Abstract. This work reports on a study of the spatially coarse-grained velocity dispersion in cosmological N-body simulations (OCDM and ΛCDM models) as a function of time (redshifts $z = 0–4$) and of the coarsening length ($0.6–20 h^{-1}$Mpc). The main result is the discovery of a polytropic relationship $I_1 \propto \rho^{2-\eta}$ between the velocity-dispersion kinetic energy density of the coarsening cells, $I_1$, and their mass density, $\rho$. The exponent $\eta$, dependent on time and coarsening scale, is a compact measure of the deviations from the naive virial prediction $\eta_{\text{virial}} = 0$. This relationship supports the “polytropic assumption” which has been employed in theoretical models for the growth of cosmological structure by gravitational instability.

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

1. Introduction

Some recent works (Barbero et al. 1997; Buchert & Domínguez 1998; Buchert et al. 1999; Adler & Buchert 1999; Adler et al. 1999; Maartens et al. 1999; Buchert et al. 1999; Maartens & Tatekawa 2001; Domínguez 2000; Domínguez & Tatekawa 2002; Tatekawa et al. 2002) have explored a formulation of hydrodynamic kind for the formation of cosmological structures by gravitational instability. It intends to describe the dynamical evolution of the few most relevant fields (typically the coarse-grained mass density and velocity fields) in terms of a set of autonomous equations for those fields, much in the same way as the hydrodynamic equations for usual fluids. The widely used dust model (Peebles 1980; Sahni & Coles 1995) belongs to this class, but it has shortcomings, most noticeably the emergence of singularities, beyond which its application is invalid. An interesting result of the systematic study of the hydrodynamic formulation are the corrections to the dust model. They arise from the nonlinear coupling of the evolution to the structure below the coarsening length, and turn out to be relevant in the nonlinear regime ($\leftrightarrow$ the regime of large density fluctuations about homogeneity). The corrected equations are generalizations of the adhesion model (Kofman & Shandarin 1988; Gurbatov et al. 1989; Kofman et al. 1992; Melott et al. 1994).

Sathyaprakash et al. 1995, which is able to reproduce successfully the gross features of the structure evolved by gravitational instability in different cosmological scenarios. The hydrodynamic formulation requires the corrections to dust to be expressed as functions of the coarse-grained mass density and velocity fields, so as to get a closed set of equations for these fields. This is, however, a major theoretical problem, since one cannot follow the standard procedure to close the hydrodynamic hierarchy by invoking “local thermal equilibrium” (Huang 1987; Balescu 1991): the ideas and the formalism of thermodynamics cannot be applied straightforwardly to a system dominated by its own gravity, this being in fact still an open question (see, e.g., the concise review by Hut (Hut 1997)).

In this work I report on the empirical search for closure relationships with the help of N-body simulations of large-scale structure formation. I consider in particular the velocity dispersion of the particles contained in any coarsening cell, which shows up in the equation for momentum conservation (in the hydrodynamic parlance, the kinetic contribution to the pressure and to the viscous stresses). The simulation results for the trace of the velocity dispersion (the internal kinetic energy density of the coarsening cells) can be fitted quite well by a “polytropic relationship”, borrowing the terminology from thermodynamics: $I_1 \propto \rho^{2-\eta}$. This result supports the polytropic approximation used in the theoretical derivation of adhesion-like models (Buchert et al. 1999). The poly-

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tropic relationship improves with time, and so I conclude that it must be a consequence of the evolution by gravitational instability. For small coarsening lengths or large times, the exponent \( \eta \) is close to, but significantly different from the virial prediction following from the simple model of isolated, relaxed, structureless halos.

The degree of anisotropy of the velocity dispersion (the departure from a spherically symmetric distribution of the dispersion) has also been studied, but in this case the scatter of the data is large and the results do not provide a significant conclusion. The anisotropy tends to decrease with increasing comoving smoothing scale \( \Lambda \). The degree of anisotropy of the velocity dispersion (the scatter) where

\[
\frac{\sigma_{\perp}}{\sigma_{\parallel}} = \left( \frac{aL}{m} \right) \sum_{\alpha=1}^{N} \left[ \mathbf{u}_\alpha(t) - \mathbf{u}(x, t) \right] \otimes \left[ \mathbf{u}_\alpha(t) - \mathbf{u}(x, t) \right] W \left( \frac{x - x_\alpha}{L} \right).
\]

