A new method for accurate estimation of velocity field statistics

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ABSTRACT

We introduce two new methods to obtain reliable velocity field statistics from N-body simulations, or indeed from any general density and velocity fluctuation field sampled by discrete points. These methods, the Voronoi tessellation method and Delaunay tessellation method, are based on the use of the Voronoi and Delaunay tessellations of the point distribution defined by the locations at which the velocity field is sampled. In the Voronoi method the velocity is supposed to be uniform within the Voronoi polyhedra, whereas the Delaunay method constructs a velocity field by linear interpolation between the four velocities at the locations defining each Delaunay tetrahedron.

The most important advantage of these methods is that they provide an optimal estimator for determining the statistics of volume-averaged quantities, as opposed to the available numerical methods that mainly concern mass-averaged quantities. As the major share of the related analytical work on velocity field statistics has focused on volume-averaged quantities, the availability of appropriate numerical estimators is of crucial importance for checking the validity of the analytical perturbation calculations. In addition, it allows us to study the statistics of the velocity field in the highly non-linear clustering regime.

Specifically we describe in this paper how to estimate, in both the Voronoi and the Delaunay methods, the value of the volume-averaged expansion scalar $\theta = H^{-1} \nabla \cdot \mathbf{v}$ (the divergence of the peculiar velocity, expressed in units of the Hubble constant $H$), as well as the value of the shear and the vorticity of the velocity field, at an arbitrary position. The evaluation of these quantities on a regular grid leads to an optimal estimator for determining the probability distribution function (PDF) of the volume-averaged expansion scalar, shear and vorticity. Although in most cases both the Voronoi and the Delaunay methods lead to equally good velocity field estimates, the Delaunay method may be slightly preferable. In particular it performs considerably better at small radii. Note that it is more CPU-time intensive while its requirement for memory space is almost a factor 8 lower than the Voronoi method.

As a test we here apply our estimator to that of an N-body simulation of such structure formation scenarios. The PDFs determined from the simulations agree very well with the analytical predictions. An important benefit of the present method is that, unlike previous methods, it is capable of probing accurately the velocity field statistics in regions of very low density, which in N-body simulations are typically sparsely sampled.

In a forthcoming paper we will apply the newly developed tool to a plethora of structure formation scenarios, of both Gaussian and non-Gaussian initial conditions, in order to see to what extent the velocity field PDFs are sensitive discriminators, highlighting fundamental physical differences between the scenarios.

Key words: methods: numerical – methods: statistical – cosmology: theory – large-scale structure of Universe.

1 INTRODUCTION

Besides the distribution of galaxies and the temperature fluctuations in the cosmic microwave background, and possibly weak gravitational lensing of background galaxies by large-scale structures (see e.g. Villumsen 1995), the velocity field on cosmological scales is one of the main sources of information on the formation and evolution of structure in the Universe.
Early work indicated the existence of large-scale velocity flows (Rubin et al. 1976) and established the existence of the motion of the Local Group with respect to the rest-frame defined by the microwave background (Smoot & Lubin 1979). However, it was the work by Burstein et al. (1987) that established beyond doubt that the Local Group is participating in a large-scale streaming motion.

The advent of reliable redshift-independent distance estimators led to an enormous growth of activity in the field of measuring and interpreting the peculiar velocities of galaxies. This growth of attention was evidently fed by the fact that the velocity field provides direct information on the dynamics of the Universe on scales of more than a few Mpc. Above these scales dynamical relaxation has not had yet a chance to wash out the memory of the conditions in the early Universe. The velocity field can therefore be fruitfully investigated by means of perturbation analysis. Particularly useful is the (Ω-dependent) velocity–density relationship that follows from linear theory (see e.g. Peebles 1980). Moreover, a general result of perturbation theory predicts that the rotational part of the velocity field vanishes. Based on this observation Bertschinger & Dekel (1989) developed the non-parametric POTENT method in which the local cosmological velocity field is reconstructed from the measured line-of-sight velocities. In a series of papers (e.g. Bertschinger et al. 1990), they applied their method to the existing catalogues of galaxy peculiar velocities.

