{th}}(k)^2 = \frac{4\pi^2}{V k^2 \Delta k} \left(P(k) + \frac{1}{n}\right)^2.
\]

Where $\Delta k$ is the bin width over which the power spectrum $P(k)$ has been measured.

The **Fixed** and **Paired** technique was introduced in Angulo & Pontzen (2016) precisely to reduce that variance on simulations. On the one hand, fixing the amplitude of the primordial overdensities, reduces de variance of the late-time overdensities. On the other hand, pairing two simulations with inverse phases cancels out certain terms, reducing again the variance (see Angulo & Pontzen 2016; Maion et al. 2022).

From this point, when we refer to results derived from the **Paired** simulations (either **Normal** or **Fixed**), it means that we have taken the average of each simulation with its **Inverted** partner:

\[
P_{\text{Paired,}i}(k) = \frac{1}{2} \left(P_{\varphi_i}(k) + P_{\varphi_i+\pi}(k)\right).
\]

When we compute the standard deviation of **Paired** simulations, we first average over the couple, then compute the standard deviation and finally, multiply by $\sqrt{2}$ to compensate for doubling the volume:

\[
\sigma_{\text{Paired}} = \sqrt{2} \cdot \text{std} \left(\frac{1}{2} \left(P_{\varphi_i}(k) + P_{\varphi_i+\pi}(k)\right)\right).
\]

In Figure 2, we show the standard deviation obtained from the 41 cases of **Normal**, **Fixed**, **Normal-Paired** and **Fixed-Paired** simulations (the last two, using Equation 12). On the solid red line, we also represent the theoretical Gaussian expectation, given by Equation 10.

We find that the scatter of the **Normal** simulations (red) is well described by Equation 10, at least at large scales. On the other hand,

\[\text{https://github.com/bccp/nbodykit}, (Hand et al. 2018)\]
the **Fixed** simulations present a large reduction at small $k$, as expected and previously found. Remarkably, whereas the **Fixed-Paired** case shows a slight further reduction at intermediate scales over the **Fixed** case, the **Normal-Paired** case shows an increment of scatter with respect to the **Normal** case.

When comparing the $f_{NL} = 0$ and $f_{NL} = 100$ simulations, we find very similar results in the ratios of the simulation variances to the expected Gaussian variance (Equation 10). Hence, by combining the results from Figure 1 & Figure 2, we conclude that the **Fix & Pair** technique can be use for local Primordial Non-Gaussianities in the same manner it is used for the Gaussian simulations.

In this study, we fit the scale-dependent variance reduction with the following phenomenological expression:

$$
\sigma_1(k) = \sqrt{\frac{4\pi^2}{V k^2 \Delta k}} P(k) \left( R_{CV} - (1 - R_{CV}) \cdot \frac{2}{\pi} \arctan\left( \frac{k}{k_{soft}} \right) \right) \frac{1}{n \cdot f_{sn}} \cdot \frac{1}{\sqrt{N_{sim}}},
$$

(13)

with the aim of having a less noisy version of the uncertainties presented in Figure 2. Note that this is simply a slight modification of Equation 10, where we introduce a smooth step function (with softening scale $k_{soft}$) between a large-scale reduced cosmic variance (by a factor $R_{CV}$) and the standard value at small scales (large-$k$). We also consider a super-Poissonian shot-noise factor $f_{sn}$. This last factor is used to account for an excess scatter observed at large $k$, which is not specific to the **Fixed** simulations as it is also found in the **Normal** simulations. The existence of excess shot-noise due to halo formation being a non-Poissonian process is well documented in the literature (Hamaus et al. 2010; Baldauf et al. 2013; Desjacques et al. 2018). We note, however, that this affects only large $k$, whereas we will focus later on the small-$k$ ($k < 0.09h^{-1}\text{Mpc}$). Nonetheless, we fit the expression above for all the scales $k < 0.4h^{-1}\text{Mpc}$, finding good agreement.

The fits with Equation 13 to the **Fixed** and **Fixed-Paired** variances...
is shown in Figure 2 (blue for Fixed, cyan for Fixed-Paired) and the best-fit values of the parameters are presented in Table 2. The error on the scatter ($\Delta(\sigma)$) plotted in Figure 2 and considered for the fits has been estimate as (Lehmann & Casella 1998):

$$\Delta(\sigma) = \frac{1}{\sqrt{2(N_{\text{sim}} - 1)}} \sigma.$$  \hspace{1cm} (14)

Table 2. Best fit parameters of Equation 13 for the standard deviation measured on the Fixed simulations and the Fixed & Paired (using Equation 12) simulations. These parameters and equation will be used as the error for most of the analysis of the paper.

| $f_{NL}$ | $\sigma$ | $R_{cv}$ | $k_{soft}$ [h/Mpc] | $f_{sn}$ |
|----------|----------|----------|---------------------|---------|
| $0$      | $\sigma$ | $0.141$  | $0.114$             | $1.174$ |
| $0$      | $\sigma_{FP}$ | $0.177$  | $0.224$             | $1.224$ |
| $100$    | $\sigma$ | $0.110$  | $0.110$             | $1.081$ |
| $100$    | $\sigma_{FP}$ | $0.120$  | $0.156$             | $1.056$ |
4 HALO BIAS ON THE GOLIAT-PNG SIMULATIONS

4.1 Modeling

Dark matter halos and galaxies are biased tracers of the underlying matter distribution. At large scales, this can be described by a linear relation between the matter overdensity ($\delta$) and the halo overdensity ($\delta_{\text{halo}}$) (Bardeen et al. 1986; Desjacques et al. 2018):

$$\delta_{\text{halo}} = b \cdot \delta,$$

with $b$ defined as the linear bias.

Hence, the power spectrum, which is simply the Fourier 2-point function of $\delta$, is described as

$$P_{\text{halo}}(k) = b^2 \cdot P(k),$$

with $P(k)$ being the dark matter power spectrum, which we will be modelling with the CAMB linear power spectrum\(^{12}\).

Whereas for Gaussian initial conditions, the bias is found to be constant at large scales $b = b_g$, in the presence of local Primordial Non-Gaussianities, the bias has been found to follow (Dalal et al. 2008; Slosar et al. 2008):

$$b(k) = b_g + 2\delta_c(b_g - p) \cdot f_{\text{NL}} \cdot \frac{1}{a(k,z)},$$

with $b_g$ and $p$ being a priori free parameters. $a(k,z)$ is defined in Equation 2 and has a $k^2$ dependence, which will dominate the clustering at large scales. It was originally proposed that $p = 1$ (Dalal et al. 2008) in what is called the Universality Relation (assuming that halo bias only depends on mass), motivated by the Peak-Background Universality Relation.

