Newtonian kinematical backreaction in cosmological \( N \)-body simulations with Delaunay Tessellation: “zero test” and scale dependence

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The backreaction of inhomogeneities describes the effect of inhomogeneous structure on average properties of the Universe. We investigate this approach by testing the consistency of cosmological \( N \)-body simulations as non-linear structure evolves. Using the Delaunay Tessellation Field Estimator (DTFE), we calculate the kinematical backreaction \( Q \) from simulations on different scales in order to measure how much \( N \)-body simulations should be corrected for this effect. This is the first step towards creating fully relativistic and inhomogeneous \( N \)-body simulations. In this paper we compare the interpolation techniques available in DTFE and illustrate the statistical dependence of \( Q \) as a function of length scale.

Keywords: large–scale structure, statistics, \( N \)-body simulations, interpolation techniques

1. Introduction

Inhomogeneous structure of the Universe at scales below \( 500 h^{-1} \) Mpc is an undeniable fact. The standard approach to model it (i.e., in the standard \( \Lambda \)CDM model approach) is to perturb the homogeneous solution of the Einstein equations, i.e. the Friedmann–Lemaître–Robertson–Walker (FLRW) metric. However, there are strong suggestions that this approach may not be the best one especially for the late times (i.e. small redshifts \( z \leq 3 \)) of the Universe evolution (e.g., Ref. 1).

Another approach, scalar averaging using general relativity (GR), introduces kinematical and curvature backreaction of the inhomogeneous structure of the Universe, in principle without assuming a homogeneous background. Here we focus only on the Newtonian version of this approach \([2, 3]\) since current \( N \)-body simulations are Newtonian (within the expanding FLRW background, which is rigid in comoving coordinates). Our motivation is to investigate whether the effect, namely kinematical backreaction \( Q \), described in Ref. 2, exists in \( N \)-body simulations as the model predicts, and check how big this effect is compared to that expected analytically.

2. Method

In the Newtonian approach there is only the kinematical backreaction\(^a\) \( Q \) which occurs in the generalised acceleration law:\([2, 3]\)

\[
3 \frac{\ddot{a}^D}{a^D} + 4\pi G \langle \rho \rangle^D - \Lambda = Q^D,
\]

\(^a\)Curvature backreaction is obviously zero because of the flat Euclidean spatial section.
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where

$$Q_D := \frac{2}{3} \left( \langle \theta^2 \rangle_D - \langle \theta \rangle_D^2 \right) + 2 \langle \omega^2 - \sigma^2 \rangle_D. \quad (2)$$

The volume-weighted average $\langle \cdot \rangle_D$ is defined as a volume integral normalised by the volume of the domain $D$ for which averaging is performed. The quantities $\theta$, $\omega$ and $\sigma$ are respectively the expansion rate and the rates of vorticity and shear, defined in the standard way as elements of the decomposition of the velocity gradient tensor $v_{i,j}$ in three parts: the trace $\theta$, the symmetric part $\sigma_{ij}$ and the antisymmetric part $\omega_{ij}$. Equation 2 can be rewritten in terms of the tensor invariants:

$$Q_D = 2 \langle \mathbf{I}(v_{i,j}) \rangle_D - \frac{2}{3} \langle \mathbf{II}(v_{i,j}) \rangle_D^2, \quad (3)$$

where

$$\mathbf{I}(v_{i,j}) = \text{tr}(v_{i,j}) = \theta, \quad (4a)$$

$$\mathbf{II}(v_{i,j}) = (\text{tr}(v_{i,j}))^2 - \text{tr}((v_{i,j})^2) = \omega^2 - \sigma^2 + \frac{1}{3} \theta^2 \quad (4b)$$

and $v_{i,j} := \partial_j v_i$.