The POTENT analysis also paves the way for a more quantitative analysis of the velocity field, estimating various statistical properties and their relation to the properties of the density field. For instance, via the velocity–density relationship it is possible to reconstruct the corresponding density field or, by comparison with a uniformly sampled galaxy redshift catalogue (in particular the IRAS-based redshift catalogues, e.g. Strauss et al. 1990), obtain an idea of to what extent the galaxy distribution forms a biased tracer of the underlying mass distribution. If it is assumed that this bias can be simply represented by a linear bias factor b, the value of \(b^2\) can be estimated from the measured peculiar velocity field and a uniformly sampled redshift catalogue (e.g. Yahil et al. 1991).

A variety of other methods have been proposed to determine this combination of \(Ω\) and \(b\) (see the review paper of Dekel 1994 and references therein). On the basis of a more specific statistical analysis, in particular of the velocity divergence, other studies managed to determine these two parameters separately. For example, Nusser & Dekel (1993) proposed to use a reconstruction method assuming Gaussian initial conditions to constrain \(Ω\), while Dekel & Rees (1994) used voids to achieve the same goal.

Another approach has been proposed by Bernardet et al. (1995) and Bernardau (1994a). This is based on the use of statistical properties of the divergence of the locally smoothed velocity field, its skewness (the third-order moment) and its kurtosis (fourth-order moment). It was shown that these statistical quantities are potentially very valuable to measure \(Ω\) or to test the gravitational instability scenario. The early analytical work was subsequently extended towards the determination of the complete velocity divergence probability distribution function for gravitational instability scenarios starting from Gaussian initial conditions in the case that the velocity field is filtered by a top-hat window function. Preliminary comparisons with numerical simulations (Bernardeau 1994b; Juszkiewicz et al. 1995; Łokas et al. 1995) yielded encouraging results. However, a comparison of the analytical results with the PDFs determined from N-body simulations is complicated considerably by the fact that in the latter velocities are only known at (non-uniformly distributed) particle locations.

In this paper we address specifically the issue of the discrete nature of the velocity sampling, which leads to the development of a numerical method to obtain reliable velocity field statistics from N-body simulations. The goal is threefold. First of all, we wish to have an independent way of checking whether the perturbation calculations that yield the quasi-linear results are indeed valid. Secondly, if so, these analytical results form a good ‘calibration’ point for the numerical tool that we have developed here, so that we can use it with confidence in highly non-linear conditions. Finally, because the velocity field in observational samples is also only known at a discrete number of positions, the locations of galaxies, we may be able to apply the developed method, in adapted form, to the available catalogues of measured galaxy peculiar velocities.

The central problem that we address here is that, while almost all analytical results concern volume-averaged quantities, almost all available numerical estimators in essence only yield mass-averaged quantities. This may considerably complicate any comparison, and even lead to false conclusions regarding e.g. the validity of perturbation theory. To improve upon this situation we introduce two new numerical methods, the Voronoi tessellation method and the Delaunay tessellation method. Both methods are based on two important objects in stochastic geometry, the Voronoi and the Delaunay tessellations of the point set consisting of the points at which the velocity field has been sampled. A Voronoi tessellation of a set of nuclei is a space-filling network of polyhedral cells, each of which delimits that part of space that is closer to its nucleus than to any of the other nuclei. The Delaunay tessellation is also a space-filling network of mutual disjoint objects, tetrahedra in 3D. The four vertices of each Delaunay tetrahedron are nuclei from the point set, such that the corresponding circumscribing sphere does not have any of the other nuclei inside. The Voronoi and the Delaunay tessellations are closely related, and are dual in the sense that one can be obtained from the other.

The earliest use of Voronoi tessellations can be found in the work of Dirichlet (1850) and Voronoi (1908) in their work on the reducibility of positive definite quadratic forms. However, their application to random point patterns has caused this concept to arise independently in various fields of science and technology, ranging from molecular physics to forestry (see Stoyan, Kendall & Mecke 1987 for references). Because of these diverse applications they acquired a set of alternative names, such as Dirichlet regions, Wigner–Seitz cells, and Thiessen figures. Despite the simplicity of its definition, analytical work on the statistics of Voronoi tessellations has appeared to be rather complicated and cumbersome, so that present analytical knowledge is mainly restricted to a few statistical moments of the distribution function of geometrical properties of Voronoi tessellations generated by homogeneous Poisson processes (see e.g. Meyer 1953; Gilbert 1962; Miles 1970; Møller 1989). For the time being, numerical work is therefore an inescapable necessity for any progress in this field (see e.g. van de Weygaert 1991b, 1994).