4.2 Fits to the simulations

4.2.1 Methods

We are now prepared to fit the modelling described in subsection 4.1 to the halo power spectrum measured in subsection 3.1, using the variance described in subsection 3.3. Since the covariance we are using is diagonal, the $\chi^2$ reads:

$$\chi^2(\vec{\theta}) = \sum_k \frac{\left(P_{\text{halo}}(k) - b(k, \vec{\theta})^2 P_{\text{lin}}(k)\right)^2}{\sigma(k)^2},$$

where $k_{\text{max}}$ is the maximum wave-number considered. We find that our results are very stable against $k_{\text{max}}$ variations up to $k_{\text{max}} = 0.09h^{-1}\text{Mpc}$. Hence, we fix that maximum $k$ for the rest of the analysis. $\vec{\theta}$ represents the free parameters considered, namely combinations of $b_g$, $p$ and $f_{\text{NL}}$.

We then consider the standard Gaussian likelihood

$$\mathcal{L}(\vec{\theta}) \propto \exp(-\chi^2(\vec{\theta})/2).$$

\(^{12}\) https://camb.info/sources/: Lewis & Bridle (2002).

4.2.2 $f_{\text{NL}} = 0$ simulations

We start by fitting a constant bias $b(k) \equiv \sqrt{P(k)/P_{\text{lin}}(k)} = b_g$ to the $f_{\text{NL}} = 0$ simulations in Figure 3. First, we consider the mean of all the Normal simulations\(^{13}\), with the expected error of a single simulation, $\sigma_{\text{th}}$, given by Equation 10 and show the results in solid red. We repeat this process for all the Fixed simulations considering either the error fitted to the Fixed case, $\sigma_F$, or the error fitted to the Fixed-Paired case, $\sigma_{FP}$ (Equation 13, Table 2). We find that the error on the bias is reduced by a factor $\sim 2$ when Fixing the initial conditions, whereas adding the Pairing further reduces the error another $\sim 10\%$. In order to make sure that our approximations to the errors $\sigma(k)$ do not introduce any significant changes, we also plot in dotted lines the results when using directly the standard deviation measured in the simulations, finding the differences negligible.

In Figure 4 we show the bias measured from the simulations when using linear theory as a reference. We find that our constant bias fits (bands) represent a good description up to $k_{\text{max}} = 0.09h^{-1}\text{Mpc}$. In general, we have found a good consistency in our description of the bias for the $f_{\text{NL}} = 0$ simulations for the different types of simulations considered (Normal and Fixed) and the different error estimations.

\(^{13}\) Recall that at this stage the average of all Normal simulations include already the Original-Paired. And similarly for the Fixed.

Figure 3. Probability Distribution Function (PDF) for the likelihood (Equation 18, Equation 19) of fitting the measured halo bias on the $f_{\text{NL}} = 0$ GOLIAT-PNG simulations to a constant $b_g$. By default (solid lines, and reported values) we use the errors, $\sigma$, given by the theoretical/fitting functions described by Equation 10 and Equation 13, whereas the dotted lines represent the PDF derived by using the standard deviation measured in the simulations. The results for the Normal (Normal-Original + Normal-Paired) simulations is shown in red. For the Fixed (Fixed-Original + Fixed-Paired) simulations we consider both the cases of the errors given by only Fixing (blue) and by both Fixing & Pairing (cyan).
we consider three fitting procedures: We perform a similar analysis for the \( f_{\text{NL}} \) simultaneously for the \( f_{\text{NL}} \) deviation from universality, see subsection 4.1), and then, it is worth

4.2.3 \( f_{\text{NL}} = 100 \) simulations

We perform a similar analysis for the \( f_{\text{NL}} = 100 \) simulations. Here, we consider three fitting procedures:

i) Fixing \( p = 1 \) and \( f_{\text{NL}} = 100 \), while letting \( b_\ell \) free.

ii) Fixing \( f_{\text{NL}} = 100 \), while letting \( b_\ell \) and \( p \) free.

iii) Fixing \( p = 1 \), while letting \( b_\ell \) and \( f_{\text{NL}} \) free.

We show the \( b(k) \) measurements from the simulations in Figure 5, together with the best fit for the three cases described above. We find that cases ii) and iii) give mathematically equivalent results for the \( b(k) \) since there is a complete degeneracy between \( p \) and \( f_{\text{NL}} \) in Equation 17. Precisely, we show both ii) and iii) to emphasize that a bias on the assumed \( p \) can bias the obtained \( f_{\text{NL}} \) and that there is an direct propagation from the error on one to the other one. We also find consistent results between the Normal and for the Fixed simulations.

Case i) shows slightly worse fit than ii) and iii), as expected since it has one parameter less. Given that case i) still shows a good fit and that \( p \) is found compatible with 1, one may consider whether it is necessary to consider \( p \) different to unity. So far, we have been only considering the error equivalent to a single \( V = (1h^{-1}\text{Gpc})^3 \) simulation, as the focus of the paper is to understand what we can infer from single simulations (or pairs), at fixed computational cost. However, for a moment we can consider the error on the ensemble average of the 2 \( \times \) 41 simulations. This is shown on Figure 6 in green, where we find \( p = 0.902 \pm 0.017 \), hence, we know that the ensemble of our mocks are best described with \( p \neq 1 \) (implying a deviation from universality, see subsection 4.1), and then, it is worth considering this parameter as free.

In Figure 6 we also show the constraints on the \( \{p, b_\ell\} \) plane on the Normal and Fixed cases, similarly to what was done in Figure 4 for only \( b_\ell \). We find that Fixing the initial conditions can reduce the error by a factor \( \sim 4 \) on \( p \) and by a factor \( \sim 3 \) on \( b_\ell \), when fitted simultaneously for the \( f_{\text{NL}} = 100 \) GOLiat-PNG simulations. Adding the Pairing gives us an additional \( \sim 5\% \) and \( \sim 10\% \) gain, respectively.

We checked again that using the standard deviation instead of the fitted errors gives similar results.