### 2.1. Interpolating and averaging fields from N-body simulations

In order to calculate $Q$ from N-body simulations for a given domain $D$ one needs to interpolate the velocity field (and its gradient) from a discrete set of points, since in N-body simulations all information about fields is encoded in particles. There are several methods for interpolating fields from a set of points (e.g. SPH, CIC). We chose the Delaunay Tessellation Field Estimator\(^b\) (DTFE) \(^c\) method, which is based on Delaunay Triangulation (DT).\(^5\) The advantage of this choice is that it interpolates the velocity field and its gradients in a very natural way, i.e. by linear interpolation inside every Delaunay cell (a tetrahedron in the 3D case).\(^6\) Cells are constructed from a discrete set of points (particles) in such a way that every tetrahedron constructed from 4 particles fulfills the requirement that there is no other particle inside a sphere circumscribed on that tetrahedron.

### 2.2. “$Q_C = 0$” test for periodic boundary condition

From (2) and (1) it is clear that the backreaction $Q$ in the Newtonian approach is purely of a kinematical origin. Moreover, because of the way in which it is defined, it will always be zero if there is no boundary, e.g. if the “boundaries” are periodically identified, as is the case for cosmological numerical simulations.\(^c\) This is due to the

\(^b\) The code is free-licensed and available at: [http://www.astro.rug.nl/~voronoi/DTFE/dtfe.html](http://www.astro.rug.nl/~voronoi/DTFE/dtfe.html). DTFE uses CGAL—the Computational Geometry Algorithms Library, also free-licensed ([http://www.cgal.org/](http://www.cgal.org/)).

\(^c\) The problem of boundaries in cosmological simulations is “solved” by setting up a $T^3$ topology of the simulation box, i.e. periodic translation of the fields through the opposite faces of the simulation box.
Kinematical backreaction $Q$ with DTFE

The fact that, by using Gauss’ theorem, $Q_D$ in comoving coordinates can be expressed as an integral over the surface $\partial D$ (see eq. (10) of [2]). This gives the possibility to test existing simulations for consistency if they preserve $Q_C = 0$ ($C$ denotes the whole simulation domain with $T^3$ topology, “periodic boundary conditions”). If one divides the whole simulation box domain onto $N^3$ smaller cubes (or domains of another shape) of equal volume $|D_n| = |C|/N^3$, then the following equation will be valid:

$$Q_C = 2\langle \Pi_C \rangle - \frac{2}{3} \langle I_C \rangle^2 = \frac{2}{N^3} \sum_{n=1}^{N^3} \Pi_{D_n} - \frac{2}{3} \left( \frac{1}{N^3} \sum_{n=1}^{N^3} I_{D_n} \right)^2 = 0 \quad (5)$$

for $N > 0$.

3. Results

For calculations we used Einstein–de Sitter ($\Omega_m = 1, \Omega_\Lambda = 0$) $N$-body simulations: (i) a Virgo Consortium (VC) simulation from [7] (simulation SCDM1, hereafter VC EdS) and (ii) our own simulation performed with Gadget-2 (hereafter, Gadget-2 EdS) with the same box size and number of particles and cosmological parameters as in VC EdS (simulation box size: $240h^{-1}$ Mpc, $256^3$ particles, $h = 0.5$).

We tested vanishing $Q_C$ with periodic boundary conditions (the “$Q_C = 0$” test) with $4 \leq N \leq 512$. For any $N$, this sets up the grid resolution which corresponds to sub-box domains $D_n$ of a fixed size ($n = 1, \ldots, N$); and probes all ranges of scales from $L_C/512$ to $L_C/4$ for a simulation with a box side length $L_C$. The velocity gradient was calculated using DTFE with the default volume averaging method, i.e. Monte Carlo sampling over DT cells with approximately 100 samples$^3$ per each grid cell for a given estimate.

Figure 1 shows $Q_C$ as a function of the size $L_{D_n} = L_C/N$ of sub-domains $D_n$ (eq. 5), or equivalently, as a function of $N$. $Q_C$ does not stay close to zero for every $N$, particularly for $N$ ranging from 128 to 512, where $Q_C$ is negative for both the VC EdS and Gadget-2 EdS simulations (top panels of fig.1). This corresponds to $2h^{-1}$ Mpc $\gtrsim D_n \gtrsim 0.5h^{-1}$ Mpc. Moreover fig. 1 shows $\langle I \rangle_C$ (middle panels) and $\langle \Pi \rangle_C$ (bottom panels) from which—with respect to the $D_n$—$Q_C$ was calculated. It is clear that negative values of $Q_C$ comes from $\langle \Pi \rangle_C$. Equation (4b) shows that this significant deviation from zero values comes either from overestimation of $\sigma$ or underestimation of $\omega$ and/or $\theta$, since the square of the former provides a negative contribution and square of the latter two positive input to $\langle \Pi \rangle_C$ (see eq. (4b)).