Within astronomy, and in particular cosmology, Voronoi...
A new method for accurate estimation of velocity field statistics

Juszczakiewicz

In this paper, we start by briefly discussing the conventional methods to sample the value of velocity fields on grid positions from the value of the velocity at a discrete number of points. In particular we stress the fundamental difference between mass- and volume-weighted velocity averages. Conventional estimators are almost always based on mass-weighted velocity fields. This may induce complications in the comparison with theoretical predictions. This leads to the introduction in Section 3 of the Voronoi and the Delaunay methods. Both are good estimators for volume-weighted velocity fields, and are therefore instrumental in improving comparisons between theoretical predictions and the results of N-body simulations. The accompanying Appendices A and B contain detailed descriptions of the geometrical details of these sampling techniques. Computational considerations are discussed in Section 4, while Section 5 contains a discussion of an application of both methods to an N-body simulation of galaxy clustering, determining the values of the divergence, vorticity and shear of the velocity field on a regular grid. These values are compared with each other as well as with the ones determined by a conventional estimator. Finally, in Section 6 we conclude with a discussion of the virtues of the new methods, and suggestions for future applications.

2 DISCRETELY SAMPLED VELOCITY FIELD

The fact that the velocity field is only known at a finite number of discrete positions is a major technical obstacle for obtaining reliable estimates of statistical parameters of the velocity field. It is of importance in the observational data as well as in N-body simulations. One possibility is to smooth the galaxy velocity field with a filter. For example, Bertschinger et al. (1990) chose to filter the measured galaxy velocities with a Gaussian smoothing function. In one case they took a fixed smoothing length, to be preferred for a rigorous statistical analysis, while for an optimal representation of the velocity and density field they adopted a filter with an adaptive smoothing length. By taking this length to be equal to the distance to the fourth nearest neighbour, the analysis automatically becomes better in the well-sampled high-density regions, thereby reducing the problem of noisy data and sparsely sampled underdense regions. In their analysis of numerical simulations, Juszczakiewicz
et al. (1995) and Lokas et al. (1995) also used smoothing of the velocity field by a Gaussian filter with a fixed smoothing length to obtain the local velocity field on a regular grid. Effectively these are mass-weighted velocity fields,

\[ \mathbf{v}_{\text{mass}}(x_0) = \frac{\int \mathrm{d}x \, v(x) \rho(x) W_M(x, x_0)}{\int \mathrm{d}x \, \rho(x) W_M(x, x_0)} , \]

where \( W_M(x, x_0) \) is the adopted filter function defining the weight of a mass element in a way that is dependent on its position with respect to the position \( x_0 \). In other words, \( \mathbf{v}_{\text{mass}} \) is effectively the velocity corresponding to the average momentum within the filter volume. For a discrete particle distribution, \( \mathbf{v}_{\text{mass}} \) reduces to

\[ \mathbf{v}_{\text{mass}}(x_0) = \frac{\sum_i \delta_D(x - x_i) v_i W_M(x, x_0)}{\sum_i \delta_D(x - x_i) W_M(x, x_0)} = \frac{\sum_i w_i v_i(x_i)}{\sum_i w_i} , \]

where \( w_i = W_M(x_i, x_0) \) and \( \delta_D(x - x_i) \) is the Dirac delta function. A major complication of such an analysis is that a comparison with the known analytical results is not straightforward. Almost without exception these analytical results are based on the volume-weighted filtered velocity field \( \mathbf{\tilde{v}} \),

\[ \mathbf{\tilde{v}}(x_0) = \frac{\int \mathrm{d}x \, v(x) W_V(x, x_0)}{\int \mathrm{d}x \, W_V(x, x_0)} , \]

where \( W_V(x, x_0) \) is the used weight function. At the present the only analytical work that has treated certain aspects of the statistics of the mass-averaged velocity, namely the skewness of \( \theta = H^{-1} \nabla \cdot v \), is the work by Bernardeau et al. (1995). A major complication is that this quantity involves the density field, and therefore would introduce the unknown bias between mass and galaxy density field in a practical implementation.

