The Initial Conditions of the Universe from Constrained Simulations

Francisco-Shu Kitaura*
Leibniz-Institut für Astrophysik Potsdam (AIP), An der Sternwarte 16, D-14482 Potsdam, Germany

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ABSTRACT

I present a new approach to recover the primordial density fluctuations and the cosmic web structure underlying a galaxy distribution. The method is based on sampling Gaussian fields which are compatible with a galaxy distribution and a structure formation model. This is achieved by splitting the inversion problem into two Gibbs-sampling steps: the first being a Gaussianisation step transforming a distribution of point sources at Lagrangian positions—which are not a priori given—into a linear alias-free Gaussian field. This step is based on Hamiltonian sampling with a Gaussian-Poisson model. The second step consists on a likelihood comparison in which the set of matter tracers at the initial conditions is constrained on the galaxy distribution and the assumed structure formation model. For computational reasons second order Lagrangian Perturbation Theory is used. However, the presented approach is flexible to adopt any structure formation model. A semi-analytic halo-model based galaxy mock catalog is taken to demonstrate that the recovered initial conditions are closely unbiased with respect to the actual ones from the corresponding N-body simulation down to scales of a ~5 Mpc/h. The cross-correlation between them shows a substantial gain of information, being at k ~ 0.3 h/Mpc more than doubled. In addition the initial conditions are extremely well Gaussian distributed and the power-spectra follow the shape of the linear power-spectrum being very close to the actual one from the simulation down to scales of k ~ 1 h/Mpc.

Key words: (cosmology:) large-scale structure of Universe – galaxies: clusters: general – catalogues – galaxies: statistics

1 INTRODUCTION

The primordial density fluctuations of the Universe comprise all the information of the cosmological large-scale structure at any later time assuming that the theory of structure formation is known. Accurate estimates of the initial cosmic density field would hence also lead to a reconstruction of the formation of cosmic structures. This is one of the main motivations underlying constrained simulations of the local Universe (see e.g. Mathis et al. 2002, Klypin et al. 2003, Lavaux 2010). The reconstructed density field is especially valuable as it permits one to study the cosmic web and perform environmental studies (see e.g. Hahn et al. 2007, Forero-Romero et al. 2009, Jasche et al. 2010, Muñoz-Cuartas et al. 2011, Wang et al. 2012, Platen et al. 2011). Moreover, undoing the major effects of gravity on large scales has been shown to increase the cosmological information. For this purpose a large amount of techniques (mostly based on local transformations) has been developed which Gaussianise the cosmic density field (see e.g. Klypin et al. 2003, Lavaux 2010). I refer to a similar approach consisting on relating the observed positions of matter tracers (e.g. galaxies) in a geometrical way to a homogeneous distribution by minimizing a cost function (see e.g. Branchini et al. 2002). A similar approach consists on relating the observed positions of matter tracers (e.g. galaxies) in a geometrical way to a homogeneous distribution by minimizing a cost function (see e.g. Lavaux et al. 2008). One still needs then to find the corresponding Gaussian field to that point source distribution (see e.g. Lavaux 2010).

Ideally, one would wish to sample the density field δ(q) at the initial conditions {q} (Lagrangian positions) given the data at the present, in our case study, given a set of galaxies with their Eulerian coordinates {xG}:

\[
\delta\{q\} \sim P(\delta\{q\} | \{x_G\}),
\]

where the arrow indicates the sampling process. The relationship between both coordinate systems is summarised by the following equation: x = q + \Psi, where \Psi is the displacement which a particle suffers to go from its initial position q to its final position x. One

* E-mail: kitaura@aip.de, Karl-Schwarzschild-fellow

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should note that the structure formation model is encoded in the
displacement field $\Psi$. However, this direct approach is extremely
complex since the PDF is highly non-Gaussian as the galaxies live
in structures which have undergone nonlinear structure formation.
An attempt to find a statistical formulation of such a PDF im-
plies including the biased nature of a galaxy distribution beyond
the Poisson statistics (Kitaura 2012a) and higher order correlation
functions beyond the 2-point statistics (Kitaura 2012b). Such a sta-

tistical description could be relevant to deal with primordial non-
Gaussianities which will not be considered in this work.

I suggest in this letter to radically simplify the problem splitting
it into well defined ones which encode our physical understanding of
structure formation on large scales in a forward approach. In the next section, the method is presented in detail followed
by a validation section based on tests with synthetic data. Finally
the conclusions and discussion section is presented.