We have found, as motivated in section 1, that the gain of using Fixed initial conditions is huge when we want to constrain the bias parameters (\( b_\ell \), \( p \)) associated to the PNG halo clustering. Pairing can give us some mild additional constraint. In the next section, we will study how this gain can also be used in the context of model validation.

5 MODEL TESTING WITH PNG FIXED, PAIRED & MATCHED SIMULATIONS

5.1 Individual fits

Up to this point, we have always worked with the average of all simulations and their variance. We now turn to analyse the simulations individually or in pairs, in order to show the statistical power of using the Fix, Pair and Match techniques. In particular, we will work with \( b_\ell \) and \( f_{\text{NL}} \) as free parameters with \( p = 1 \) (case iii) above) and we choose the peak of the \( f_{\text{NL}} \) posterior as our estimator: \( \hat{f}_{\text{NL}} \).

Since we are using the same stochastic part of the ICs (the phases and, for Normal simulations, also the noise in the amplitude, see subsection 2.1) for the \( f_{\text{NL}} = 0 \) and the \( f_{\text{NL}} = 100 \) cases, their statistics will be highly correlated. This means that if a single realisation has some large scale \( P(k) \) fluctuations that favour a higher measured \( f_{\text{NL}} \) for the \( f_{\text{NL}} = 100 \) simulation (from now \( f_{\text{NL}}^{100} \)), we should also expect a higher estimation of \( f_{\text{NL}} \) for the \( f_{\text{NL}} = 0 \) simulation (\( f_{\text{NL}}^{0} \)), if we run the same analysis for both. This is precisely what we can see in the top panel of Figure 7. Here, we have fitted individually all the 41 \( f_{\text{NL}}^{100} \) and 41 \( f_{\text{NL}}^{0} \) simulations for the Normal, the Fixed and the Fixed-Paired cases. For the Normal cases, we join the simulations with the same initial phases by a line. We find that, whereas the individual fits have a huge scatter (with the distribution of the \( f_{\text{NL}} = 0 \) and \( f_{\text{NL}} = 100 \) best fits even overlapping), the length and orientation of the magenta line remains relatively constant.

For the Fixed and Fixed-Paired cases, we find that the scatter in the best fits \( f_{\text{NL}} \) is greatly suppressed, as anticipated. At the bottom panel of Figure 7 we show the 2D constraints derived in the mean of the Normal and Fixed simulations, similar to what was shown in Figure 6 but now on the \( (f_{\text{NL}}, b_\ell) \) plane. However, note that here we divide by \( \sqrt{2} \) the \( \sigma_{\text{PP}} \) error as we want to compare it with the scatter of the Fixed & Paired simulations, whose scatter will be intrinsically reduced by the doubling of volume. Qualitatively, the scatter of the best fits in the top panel follows the ellipses shown in the bottom panel.

More quantitative results are given on the marginalised results on \( f_{\text{NL}} \). The histogram of the distributions of \( f_{\text{NL}} \) for the \( f_{\text{NL}} = 0 \) and \( f_{\text{NL}} = 100 \) simulations is given in the first two panels of Figure 8 and their mean and standard deviation reported in the Table 3 (1st and 3rd columns). Next to them, we also show the 68\% c.r. of the posterior on \( f_{\text{NL}} \) on the mean of all the simulations (represented by the center and semi-width under the label ’Mean’), with the posterior of the mean represented also in Figure 8 as solid lines. We find good consistency between the distribution of the individual fits and the fit on the mean of the mocks (note that we expect a 11\% level of statistical uncertainty on the std and 15\% on the mean, given that we are using \( N_{\text{mc}} \) = 41 mocks; see Equation 14).

When using Fixed initial conditions, we find a drastic (\( \times \sim 4 \)) reduction in the uncertainty (and scatter) of \( f_{\text{NL}} \) with respect to the Normal simulations. However, when also Pairing them, we do not find evidence for an improvement on \( \sigma(\hat{f}_{\text{NL}}) \) beyond the one expected.
Hence, we simply conclude that Pairing does not add a significant improvement to the measurement of $f_{\text{NL}}$ with our analysis pipeline.

5.2 Correlating Matched ICs

Motivated by the top panel of Figure 7, we can now consider our new estimator as the difference between the best fit value of $f_{\text{NL}} = 100$ and the $f_{\text{NL}} = 0$ simulations:

$$\Delta \hat{f}_{\text{NL}} = \hat{f}^{100}_{\text{NL}} - \hat{f}^{0}_{\text{NL}}.$$  \hspace{1cm} (20)

Then, the propagated error on this estimator, taking into account the Pearson correlation coefficient $\rho$ between $\hat{f}^{0}_{\text{NL}}$ and $\hat{f}^{100}_{\text{NL}}$, is

$$\sigma(\Delta \hat{f}_{\text{NL}})^2 = \sigma(\hat{f}^{100}_{\text{NL}})^2 + \sigma(\hat{f}^{0}_{\text{NL}})^2 - 2 \cdot \rho \cdot \sigma(\hat{f}^{100}_{\text{NL}}) \sigma(\hat{f}^{0}_{\text{NL}}).$$  \hspace{1cm} (21)

For this purpose, we measure the correlation coefficients between the best fits of the $f_{\text{NL}} = 0$ and $f_{\text{NL}} = 100$ simulations for the Normal, Fixed and Fixed-Paired cases, shown in Table 3.

On the right panel of Figure 8 we show the histogram of the difference of best fits, $\Delta \hat{f}_{\text{NL}}$. Indeed, we find that the scatter of $\Delta \hat{f}_{\text{NL}}$ is greatly reduced if we compare it with the $f_{\text{NL}} = 100$ (or $f_{\text{NL}} = 0$) case (note the change of scale in the $x$-axis). We also infer a Gaussian PDF with the variance given by Equation 21 (inputting the $\sigma$s derived for the mean of all the $f_{\text{NL}} = 0$ simulations at the mean given by the difference of the peak of the posterior represented in the left and center panels. We find a good agreement between the errors expected by Equation 21 and the distribution of $\Delta \hat{f}_{\text{NL}}$, as reported in Table 3.