(\( \Pi \) is a second-rank tensor, \( \otimes \) denoting a dyadic product). Here, \( a(t) \) denotes the expansion factor, \( m \) is the mass of a particle, \( x_\alpha \), and \( \mathbf{u}_\alpha \) represent the comoving position and peculiar velocity, respectively, of the \( \alpha \)-th particle, and \( W(\cdot) \) is a (normalized) smoothing window. Exact dynamical equations can be derived for \( \varrho \) and \( \mathbf{u} \), expressing mass and momentum conservation; the latter equation features the velocity dispersion in the form of a term \( \nabla \cdot \Pi \). The purpose of the present study is to check if there exists any approximate relationship between \( \Pi \) and the field \( \varrho \), so that an autonomous set of equations can be written for the fields \( \varrho \) and \( \mathbf{u} \).

Starting from the coordinates \( \{ x_\alpha, \mathbf{u}_\alpha \}_{\alpha=1}^{N} \) provided by the simulation, the definitions \( \Pi \) were implemented with a cubic top-hat window,

\[
W(z) = \theta(1 - 2|z_1|) \theta(1 - 2|z_2|) \theta(1 - 2|z_3|),
\]

where \( \theta(\cdot) \) is the step function. In total 13 different values of \( L \) were explored, spanning the range from 0.6 \( h^{-1} \text{Mpc} \) up to 20 \( h^{-1} \text{Mpc} \) and equally separated in a logarithmic scale. For each value of \( L \), at least \( 2 \times 10^4 \) randomly centered, non empty coarsening cells were probed.

The velocity dispersion tensor \( \Pi_{ij}(x) \) was studied as a function of the density \( \varrho(x) \), or equivalently, of the number of particles contained in the cell at \( x \), namely \( n(x) = [m a L^3] / \varrho(x) \). For the purposes of this work, it sufficed to consider the three eigenvalues \( \lambda_i \) of the tensor \( \Pi \), or better, its three principal scalar invariants:

\[
I_1 = \text{tr} \Pi = \lambda_1 + \lambda_2 + \lambda_3,
\]

\[
I_2 = \frac{1}{2} \left[ (\text{tr} \Pi)^2 - \text{tr} (\Pi : \Pi) \right] = \lambda_1 \lambda_2 + \lambda_2 \lambda_3 + \lambda_3 \lambda_1,
\]

\[
I_3 = \det \Pi = \lambda_1 \lambda_2 \lambda_3.
\]

The quantity \( (1/2)I_1 \) is the peculiar kinetic energy per unit volume due to the motion of the particles relative to the cell.
center of mass. The other two invariants can be related to the degree of anisotropy of the tensor $\Pi$. More precisely, the dimensionless coefficients

$$\alpha = 1 - \frac{3 I_2}{I_3}, \quad \beta = 1 - \frac{27 I_3}{I_3},$$

(4)

quantify the departure from the isotropic case, $\lambda_1 = \lambda_2 = \lambda_3 = p$. I show in the Appendix that $0 \leq \alpha, \beta \leq 1$, and they vanish if and only if $\Pi$ is isotropic. Moreover, it follows from its definitions that $\beta \approx 3\alpha$ for small anisotropy.

To check that this smoothing algorithm was right, it was applied to an ideal gas simulation. The results for the dependence of the kinetic pressure $p = (1/3)\Pi_3$ and the anisotropy parameters $\alpha, \beta$ on $n$ agree with the predicted relationships (see the Appendix).

In the next Section I also discuss how the results depend on the smoothing details (e.g., on the choice of the window). I anticipate that the conclusions to be extracted are robust.

3. Results

The results concerning the three invariants as a function of the particle number are qualitatively the same in the whole range of smoothing scales and times explored, and for the two cosmological models OCDM and $\Lambda$CDM. Fig. 1 is a typical example of a $I_3$ vs $n$ scatter plot. The data suggest a polytropic relationship between the scalar invariants and $n$, more and more accurate for larger $n$. Hence, it appears that the increasingly larger scatter for smaller particle numbers is mainly due to the discrete character of the variable $n$. To eliminate this noise, the log-log plots of the raw data were binned into 40 subintervals on the $n$-axis: this effectively means averaging the scalar invariants for different fixed values of $n$ and provides also an estimate of the variance. This scatter is in fact the main source of error in the parameters $\eta$ and $\kappa$ of the fit. Fig. 2 collects a set of representative cases after implementation of this procedure, where the advocated polytropic dependence is evident. To be sure that this averaging method does not introduce artificial features, the analysis was repeated by varying the number of bins, from 10 up to the limiting case in which each possible value of the discrete variable $n$ is treated as a bin. The conclusions are robust and the results do not depend on the amount of binning. (Changes of the number of bins within this range induce variations in the best-fit parameters $\eta$ and $\kappa$ which are well within the error region in Fig. 5). The choice of 40 bins is a good compromise that efficiently discards the noise but still preserves the relevant features of the $I_3$-$n$ relationship.