2 METHOD

Let us suppose that we have an unbiased sample of matter tracers at
initial (Lagrangian) positions $\{q\}$. The problem of the reconstruc-
tion of the primordial density fluctuations would be reduced to find
the Gaussian field corresponding to a discrete point-source distri-
bution. Once we knew the initial Gaussian field, we could apply a
model of structure formation and match the structures we find in
our simulation with the actual ones given by the observed galaxy
distribution in a likelihood comparison procedure. In this way an
iterative procedure can be constructed which yields a set of Gauss-
ian fields corresponding to the initial distribution of matter tracers
constrained on some data. The set of solutions will depend on the
particular structure formation model and the matching criteria.

In terms of conditional PDFs the two steps described above can be expressed in the following way:

\[ \delta(\{q\}) \sim P(\delta(\{q\})|\{q\}) \]  
\[ (\{q\}) \sim P(\{q\}|\{x_G\},\delta(\{q\}, m_{\text{SF}})) \],

where $m_{\text{SF}}$ denotes the assumed structure formation model.

(i) Step 1 (Eq. 2): Gaussianisation step: Sampling the Gaussian
field given a set of matter tracers at the initial conditions.

The first step can be solved using Bayes theorem. The posterior distribution
$P(\delta(\{q\})|\{q\})$ is given by the product of a Gaussian prior
and a Poissonian likelihood (see Kitaura & Enßlin 2008, Kitau-
ra et al 2010). We assume a Gaussian prior $P(\delta(\{q\})|C)$ de-
scribing the initial field $\delta(\{q\})$ which only depends on the corre-
lation function (variance) C or power-spectrum and thus on a set of
cosmological parameters. The likelihood $P(\{q\}|\delta(\{q\}))$ is mod-
eled by a Poissonian PDF describing the discrete nature of the test
particles at their Lagrangian positions. In order to sample from such
a posterior PDF the efficient Hamiltonian Sampling technique is
applied (see Jasche & Kitaura 2014, Kitaura et al 2012). This step
yields Gaussian fields on a mesh with $N_c$ cells. One should note that
similar approaches exist since long in the literature usually
known under the term constrained realisations (see Bertschinger
1987, Hoffman & Ribak 1991, van de Weygaert & Bertschinet
1996).

(ii) Step 2 (Eq. 3): Structure matching step: Likelihood com-
parison: Sampling the set of matter tracers at the initial condi-
tions given an initial Gaussian field and a galaxy distribution.

The second step requires a structure formation model linking the
initial Gaussian field to the observed structures given by the set of
galaxies $\{x_G\}$ to perform a constrained simulation. We need to
take the high dimensional statistical space spanned by the en-
semble of nonlinearly evolved density fields compatible with the
data. To find computationally feasible solutions we have to assume
at this stage a simplified structure formation model which remains
accurate on large-scales. Motivated by the recent findings in the
accuracy of tracing the cosmic structures back in time and esti-
mating the peculiar velocity fields with second order Lagrangian
perturbation theory (2LPT) we have chosen here to use this ap-
proximation (see Kitaura & Angulo 2012, Kitaura et al 2013).

In this framework we can compute the displacement field $\Psi(q)$ from the Gaussian field $\delta(\{q\})$ in an efficient way with FFTs. A random
homogeneous Poisson distribution of $N_p$ particles is moved to the
redshift in which the observations are present according to the pre-
viously computed displacement field. For technical details we refer to
Buchert (1994), Bouchet et al (1995), Bernardeau et al (2002).

We then assign a number of closest particles $N_{c,\{x_G\}}$ to each galaxy,
where each particle must be closer than a certain distance $d_{\text{max}}$.
The id’s of particles and galaxies are stored on a grid permitting us to look up fast
which particles are in the surrounding of a particular galaxy. In this
way each galaxy $x_G$ is assigned a set of particles $\{x\}$ answering
the question: where does the matter come from which formed
the structures we observe today. The galaxy bias that is put in this
method is given by the 2LPT halo bias constructed around galaxies
(for a review on the halo-model see Cooray & Sheth 2002). A sim-
ilar procedure was suggested by Scoccimarro & Sheth (2002). This
bias can be improved with a stochastic halo-model on top of the
2LPT realisation as performed in the same work. More sofisticated
approaches could be done based on halo occupation distribution
models (see the recent work by Manera et al 2013 and references
therein). This point needs to be further investigated. One should
notice that the first step searches for Gaussian fields compatible with
a given power-spectrum and in this way already partly corrects for