We find a significant gain in precision, when using the correlation of phases between two simulations with Matched initial conditions. This can be used in general to validate a model or to constrain nuisance parameters associated with it. The larger the correlation, the larger the gain we can obtain from using this technique. Hence, this gain is larger for the Normal simulations, then the Fixed-Paired, and finally the Fixed. This larger correlation for the Normal simulations is expected, since much of this correlation comes from having the same cosmic variance realisation at large scales. When Fixing the

by the increment of volume; whereas the error on the mean does show some slight improvement, the measured scatter increases (when corrected by the $\sqrt{2}$ factor). Nonetheless, this subtle differences fall within the expected statistical differences by having a limited number of mocks. Additionally, for non-Gaussian likelihoods, the scatter on the peak of the posterior may not coincide with the $\sigma$ derived on the mean $P(k)$. These subtleties are beyond the scope of this paper as we focus on the large improvements obtained by the Fixing and by the usage of correlation between Matched-ICs boxes (see below).
Table 3. Summary statistics of individual and global fits to the GOLIAT-PNG simulations: 1) mean and standard deviation of the individual best fits \(f_{NL}^0\) for the \(f_{NL} = 0\) simulations; 2) 1-\(\sigma\) c.r. from the fit on the mean of the \(f_{NL} = 0\) simulations and used for its Gaussian approximation; 3) mean and standard deviation of the individual \(f_{NL}\) best fits for the \(f_{NL} = 100\) simulations; 4) 1-\(\sigma\) c.r. inferred from the fit on the mean of the \(f_{NL} = 100\) simulations; 5) gain in effective volume with respect to a standard simulation due to the type of initial conditions based on the \(\sigma\) [and based on the \(\sigma\) on the mean] on the \(f_{NL} = 100\) simulations; 6) Pearson correlation coefficient between \(\hat{f}_{NL}^0\) and \(\hat{f}_{NL}^{100}\); 7) mean and standard deviation of the Matched difference between \(\hat{f}_{NL}^0\) and \(\hat{f}_{NL}^{100}\); 8) derived \(\mu\) and \(\sigma\) parameters under the Gaussian approximation for \(\hat{f}_{NL}\); 9) total gain in effective volume with respect to a standard non-Matched simulation due to both the use of Matched-ICs and the type of initial conditions based on the \(\sigma\) [and based on the Gaussian \(\sigma\)] (with \(V_{eff} \propto 1/\sigma^2\)). Each of the three first rows represents a different case of initial conditions (Normal, Fixed or Fixed-Paired), whereas in the last row we multiply the errors of the Fixed-Paired by \(\sqrt{2}\) to compensate by the doubling of volume.

| \(f_{NL} = 0\) | \(f_{NL} = 100\) | \(f_{NL} = 0\) | \(f_{NL} = 100\) | \(\Delta f_{NL}\) | \(\Delta f_{NL}\) | \(\sigma\) | \(V_{eff}/V\) |
|---------------|----------------|---------------|----------------|----------------|----------------|------|----------------|
| Normal        | 1.9 \pm 47.0   | 1.1 \pm 40.3  | 111.4 \pm 60.5 | 108.7 \pm 50.7 | 1 [1]         | 0.97 | 109.5 \pm 18.1 | 107.6 \pm 14.6 | 11 [12] |
| Fixed         | -1.3 \pm 11.8  | -1.9 \pm 12.0 | 107.6 \pm 12.1 | 107.5 \pm 12.4 | 25 [17]       | 0.76 | 108.9 \pm 8.3  | 109.4 \pm 8.4  | 53 [36]  |
| Fixed-Paired  | -1.8 \pm 9.5   | -1.2 \pm 8.3  | 107.4 \pm 9.3  | 107.5 \pm 8.2  | -             | 0.85 | 109.2 \pm 5.2  | 108.7 \pm 4.6  | -         |
| \(\times \sqrt{2}\) | \pm 13.5       | \pm 11.8      | \pm 13.2       | \pm 11.7       | 21 [19]       | -     | \pm 7.3        | \pm 6.4       | 89 [3]    |

Figure 7. Top: We represent the position of the best fits in the \(\{f_{NL}, b_g\}\) plane for all the individual Normal and Fixed simulations and also for the Pairs of Fixed simulations (using Equation 11). We show the results for both the \(f_{NL} = 0\) and \(f_{NL} = 100\) simulations. For the Normal cases we match with a red line the simulations using the same stochastic component of the ICs (Matched), making already very apparent the correlation between the \(f_{NL} = 0\) and \(f_{NL} = 100\) best fits. Bottom: 1-\(\sigma\) and 2-\(\sigma\) contours of the likelihood on the mean of the simulations. Unlike in Figure 6, the error used here for the Fixed-Paired corresponds to the volume of the two simulations in the pairs. The scatter on the points on the top panel approximately follow the contours shown in the bottom panel.

ICs, we reduce much the cosmic variance influence, thus, reducing this correlation. Nevertheless, the Matched Fixed simulations still present smaller scatter (std(\(f_{NL}\)) \~ 8) than the Normal simulation (std(\(f_{NL}\)) \~ 18). Hence, these two techniques can be used together to gain even more information. For the Fixed-Paired case, given the larger correlation than in the Fixed case, we see a further reduction in the uncertainties. In this occasion, both estimators of the Fixed-Paired error (std and the Gaussian \(\sigma\)), go in the direction of having a more precise measurement of \(f_{NL}\) (after compensating for the \(\sqrt{2}\) factor). However, this gain is still not statistically significant for the Fixed-Paired case, given the uncertainty on the standard deviation (11%).

5.3 Model validation

With the Fixed-Paired simulations and using the Matched-ICs correlation, we obtain a value of \(\langle f_{NL}^0 \rangle = 109.2 \pm 5.2\) (or \(\Delta f_{NL} = 108.7 \pm 4.6\) for the Gaussian approximation), which is marginally in tension (almost 2\(\sigma\)) with the known \(f_{NL} = 100\) of our simulations. This can be interpreted as a hint that our model \((p = 1)\) is inaccurate, as we know it is the case: we found in Figure 6 that when combining all the 2 x 41 boxes we obtain \(p = 0.902 \pm 0.017\).

Otherwise, said, a single pair of \(f_{NL} = 100\) Fixed & Paired N-Body simulations with the properties of GOLIAT-PNG (mainly \(L = 1h^{-1}\)Gpc) Matched to another Fixed-Pair with \(f_{NL} = 0\) with the same initial phases is expected to detect a ~2\(\sigma\) discrepancy with the halo clustering predicted by the universality relation \((p = 1)\). We remind the reader that this relation is expected to break (see subsection 4.1).