For a regular grid such as the one used here, DTFE has two built-in methods of interpolating fields to a grid location followed by a local averaging procedure (hereafter, “averaged interpolation”): (i) sampling randomly over Delaunay cells (hereafter, the DT method; as in fig. 1); or (ii) sampling (randomly or not) within

$^3$The number of samples depends on the ratio between the DT cell volume and the chosen grid cell volume.
the grid cell (hereafter, the grid method). We have performed the same test for both averaged interpolation methods, and varied the numbers of random samples.

Figure 2 compares these two methods for the “$Q_C = 0$” test with the VC EdS simulation. The DT method (solid red line) is less noisy in general, but produces strong negative values for $128 \leq N \leq 512$. Grid sampling (dashed green line) is more noisy (especially for high $z$) but does not produce this feature for $N \gtrsim 120$, even though the sample size per grid cell (by default, 20 random samples) is lower than for the DT method. When $N$ is high, the number of particles per grid cell is low, so that Delaunay cells will be large compared to a grid cell; thus, a systematic error in volume-weighted averaging of the velocity gradient could occur by sampling within the local Delaunay cells rather than within the grid cell. This may explain the DT-method high-$N$ negative $Q_C$ values, in which case increasing the sample size should weaken the negative $Q_C$—figure 3 supports this.

3.1. Statistics of $Q$—early results
Motivated by the $Q_C = 0$ analysis, the DT method, with random sample size increased to 300 and grid size $N = 100$, was used to estimate probability density
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![Graph showing comparison of interpolation methods](image)

Fig. 2. Comparison of two interpolation methods: sampling over DT cells (red, solid line) and sampling over grid cells (green, dashed line) for $z = 0$ (left top pane), $z = 1.5$ (right top), $z = 5$ (left down) and $z = 10$ (right down).

functions (PDF) of $Q_D$ for the VC EdS simulation at redshift $z = 0$. Figure 4 shows PDFs for three different domain $D$ sizes, $L_D = 20, 40, 60 \, h^{-1} \text{Mpc}$; in each case, 200 domains were chosen randomly. There is clear evidence of statistical scale dependence for $Q_D$: the smaller the domain $D$, the more negative $Q$ tends to be (fig. 4). More detailed calculations will be published soon.

4. Summary

Using DTFE to perform the “$Q_C = 0$ test” for the VC EdS and Gadget-2 EdS simulations suggests that the DT method (sampling over DT cells) introduces artificial behaviour for small grid cells, i.e. when the number of grid cells is comparable to the number of particles in simulation. At early epochs, the magnitude of the effect is comparable to that of the noise of the grid-sampling averaged interpolation method for big grid cells (low numbers of grid cells). This systematic error can be reduced by increasing the number of random samples used for averaged interpolations within Delaunay tetrahedra (fig. 3), at the cost of slowing the calculation. The code could be improved by implementing an exact calculation of volume-weighted averages in each grid cell (i.e. averaging the interpolation without random sampling). The PDFs of $Q$ show statistical scale dependence (fig. 4).
Fig. 3. DT interpolation method (sampling in Delaunay cells) as a function of sample size for VC EdS, \( z = 0 \): 50 samples — green, 100 — blue (default), 200 — red.

Fig. 4. Histogram of \( Q_D \) from sample of 200 times randomly chosen domain \( D \) of three different sizes: 20\( h^{-1} \) Mpc, 40\( h^{-1} \) Mpc and 60\( h^{-1} \) Mpc divided by \( H_0^2 \) in order to have dimensionless units.

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