![Figure 1. Matter statistics. Black curve represents the PDF of the overdensity for the mean over 500 samples of the reconstructed initial Gaussian field. Shaded regions indicate 1 and 2 sigma contours. The dashed curve stands for the PDF of the nonlinear 2LPT reconstruction of the same sample. The average skewness, kurtosis and mean of the initial conditions are also indicated by $\langle S(\delta(\{q\})) \rangle$, $\langle K(\delta(\{q\})) \rangle$ and $\langle M(\delta(\{q\})) \rangle$, respectively.](image-url)
the bias in a $k$-dependent way. As we know the initial positions of the particles associated to each galaxy we obtain a distribution of Lagrangian positions $\{q\}$ which trace the initial Gaussian field. This closes one iteration permitting us to go to the first step again. In the first iteration the Gaussian field is assumed to be zero and thus the initial displacement field vanishes.

### 3 VALIDATION OF THE METHOD

In this section the numerical experiments are presented which have been performed to validate the method. As an input for our studies we have taken a galaxy catalogue which uses a semi-analytic halo-model scheme (De Lucia & Blaizot 2007) based on the Millennium Run simulation (Springel et al. 2005) with a box of 500 $h^{-1}$ Mpc side. In particular we have considered a uniform subsample of about 530 000 galaxies including all galaxy types conforming a nonlinear biased tracer of the underlying matter distribution.

This set-up permits us to test whether our reconstructions of the initial conditions and the cosmic web resemble the actual ones of the simulation.

We have made a great effort optimising our computer code KIGEN to cope with the hard computational task presented in this work (for the first version see Kitaura & Angulo 2012). We employ the Hamiltonian sampling technique in the Gaussianisation step based on the ARGO-code (first and last works Kitaura & Enßlin 2008; Kitaura et al. 2012) and the efficient 2LPT structure formation model with parallel FFTs.

To compute the Gaussianisation step (Eq. 2) and the displacement fields (Eq. 3) with FFTs we have used a mesh of $N_c=128^3$ cells. Structure formation was simulated using 2LPT with $N_p=384^3$ particles. Only particles closer than $d_{\text{max}} = 2 \, dL$ where considered to be friends of a galaxy with $dL = L/N_c^{1/3}$ being the cell side, allowing for up to $N_p^{1/3}=50$ particles associated to each galaxy. We have tested KIGEN with $N_p^{1/3}=1, 5, 10, 20, 30, 50$, finding a stable behaviour already with $N_p^{1/3}=20$. For safety we chose $N_p^{1/3}=50$ leaving a thorough analysis for future work. We gave equal weights to those particles, but could improve the method considering different weights for instance according to the luminosity of the galaxy. We have also performed tests with fewer particles finding a worse resemblance with the actual density fields from the simulation. Nevertheless, a careful study is still to be done to quantify the required number and weights of particles for a given resolution and different galaxy type. In addition, we discarded cells with less or equal 3 particles as such weak constraints correspond to very low density regions which are not correctly captured by the 2LPT approximation. Going to third order could mitigate this problem (see discussion in Scoccimarro & Sheth 2002).

We have performed 1500 iterations and found convergence in the matter statistics and the power-spectra of the reconstructed initial conditions after about 600 iterations. For safety we consider, however, only the last 500 iterations.

Let us start demonstrating that the first step in our reconstruction method leads to Gaussian distributed fields. Fig. 1 shows the matter statistics of 500 samples after convergence has been achieved. The continuous black curve shows the mean PDF of the overdensity for the 500 samples of the reconstructed initial Gaussian field after 1000 iterations. The low skewness, kurtosis and mean values indicate that it is indeed Gaussian distributed, whereas the gravitationally evolved field using 2LPT unveils a highly skewed PDF (dashed curve).

Fig. 2 shows the power-spectrum of the reconstructed initial conditions in comparison to the one corresponding to the galaxy overdensity field and the ensemble averaged power-spectrum of primordial fluctuations in a $\Lambda$-CDM Universe with the same cosmological parameters as in the Millennium Run (see Springel et al. 2005). The good agreement between the reconstruction and linear theory demonstrates that shot noise and gravitational nonlinear evolution have been removed. On large scales ($k < 0.2\,h^{-1}$ Mpc) we find that the fields reveal a great resemblance with the actual linear power-spectrum from the first snapshot of the simulation (see left panel of Fig. 2).

A visualisation of the results is given in Fig. 3. Here we show how the reconstruction of the initial field leads to constrained nonlinear density field estimates which nicely follow the structures traced by the galaxies. This is emphasised by the upper right panel in which the input galaxies are overplotted on top of the cosmic web reconstruction. It is also remarkable how difficult it is to recognise the cosmic web in the initial Gaussian field (lower left panel in the of Fig. 3), and nevertheless how accurately this field leads to the observed structures.