In order to achieve the same level of accuracy \((\sigma(\langle f_{NL} \rangle) = 5)\) with Normal non-Matched simulations (single error of \(\sigma(\langle f_{NL} \rangle) = 60\)), we would need ~ 144 individual simulations (as the error scales as \(\sigma \propto 1/\sqrt{V}\)).

If we redo our analysis with \(p = 0.902\), we obtain \(\langle \hat{f}_{NL}^0 \rangle = 101.7 \pm 4.8\) (from the Fixed, Paired & Matched mocks), an unbiased result. Another approach is to re-interpret the measured \(\Delta f_{NL}\) in terms of \(p\). Arguably, what we are able to measure is the joint \((b_g - p) f_{NL}\) factor \((\propto b_g f_{NL})\). Then, the we can estimate \(p\) as

\[
\hat{p} = b_g - (\hat{b}_g - 1) \frac{\hat{f}_{NL}}{f_{NL}} ,
\]

recovered \(\hat{p} = 0.88\) when inputting \(\frac{\hat{f}_{NL}}{f_{NL}} = 109.2\) retrieved from the Fixed, Paired & Matched mocks. Alternatively, if we apply Equation 22 with \(\hat{f}_{NL} = 100\) to each mock individually, we obtain \(\langle \hat{p}\rangle \pm \text{std}(\hat{p}) = 0.87 \pm 0.81, 0.90 \pm 0.16, 0.90 \pm 0.12\) for
the Normal, Fixed and Fixed-Paired cases, respectively, when inputting \( f_{NL}^{100} \) \((\text{non-Matched})\) and \( \hat{f} \pm \text{std}(\hat{f}) = 0.88 \pm 0.24, 0.88 \pm 0.07 \), when inputting \( f_{NL} = \Delta f_{NL} \) \((\text{i.e. Matching})\).

For the Matched + Fixed-Paired analysis, we retrieve again a 2-\( \sigma \) hint against the universal relation model \( p = 1 \).

6 SUMMARY

In this work, we have studied combinations of three techniques designed to reduce the variance associated to cosmological simulations by tweaking the Initial Conditions (ICs, section 2): the Fix & Pair technique (proposed in Angulo & Pontzen 2016) and the Matching. First, Fixing removes the variance input to the clustering of the ICs, greatly reducing the variance at the late times as well. Secondly, Pairing consists on running a second simulation with the phases Inverted on the ICs and the rest of the setup unchanged, which is able to cancel out some contributions to the variance, when combined with the Fixing. Lastly, the Matching consists of running simulations with different cosmologies but the same random realisations of the stochastic part of the ICs (for the phase and amplitude). With Matched-ICs, the retrieved clustering statistics are correlated for the different cosmologies and part of the noise can be canceled out. Whereas the three techniques have been used in the past in a qualitative/implicit way, here we have proposed a framework to utilise (combinations of) these three techniques to increase significantly the precision retrieved from simulations in a quantitative and explicit way.

In particular, we put the focus on the usage of simulations to validate galaxy/halo clustering models and also to put constraints/priors of nuisance (bias) parameters associated with them. We note that a recent work by Zennaro et al. (2021) already uses Fixed & Paired simulations to constrain (Gaussian) bias parameters down to a reduced uncertainty, with the methodology just realeased in Maion et al. (2022).

In order to illustrate the potential of these techniques, we focused on constraining local Primordial Non-Gaussianities (PNG) with the halo power spectrum \( P(k) \). PNG is parametrised by \( f_{NL} \) and it induces a scale-dependent bias at very large scales, where the Fix technique is specially powerful in reducing the variance. For that purpose, we run the G oligat-PNG suite: a set of 328 \((41 \times 2 \times 4)\) \(N\)-body simulations, for which we have 41 different initial random seeds for 2 different values of \( f_{NL} \), 0 & 100, and 4 types of ICs: the Normal-Original, the Normal-Inverted, Fixed-Original and Fixed-Inverted (subsection 3.1).

Our first goal was to validate the usage of the Fix technique with local-PNG, since Fixing already induces a type of non-Gaussianity (the Rayleigh PDF is substituted by a Dirac delta). In Figure 1 we find that the \( P(k) \) ratio of the Fixed to Normal simulations is nearly identical for \( f_{NL} = 0 \) and \( f_{NL} = 100 \) and, in both cases, within the noise level. Additionally, in the Appendix A, we include a series of tests that validate the usage of Fixed-PNG simulations not only for halo power spectrum, but also for the halo bispectrum as well as for the dark matter power spectrum and bispectrum of both initial conditions and late time (\( z = 1 \)) snapshots. Additionally, we also verify that the Fixed-PNG simulations result unbiased when studying higher resolutions or larger volumes.

On a second step, we quantified in Figure 2 the reduction on the \( P(k) \) variance \((\sigma(k)^2)\) introduced by the Fix and Pair techniques. Again, the results are found very similar for the \( f_{NL} = 0 \) and the \( f_{NL} = 100 \) cases. The Fix shows a scale-dependent variance reduction similar to Chuang et al. (2019), Ding et al. (2022) or Maion et al. (2022), which we fit here with a smoothed step function (Equation 13) that we use for the rest of the paper. When adding the Pairing to the Normal simulations, we actually obtain an increment on the variance at large \( k \) in line with Chuang et al. (2019), which goes in opposite direction to the original motivation. However, when adding the Pairing to the Fixing we find slight reduction in the variance at intermediate scales \((k \sim 0.1 \text{h}^{-1}\text{Mpc})\), which is in line with the original proposal in Angulo & Pontzen (2016).

In section 4, we studied the halo bias of the G oligat-PNG and validated our modelling and fitting pipeline. We found that we can describe well the halo clustering with a linear theory + linear bias up to \( k = 0.09 \text{h}^{-1}\text{Mpc} \) for our simulations. For that, we use a constant bias for \( f_{NL} = 0 \) and a the PNG scale-dependent bias (Equation 17) for \( f_{NL} = 100 \). When considering the ensemble of the \( 2 \times 41 \) \( f_{NL} = 100 \) Fixed & Paired simulations we find that the clustering predicted by the universal mass relation (Dalal et al. 2008, Equation 17 with \( p = 1 \)) is insufficient (as expected) and we obtain \( p = 0.902 \pm 0.017 \).

Finally, in section 5 we set up the framework to validate galaxy/halo clustering models with combinations of the Fix, Pair and Match techniques. We fitted the bias and PNG parameters \((b,f_{NL})\) individually for each the simulations (or pairs) for the Normal, Fixed and Fixed-Paired cases. We find that \( P(k) \) variance reduction due to the Fixing results in a reduction on \( \sigma(f_{NL}) \) by a factor of \( \sim 4 - 5 \) (equivalent.