Another check probed the influence of the choice of smoothing window. The differences found between different windows could be explained as a consequence of the discrete nature of $n$. Fig. 3 shows the typical result after using three different smoothing windows: a cubic top-hat, Eq. (4), a spherical top-hat, $W(z) = \theta(1 - (4\pi/3)^{1/3}|z|)$, and a Gaussian, $W(z) = \exp(-\pi|z|^2)$. The windows are normalized to unity and give the same weight ($=1$) to the origin: the comparison is then straightforward. The cubic and spherical top-hat windows yield indistinguishable results, demonstrating that window anisotropy is not relevant (this could also be

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Fig. 2. Binned log-log plot of the trace of the velocity dispersion tensor (same units as Fig. 1) vs the number of particles for the $\Lambda$CDM model. The error bars correspond to the estimated 1-$\sigma$ variance. On the left, for three redshifts (from top to bottom, $z = 3.6, 1.4, 0$) at a fixed smoothing length $L = 4.55\ h^{-1}\text{Mpc}$. On the right, for three smoothing scales (from top to bottom, $L = 1.41, 4.55, 8.33\ h^{-1}\text{Mpc}$) at a fixed redshift $z = 1.4$. The solid line corresponds to the fit (6), and the dashed line marks $n_c$, Eq. (5).
expected, see the last paragraph in this Sec.). The Gaussian smoothing also gives similar results, but now a slight difference in the small-$n$ end is observed, because the discreteness of $n$ implies (i) that $\Pi = 0$ if $n = 1$ for the top-hat windows and (ii) that for small $n$, $\Pi$ is dominated by far contributions from the Gaussian tails. However, as discussed later, the discreteness constraint $\Pi = 0$ if $n = 1$ for a top-hat window can be taken into account in a simple manner and indeed the polytropic fit holds very well even for $n \sim 1$. Hence, the cubic top-hat window was selected, because it is also most easily implemented.

A final check, carried out only for the particular time $z = 0$, was to restrict the coarsening procedure to a subvolume of the simulation box (1/64 of the total volume), so as to find out to what extent the results are exclusive of the simulation volume of $100\, h^{-1}\text{Mpc}$ side length: as expected, the quality of the fits are slightly worse because of the reduced number of particles, but the conclusions remain the same.

As exemplified by Fig. 2, one finds a well defined relationship between $I_1$ and $n$, in which three different behaviors can be identified: a polytropic dependence $I_1 \propto n^{2-\eta}$ for $n$ larger than a certain value $n_c$, a bending upwards for $1 < n < n_c$, and finally a bending downwards for $n$ close to 1 which is due to the constraint $\Pi = 0$ if $n = 1$. The intermediate behavior is absent at late times/small coarsening lengths, when it is masked by the latter constraint. The value of $n_c$ increases with the redshift and the smoothing length. A rough estimate by eye of the function $n_c(L, z)$ is given by

$$n_c = F(z)\bar{n}_L, \quad \bar{n}_L := (86\, L/100)^3.$$  

(5)

$\bar{n}_L$ is the average particle number in a cell of comoving side length $L$ (in units of $h^{-1}\text{Mpc}$), and $F(z)$ is a mild function of the redshift, $F = 1$ for $z = 3.6$ and decreases slowly for smaller $z$ ($F = 0.25$ for $z = 0$). This fit for $n_c(L, z)$ is conservative in the sense of slightly overestimating $n_c$ as $L$ decreases, however it is precise enough: Fig. 2 shows that the polytropic fit is in fact still well followed by the data for a certain range below the chosen $n_c$. The best-fit parameters $\eta$ and $\kappa$ in Eq. (6) are quite insensitive to the precise value of $n_c$. The intermediate range $1 < n < n_c$ corresponds to underdense cells ($n_c$ is associated to a density contrast $\delta_c = F(z) - 1$); the deviations from the polytropic fit may then be a remnant of the artificial discreteness, most evident in the lattice structure of the initial conditions. Nonetheless, this failure of the polytropic relationship is likely unimportant from a dynamical point of view, being restricted to ever more rarefied regions ($\delta_c \approx -0.75$ at $z = 0$).