To quantify this resemblance we have computed the cell-to-cell correlation between the initial conditions $\delta(q)$ given by the first available snapshot of the Millennium Run at redshift $z=127$ and the galaxy field $\delta^G(x)$ in comparison to our reconstructed initial field $\delta^{\text{rec}}(q)$ after 1000 iterations (see upper panels in Fig. 3 for similar studies see Kitaura and Angulo 2011). We find that the complex nonlinear and nonlocal relation between the initial and final fields including galaxy biasing is straightened to a closely unbiased relation with our reconstruction scheme.

Finally we compute the propagator from the first available snapshot of the Millennium Run at redshift $z=127$ and the sample of reconstructed initial conditions after 1000 iterations and the galaxy overdensity, finding that the correlation is more than doubled at $k = 0.3\,h^{-1}$ Mpc. We can also see however, that a number of galaxies in low density regions, mostly living in small filamentary structures, do not match any structure of the recovered cosmic web. The reason is that those isolated galaxies which do not form groups do have a low number of particles associated to them which leaves them nearly unconstrained. We should also remind that the structure formation model we are using is simplified and especially fails in low density regions (see Scoccimarro & Sheth 2002).

### 4 CONCLUSIONS AND DISCUSSION

In this work I have presented a new approach to recover the initial conditions and the cosmic web structure underlying a galaxy distribution. The method is based on sampling Gaussian fields which are constrained on a galaxy distribution and a structure formation model.

This is achieved by splitting the inversion problem into two Gibbs-sampling steps: the first being a Gaussianisation step transforming a distribution of point sources at Lagrangian positions –which are not a priori given– into a linear alias-free Gaussian field. The second step being a matching procedure in which the set of matter tracers at the initial conditions is constrained on the galaxy distribution and the structure formation model we assume. For computational reasons we use second order Lagrangian Perturbation Theory. We demonstrate taking a semi-analytic halo-model based galaxy mock catalog that the recovered initial conditions are closely unbiased with respect to the actual ones from the corresponding $N$-body simulation down to scales of a few $h^{-1}$ Mpc. The cross-correlation between them shows a substantial gain of
Figure 2. **Left panel:** Ratio between the power-spectrum of the sample of 500 reconstructed initial Gaussian fields after 1000 iterations $P(k)$ and the power-spectrum from the first available snapshot of the Millennium Run at redshift $z = 127$ gridded with nearest grid point on a mesh with $128^3$ cells ($P_L(k)$) (black curve). The excess of power at high $k$ is due to aliasing. Dashed curve: same as previous case, but with power-spectrum $P(k)$ corresponding to the galaxy overdensity. Dotted curve: Same as continuous black curve, but with $P_L(k)$ being given by the theoretical $\Lambda$-CDM model. **Right panel:** power-spectra of the sample of 500 reconstructed initial Gaussian fields after 1000 iterations (black curve), the galaxy sample (dashed curve), and the theoretical $\Lambda$-CDM model (dotted curve). Shaded regions indicate 1 and 2 sigma contours.

Figure 3. Reconstruction of the initial conditions and of the cosmic web. **Upper left panel:** slice about $4\, h^{-1}\, \text{Mpc}$ thick averaged over 9 neighbouring slices through a galaxy catalogue (about 530,000 mock galaxies in a volume of $500\, h^{-1}\, \text{Mpc}$ side (De Lucia & Blaizot 2007)). Each galaxy is represented by a red circle. **Upper right panel:** same slice through a sample after 1000 iterations showing the logarithm of the reconstructed nonlinear matter density field using $384^3$ particles gridded on a $128^3$ mesh with triangular shape cloud. The mock galaxies corresponding to the same slice are over-plotted indicating the accuracy of the reconstruction method. **Lower left panel:** same slice through the reconstructed initial conditions corresponding to the same sample which are Gaussian distributed. **Lower right panel:** same as upper right panel without the mock galaxies.
The Initial Conditions

Figure 4. Cell-to-cell correlation after Gaussian smoothing with radius 5 h−1 Mpc between: the initial conditions δ(q) given by the first available snapshot of the Millennium Run at redshift z = 127 (left panel) and the galaxy field δc(q), (right panel) and the reconstructed initial Gaussian field after 1000 iterations δrec(q). The dark colour-code indicates a high number and the light colour-code a low number of cells.

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