Figure 8. The histograms show the distribution of best fit values of \( f_{NL} \) for the \( f_{NL} = 0 \) simulations (left), the \( f_{NL} = 100 \) simulations (centre) and their differences (right). We show on top the posterior on the mean of all the 41 simulations on solid lines, and its Gaussian approximation on dashed lines (barely distinguishable). We find that the difference on the estimated PNG parameter, \( \Delta f_{NL} \), shows a much more reduced scatter than the individual cases (note the difference of scale on the x-axis). We also find that the Fixed simulations (blue) also greatly reduces the error on \( f_{NL} \) with respect to the Normal simulations (red). When we consider the Fixed-Paired case (green), it further reduces the scatter, but it is compatible with the simple effect of doubling the volume. More details in the text and in Table 3.
to gaining a factor of $\sim 20$ in simulated volume) for the $f_{\text{NL}} = 100$ simulations. Adding the Pairing does not show a significant gain beyond the doubling of volume.

The ICs Matching between the $f_{\text{NL}} = 0$ and the $f_{\text{NL}} = 100$ simulations results in a high correlation on the fitted $f_{\text{NL}}, f_{\text{NL}}^0, f_{\text{NL}}^{100}$ ($\rho = 0.97, 0.76, 0.85$, for the Normal, Fixed and Fixed-Paired, respectively). Using explicitly their correlation coefficients, we defined a new variable $\Delta f_{\text{NL}} = f_{\text{NL}}^{100} - f_{\text{NL}}^0$ (Equation 20), whose variance is greatly reduced. This allows us to constrain $\Delta f_{\text{NL}}$ with a precision increased by an additional factor of $\sim 3-4$ for the Normal, $\sim 1.5$ for the Fixed and $\sim 2$ for the Fixed-Paired (we have multiplied this value by $\sqrt{2}$ to compensate the doubling of volume) cases with respect to their equivalent non-Matched simulations.

By combining the Fix, Pair and Match techniques altogether we inferred an uncertainty on one pair of simulations of $\sigma(f_{\text{NL}}) = 5$, whereas one single simulation with $f_{\text{NL}} = 100$ yields an uncertainty of $\sigma(f_{\text{NL}}) = 60$. We would have needed 144 simulations to reach the same level of precision.

In terms of model validation, combining the Fix, Pair and Match techniques allows us to find a $\sim 2\sigma$ hint of deviation from the prediction from Dalal et al. (2008) ($p = 1$) with one single pair: $f_{\text{NL}} = 109\pm 5$ or, equivalently, $p = 0.88 \pm 0.07$ (recall that the ensemble of simulations gave us the reference value of $p = 0.902 \pm 0.017$). Thus, we have shown that explicitly using the variance reduction of Fixing, Pairing and Matching can allow us to test models down to a much smaller error on the cosmological parameters ($f_{\text{NL}}$ in our case) and, therefore, to detect inaccuracies in the clustering model that would have otherwise been undetected. Alternatively, these techniques can also be used to constrain nuisance/bias parameters ($p$ in our case) to a much higher precision. These constraints can later be used to construct informative priors to constrain the data. This is particularly important for PNG analysis with the 2-point statistics, since $f_{\text{NL}}$ and $p$ are completely degenerated.

7 OUTLOOK

We have shown that explicitly using the variance reduction of Fixed, Paired and Matched simulations can lead us to a better understanding of halo/galaxy clustering models. In particular, these simulations can be used to validate down to an increased accuracy the analysis tools that we intend to implement in data. Alternatively, we can use these simulations to tighten the priors on nuisance parameters such as the PNG response $p$ studied here or other bias parameters, such as the ones studied in Zennaro et al. (2021). If one only wanted to put priors on bias parameters, an alternative approach is to use the simulation dark matter power spectrum as our theory (as done in Zennaro et al. 2021), this would likely capture most of the information that we are here capturing with the Matching. However, in this paper we put the focus on the validation a galaxy clustering models that we would plan to use on data, hence our theory may not rely on information that we are not able to retrieve from the data (such as the matter power spectrum).

Constraining PNG is one of the main goals for surveys such as DESI\footnote{https://www.desi.lbl.gov/}, Euclid\footnote{https://sci.esa.int/web/euclid} or SphereX and one of the main motivations for an intensity mapping program on the SKAO (DESI Collaboration et al. 2016; Levi et al. 2019; Laureijs et al. 2011; Doré et al. 2014, 2018; SKA Cosmology SWG et al. 2020). However, without any prior on $p$ (Equation 17, or $b_\phi$, as done in Barreira 2022), the PNG constraints are completely degenerated with it (as we displayed in Figure 5). Hence, building simulation efforts to put tight and robust priors on the PNG bias parameters is a necessary step to measure accurate and precise constraints on $f_{\text{NL}}$ by using the LSS. With the methodology proposed here we have shown that a single Fixed-Pair of $V = 1[h^{-1}\text{Gpc}]^3$ simulations with $f_{\text{NL}} = 100$ Matched to an existing $f_{\text{NL}} = 0$ Fixed-Pair can be used to test the PNG halo clustering modelling down to an uncertainty of $\sigma(f_{\text{NL}}) = 5$, comparable with current CMB constraints and upcoming constraints from Euclid or DESI (Laureijs et al. 2011; DESI Collaboration et al. 2016). This implies a reduction of the computational costs invested in simulations by a factor $\sim 140$ with respect to using Normal non-Matched simulations.

The techniques proposed here can be used with existing Fixed and Paired simulation suits such as UNITsims (Chuang et al. 2019), BACCO (Angulo et al. 2021) or Quijote (Villaescusa-Navarro et al. 2020) and possible extensions of them. An additional advantage of using Fix, Pair and Match together is that one can use a high mass resolution in order to resolve well the halos of interests for future surveys (log$M_h \sim 11$ for Euclid and DESI) in a $V \sim 1[Gpc/h]^3$ box with reasonable computing resources ($N = 4096^3$ in UNITsim), while keeping a reduced uncertainty on $f_{\text{NL}}$ (or $p$ or $b_\phi$). This way, one could also use semi-analytical models of galaxy formation (as recently done in Zhai et al. 2021; Knebe et al. 2022), to populate UNITsim with H-$\sigma$ galaxies for Roman/Euclid) to understand the effect of galaxy formation on $p$ or $b_\phi$ for different tracers (as done in Barreira et al. 2020; Barreira 2021).