The binned data in the range $n > n_c$ were fitted to the polytropic relationship

$$I_1 = \frac{m}{(aL)^3} \kappa (n - 1)^{2-\eta}. \tag{6}$$

The factor $n - 1$ enforces the discreteness constraint $I_1 = 0$ for $n = 1$. This improves the fit on the small-$n$ region in the cases that it extends down to $n \sim 1$ and it is also suggested by the simulated ideal gas: the ideal gas pressure-density relation is still obeyed with the replacement $n \rightarrow n - 1$ when the smoothing length is so small that most of the coarsening cells contain just a few particles. The parameters $\eta$ and $\kappa$ were determined by the least-squares method. The fit was carried out only when the fit range in $n$ spanned at least a decade (in which case the range in $I_1$ always extends over at least two decades); the polytropic fit is still consistent when this condition is not met, but the large errors deprive it of significance. In the best cases, the fit range in $n$ included three decades. The time and smoothing-length dependences of the parameters $\eta$ and $\kappa$ for the CDM model are plotted in Fig. 3. The results for the OCDM model are very close.

The other two invariants, $I_2$ and $I_3$, are also fitted by a polytropic dependence. In fact, it turns out that the anisotropy parameters $\alpha$ and $\beta$ computed with the fitting functions are extremely small and $n$-independent. The reason is that the binned (=averaged) velocity dispersion, being only a function of the scalar $n$, must be isotropic. The anisotropy parameters must be calculated for the raw data, before binning: Fig. 3 shows a typical $\alpha$ vs $n$ scatter plot. The plots of the parameter $\beta$ look similar (in fact, the relation $\beta \approx 3\alpha$ is a very good approximation already for $\alpha \approx 0.1$: then, one should rather study, e.g., $\beta - 3\alpha$ to gain non-redundant information). Apart from the large scatter for small particle number due to the discreteness of $n$, there is also an important dispersion even for large $n$, because the anisotropy must be determined by something else than only a scalar. Moreover, unlike the “extensive” scalar invariants (= sums of positive contributions from many particles), the anisotropy parameters, being essentially the difference between eigenvalues, Eqs. (5), are more sensitive to the discreteness of $n$. Thus, the data quality just allows to confirm that $\alpha$ and $\beta$ tend to decay with increasing $n$ but to remain somewhat larger than the average ideal gas anisotropy, $\alpha_{\text{ideal}} \approx 5/(3n)$ (see the Appendix). No significant dependence (if any) with time and smoothing length could be detected.
4. Discussion and conclusion

The simulations show a clear evidence for a polytropic relationship between the density and the scalar invariants of the velocity dispersion tensor. The fits improve with decreasing redshift or smoothing scale; hence one is lead to view them as a general consequence of the evolution by gravitational instability in a hierarchical scenario. The points for \( n = 1.4 \) are close to the virial predictions for small scales/large times; but the deviations of \( \eta \) are about the same size as the plot symbols. The virial prediction reads \( \eta = 0 \) and \( \kappa \propto 1/L \) (solid line in the \( \kappa \)-plot).

A theoretical argumentation by Buchert and Domínguez (Buchert & Domínguez 1998) provides a polytropic relationship with a fixed \( 2 - \eta = 5/3 \); this is equivalent to the adiabatic evolution of an ideal gas and was justified for early times and under restrictive initial conditions. However, Fig. 4 shows that, precisely in the opposite limit of nonlinearity, \( \eta \) is close to this “adiabatic value”, which even seems to be an asymptote. But the errors are too large and the probed range of nonlinear lengths too narrow to draw a firm conclusion.