One caveat could be the need of many simulations to measure on the one hand the variance reduction induced by the Fixing and Pairing (which Zhao et al. 2021 showed that are very sample dependent) and, on the other hand the correlation coefficient associated to the Matching. However, on the other hand simulation suites such as UNITsims (Chuang et al. 2019), FastPM (Feng et al. 2016), HALOGEN (Avila et al. 2015) or EZmocks (Chuang et al. 2015).

We envision this paper as a first step into building a suite of simulations specifically aimed at understanding the bias parameters associated to PNG well enough to put informative and robust priors on them. Simultaneously, this set of simulations will also serve to validate PNG analysis pipelines and for preparation of upcoming LSS surveys (particularly, DESI and Euclid), not only by using the halo power spectrum, but also other observables such as the Halo Mass Function, the galaxy bispectrum, the probability distribution functions, zero-bias tracers, etc (Matarrese et al. 2000; LoVerde et al. 2008; Cabass et al. 2022; Friedrich et al. 2020; Castorina et al. 2018).

Additionally, we expect that part of the methodology used here can be used to validate galaxy clustering models beyond PNG analysis and to enhance the statistical power of cosmological simulations in general.

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We discussed in section 2 that Fixing initial conditions modifies the Gaussianity of the initial conditions. This a priori means that we need to treat with special care Fixed-PNG simulations. In subsection 3.2 we already showed that for the halo power spectrum, main focus of this paper and of most interest for future surveys, we do not find any spurious PNG signal due to Fixing and that Fixed simulations behave in the same way for $f_{\text{NL}} = 100$ as they do for $f_{\text{NL}} = 0$. Said otherwise, they give unbiased halo power spectrum, whereas the error of the Fixed simulations is reduced.

The aim of this Appendix is to further validate the usage of Fixed-PNG by testing other statistics (initial and late bispectra and power spectra of dark matter and halos) and in other configurations (increasing the size or the mass resolution of the simulation).

A1 Initial DM power spectrum

As both PNG and Fixing modify only the initial conditions, this is a very clean place to look for possible spurious signals.

In Figure A1, we show the dark matter power spectra measured in the initial conditions, set at $z = 32$. We find similar power spectra for $f_{\text{NL}} = 0$ and $f_{\text{NL}} = 100$, as the PNG is only expected to affect higher order statistics. Also, we see that the variance in the Fixed power spectra is negligible as expected by construction for this method. Looking at the Fixed to Normal ratios of dark matter power spectra, $f_{\text{NL}} = 100$ simulations appear identical to the $f_{\text{NL}} = 0$ case.

A2 Initial DM bispectrum

Whereas no signal coming from PNG was expected in the power spectra, we expect to find the net signal induced by $f_{\text{NL}} \neq 0$ on the initial dark matter bispectrum. We compute the bispectrum using the library pySPECTRE\textsuperscript{16}, considering a binning of $\Delta k = 3 \cdot k_f$ for all the closed triangles up to a $k_{\text{max}}$ of $120k_f$. We show all the resulting configurations in Figure A2. Again, we do not find any evidence of spurious PNG signal introduced by the Fixing. The residuals of the comparison between Normal and Fixed simulations look very alike for $f_{\text{NL}} = 0$ and $f_{\text{NL}} = 100$.

In Figure A3, we focus on the squeezed configuration, defined by triangles having a small $k$ and two large $k$. In this case, we fix $k_3 = \Delta k = 3k_f$ and $k_1 = k_2 = k$, leaving $k$ as a variable. This configuration is where the local-PNG is expected to create a signal, not present for the Gaussian case. Indeed, for this configuration, we find a significant bispectrum signal for the ensemble of $f_{\text{NL}} = 100$ simulations, whereas, for $f_{\text{NL}} = 0$ the signal is comparable with the noise. As in previous tests, we do not find differences between the Fixed and the Normal simulations. Hence, we do not find any evidence of spurious local-PNG signal.

A3 Late DM power spectrum

 Whereas we have already studied in detail the initial conditions, where the PNG signal and the Fixing are input to the simulations, we now check similar statistics at late time, in order to search for possible spurious signals. We start by studying in Figure A4 the dark matter power spectrum at $z = 1$, redshift of study for the main body of the paper. Again, we find the Fixed and Normal simulations compatible and their ratio nearly indistinguishable for the $f_{\text{NL}} = 0$ and $f_{\text{NL}} = 100$ cases. Thus, we do not find any spurious signal introduced by Fixing the PNG simulations.

A4 Late DM bispectrum

We now put our attention on the dark matter bispectrum at redshift $z = 1$. First, we remind the reader that this signal is expected to be dominated by late non-Gaussianities induced by non-linear gravitational evolution of density perturbations. Also, that the different triangle configurations will be highly correlated. The main conclusion of this subsection can be drawn from the residual plots at the bottom of Figure A5, where we find the same pattern for $f_{\text{NL}} = 0$ and $f_{\text{NL}} = 100$. Again, pointing us to the conclusion that the Fixed initial conditions can be used in the same way for local-PNG as we use them for Gaussian cosmologies.

We do appreciate an offset with respect to a null residual for both $f_{\text{NL}} = 0$ and $f_{\text{NL}} = 100$. However, this is at the level of $\sim 0.2\sigma$. Said otherwise, they give unbiased halo power spectrum, whereas we do not find any evidence of biasing this statistics, and we find the $f_{\text{NL}} = 0$ and $f_{\text{NL}} = 100$ residuals to behave similarly.

For the squeezed configuration (as in Figure A3), we found again nearly indistinguishable results for the Fixed to Normal ratios for $f_{\text{NL}} = 0$ and $f_{\text{NL}} = 100$. We omit this figure for brevity.

A5 Late halo bispectrum

We now come back to studying the clustering of halos (at late times, in this case $z = 1$). As we validated the halo power spectrum in the main text (subsection 3.2) we now focus in another promising observable (see e.g. Cabass et al. 2022): the halo bispectrum (as a proxy for galaxy bispectrum). We show all the configurations in Figure A6 and we focus on the squeezed ones in Figure A7. In the latter, we can appreciate the signal introduced by local-PNG on this configuration. Besides that, we do not find any evidence of biasing this statistics, and we find the $f_{\text{NL}} = 0$ and $f_{\text{NL}} = 100$ residuals to behave similarly.