This flattening of \( \eta(L) \) suggests another possible explanation of the polytropic relationship. It seems sensible to hypothesise that, for smoothing lengths \( L \) well in the nonlinear regime, the kinetic energy should be fixed by the virial theorem: if the coarsening cells can be idealized as virialized, structureless halos, then \( (aL)^3 I_1 \) should be proportional to the potential gravitational energy of the coarsening cell, which could in turn be estimated as \( \sim G (m n)^2 / a L \). This implies immediately a polytropic dependence with \( \eta_{\text{virial}} = 0 \) and \( \kappa_{\text{virial}} \propto (aL)^{-1} \). This idealized model was employed to simulate scatter plots as Fig. 1 assume exact isotropy (\( \alpha = \beta = 0 \)) and the same distribution of particle numbers \( n \) as obtained in the simulations, and compute \( I_1 \) from the condition that the differences \( u_n - u \) in the definition of \( I_1 \) of \( \Pi \) are independent, Gaussian distributed random variables with zero mean and a variance given by the virial theorem. In this way, an estimated \( \sigma < 2 \cdot 10^{-3} \) for \( \eta_{\text{virial}} \) was gained. Fig. 4 shows that the best-fit values of \( \eta \) and \( \kappa \) are close to the virial predictions for small \( L \); but the deviations of \( \eta \) are well above the estimated fluctuations in \( \eta_{\text{virial}} \).

Fig. 4. Plot of the best-fit parameters in Eq. (6) vs the smoothing length for the \( \Lambda \)CDM model at the three times studied; \( \kappa \) in units of \( \text{km}^2 \text{s}^{-2} \). The scale of nonlinearity is \( r_0 \), Eq. (4). The two lines in the \( \eta \)-plot delimit the estimated 1-σ error region at time \( z = 0 \) (the errors are of the same size at the other times and they have been omitted for clarity). The error bars for \( \kappa \) are about the same size as the plot symbols. The virial prediction reads \( \eta = 0 \) and \( \kappa \propto 1/L \) (solid line in the \( \kappa \)-plot).
APPENDIX A: THE ANISOTROPY PARAMETERS $\alpha$ AND $\beta$

In this Appendix I derive some properties of the anisotropy parameters defined in Eqs. (4). Since the tensor II is positive-definite, then $\lambda_i \geq 0$. This implies the bounds $0 \leq \alpha, \beta \leq 1$. In fact, $\mathcal{I}_i \geq 0$ yields immediately that $\alpha, \beta \leq 1$. On the other hand, for any triplet of non-negative numbers, the following inequalities hold (Abramowitz & Stegun 1965):

$$\sum_{i=1}^{3} \lambda_i^2 \geq \lambda_1 \lambda_2 + \lambda_2 \lambda_3 + \lambda_3 \lambda_1,$$

$$\frac{1}{3} \sum_{i=1}^{3} \lambda_i \geq (\lambda_1 \lambda_2 \lambda_3)^{1/3},$$

and the equality is satisfied if and only if all three numbers are equal. Combining these inequalities with the definitions (4), it is found that $\alpha$ and $\beta$ must be non-negative, and they are zero if and only if the tensor II is isotropic.

Let us write $\lambda_i = \frac{1}{3} \mathcal{I}_i + \delta \lambda_i$, so that the coefficients $\delta \lambda_i$ represent the deviation from isotropy and satisfy $\sum_i \delta \lambda_i = 0$. Then:

$$\alpha = -\frac{3}{\mathcal{I}_1} \sum_{i<j} (\delta \lambda_i)(\delta \lambda_j),$$

$$\beta = 3\alpha - \frac{27}{\mathcal{I}_1} (\delta \lambda_1)(\delta \lambda_2)(\delta \lambda_3),$$

and in the limit of small anisotropy, $|\delta \lambda_i| \ll \mathcal{I}_1$, the equality $\beta \approx 3\alpha$ holds.

The simulations of the ideal gas provide $\langle \alpha_{\text{ideal}} \rangle_n \approx 5/(3n)$ with a large scatter, for the reason discussed towards the end of Sec. 5. Therefore, a very interesting result is that the violations to the “virialized halo” conditions (i-ii) do not destroy the polytropic relationship itself predicted by the virial theorem, but only change the values of the parameters.

In conclusion, N-body simulations have provided evidence for a polytropic relationship between the coarse-grained mass density and the peculiar kinetic energy. This relation can be characterized by an exponent $\eta$ which measures the (scale and time dependent) departures from the “virialized halo” prediction. It was found that, for smoothings lengths well in the nonlinear regime, $\eta$ is significantly larger than zero. There still remains the task of theoretically explaining this polytropic dependence. Future work in this direction will address scale-invariant cosmological models: they provide testbed cases which can be easily controlled in simulations and easily analyzed theoretically.

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