A6 Late halo power spectrum: higher resolution or larger box

In the main text, we validated the usage of Fixed-PNG simulations to get unbiased halo power spectra in our default configuration (Table 1). In previous subsections of this Appendix, we have looked at other statistics of the same simulations, not finding any evidence of getting biased statistics by Fixing local-PNG simulations. Finally, here, we study again the halo power spectrum, this time when changing the mass resolution or the box size of our simulations.

\footnote{https://github.com/changhoonhahn/pySPECTRE}
Figure A1. Mean of dark matter power spectra of the initial conditions at $z = 32$ for Fixed and Normal simulations (Top) and their ratios (Bottom). The standard deviation is shown in a light shaded area, whereas the dark shaded area represents the expected error on the ensemble mean. The left subfigure shows the $f_{\text{NL}} = 0$ simulations, whereas the right subfigure shows the $f_{\text{NL}} = 100$ case.

We ran a few new simulations with 8 times more particles ($N = 1024^3$) for the same box configuration (‘High-Res’) and with double the box size ($L = 2\text{Gpc}/h$, keeping the same mass resolution). In this case, in order to keep the computing time short, we only ran one seed for each of the four combinations with Normal and Fixed ICs for both $f_{\text{NL}} = 0$ and $f_{\text{NL}} = 100$. In Figure A8, we plot again the Fixed to Normal ratios shown at the bottom of Figure 1 (labeled as ‘default’), and overplot the new results with higher resolution and larger box. Taking into account that we are only plotting one realisation for the new cases (hence, with the light-shaded region as reference uncertainty), we find that both cases follow the same trend as our default case and, again, very similar results for $f_{\text{NL}} = 100$ and $f_{\text{NL}} = 0$.

Remarkably, the largest scales shown for the $L = 2\text{Gpc}/h$ case are already dominated by $f_{\text{NL}}^2$ terms of the halo power spectrum, being able to probe new regimes of the validity of our method. Additionally, in a follow-up study (Adame et al. prep), we have further validated these findings (that we still recover unbiased halo power spectra at larger scales and higher mass resolutions) with 10 Fixed and 100 Normal FastPM simulations (Feng et al. 2016) with $L = 3\text{Gpc}/h$ and $N = 2560^3$ (we leave the full description of these simulations to a follow-up paper as their configuration is very different to Table 1).

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Figure A2. All configurations of the ICs ($z = 32$) dark matter bispectrum for $\{k_1, k_2, k_3\}$ being multiples of $3k_f = 0.19 h/\text{Mpc}$ up to $120k_f = 0.75 h/\text{Mpc}$, with $k_f$ being the fundamental mode. On the top panel we compare the mean bispectrum of 41 Normal simulations to the mean of 41 Fixed simulations, in both cases with $f_{NL} = 100$. On the next two panels we show the difference between the mean Fixed bispectrum and the mean Normal bispectrum over the Normal standard deviation for the case of $f_{NL} = 0$ and the case of $f_{NL} = 100$, respectively. Finally, the last three panels show the value of $\{k_1, k_2, k_3\}$ for each of the triangles indexed on the $x$-axis. We do not find significant biases and obtain similar results for $f_{NL} = 100$ and $f_{NL} = 0$. 

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Figure A3. Squeezed bispectrum of the dark matter at the initial conditions \((z = 32)\) for \textit{Fixed} (blue) and \textit{Normal} (red) simulations. We show the average (lines) and standard deviations (light shaded) of the 41 realisations studied. On dark-shaded regions we show the estimated error on ensemble average.
Figure A4. Dark matter power spectrum at redshift $z = 1$. We compare the $f_{\text{NL}} = 0$ case (left) to the $f_{\text{NL}} = 100$ simulations (right), and the Fixed simulations (blue) to the Normal ones (red). We find that the Fixed to Normal ratios are very similar for the $f_{\text{NL}} = 0$ and $f_{\text{NL}} = 100$ cases.
Figure A5. All configurations of the late ($z = 1$) dark matter bispectrum for $\{k_1, k_2, k_3\}$ being multiples of $3k_f = 0.19h$/Mpc up to $120k_f = 0.75h$/Mpc, with $k_f$ being the fundamental mode. On the top panel we compare the mean bispectrum of 41 Normal simulations to the mean of 41 Fixed simulations, in both cases with $f_{NL} = 100$. On the next two panels we show the difference between the mean Fixed bispectrum and the Normal bispectrum over the Normal standard deviation for the case of $f_{NL} = 0$ and the case of $f_{NL} = 100$, respectively. The $x$-axis represents the index of the triangle, each of them with a different $\{k_1, k_2, k_3\}$, as shown in Figure A2. We find the $f_{NL} = 0$ and the $f_{NL} = 100$ simulations to behave in the same way when Fixing the initial conditions.

Figure A6. All configurations of the late ($z = 1$) halo bispectrum for $\{k_1, k_2, k_3\}$ being multiples of $3k_f = 0.19h$/Mpc up to $120k_f = 0.75h$/Mpc, with $k_f$ being the fundamental mode. On the top panel we compare the mean bispectrum of 41 Normal simulations to the mean of 41 Fixed simulations, in both cases with $f_{NL} = 100$. On the next two panels we show the difference between the mean Fixed bispectrum and the Normal bispectrum over the Normal standard deviation for the case of $f_{NL} = 0$ and the case of $f_{NL} = 100$, respectively. The $x$-axis represents the index of the triangle, each of them with a different $\{k_1, k_2, k_3\}$, as shown in Figure A2.
Figure A7. Squeezed halo bispectrum of Fixed and Normal simulations (top), together with their ratio (bottom). We do not find biases induced by Fixing for either $f_{\text{NL}} = 0$ (left) or $f_{\text{NL}} = 100$ (right).

Figure A8. Fixed to Normal halo power spectra ratios. On solid lines and light-shaded regions we show the mean and standard deviation of the 41 default ($L = 1\text{Gpc}/h, N = 512^3$) configuration simulations described in the main text (i.e., they replicate the bottom panels of Figure 1). The dotted line represents the large box-run ($L = 2\text{Gpc}/h, N = 1024^3$) and the dashed line represents the higher resolution run ($L = 1\text{Gpc}/h, N = 1024^3$). The latter ones only represent one realisation of each type and were only discussed in subsection A6.