In order to get an estimate of the volume-averaged velocity, Juszkiewicz et al. (1995) use a two-step scheme, wherein they first determine a velocity on a grid according to equation (2), and then use the resulting grid of velocities to determine volume-averaged velocities according to equation (3), the volume averaging being accomplished by Gaussian filtering. Bernardeau (1994b) followed a similar procedure, whereby he used a top-hat filter for the volume averaging. Such a scheme would yield reliable results if the filter length of \( W_M \) were much smaller than that of \( W_V \). However, for technical reasons this is often difficult to attain. For example, it requires a very small grid size which would be excessively computer time and memory consuming.

In the study of Lokas et al. (1995) the same approach was followed in a comparison between N-body simulations and analytical perturbation calculations. While they found good agreement with the obtained density field moments, there already appeared to be substantial discrepancies in the case of the velocity divergence \( \theta \) by the time its variance \( \sigma_\theta \approx 0.1 \). They suggested as possible causes for the disagreement that (1) the perturbation approximation has already started to break down by the time \( \sigma_\theta \approx 0.1 \), (2) the N-body simulations do not evolve the velocity divergence field with sufficient accuracy and (3) the estimator of the smoothed velocity divergence from the N-body simulations is too noisy or too inaccurate. In order to improve upon this situation it is therefore highly desirable to develop a more reliable estimator, preferentially more closely related to the 'volume-averaged' nature of the perturbation calculations. In the following sections we will introduce two new methods that overcome the dilemma of a required very small initial smoothing length by constructing the Voronoi and Delaunay tessellations of the point distribution.

3 VORONOI AND DELAUNAY TESSELLATIONS

The first new estimator that we introduce here is based on Voronoi tessellations. It follows in a rather direct way from an asymptotic interpretation of the definition of mass-filtered quantities (equation 2). Although it leads to good results, it corresponds to an artificial situation of a discontinuous velocity field. This is successfully improved upon by a subsequent further elaboration and extension of the Voronoi method to a second estimator, based on the division of space into Delaunay tetrahedrons.

3.1 The Voronoi tessellation

In Section 2 we made the observation that a good approximation of volume-averaged quantities is obtained by volume averaging over quantities that were mass-filtered with, in comparison, a very small scale for the mass-weighting filter function. We can then make the observation that the asymptotic limit of this, namely using a filter with an infinitely small filter length (see equation 2),

\[ \mathbf{v}_{\text{mass}}(x_0) = \frac{\sum_i w_i v_i(x_i)}{\sum_i w_i} \]

where we have ordered the locations \( i \) by increasing distance to \( x_0 \) and thus by decreasing value of \( w_i \), is in fact taking the velocity \( v(x_i) \) of the closest particle as the estimate of the mass-averaged velocity. In other words, we can divide up space into regions consisting of that part of space closer to a particular particle than to any other particle, and taking the velocity of that particle as the value of the velocity field in that region. The search for the closest particle to each point of the field naturally leads to the construction of the Voronoi tessellation associated with the particle distribution. This division of space is a familiar and important concept in the field of stochastic geometry (see Stoyan et al. 1987 for an overview of this field). It consists of a space-covering and mutual disjunct set of convex...
cells, each of which contains a particle of the original particle distribution, enclosing the points of space for which the closest particle is precisely the one in the cell.

Formally a Voronoi tessellation (Voronoi 1908; Dirichlet 1850) can be defined as follows. Assume that we have a distribution of a countable set \( \Phi \) of nuclei \( \{x_i\} \) in \( \mathbb{R}^d \). Let \( x_1, x_2, x_3, \ldots \) be the coordinates of the nuclei. Then, the Voronoi region \( \Pi_i \) of nucleus \( i \) is defined by the following set of points \( x \) of the space:

\[
\Pi_i = \{ x | d(x,x_j) < d(x,x_j) \quad \text{for all} \; j \neq i \},
\]

where \( d(x,y) \) is the Euclidian distance between \( x \) and \( y \). In other words, \( \Pi_i \) is the set of points that is nearer to \( x_i \) than to \( x_j, \; j \neq i \). Each region \( \Pi_i \) therefore consists of the intersection of the open half-spaces bounded by the perpendicular bisectors of the segments joining \( x_i \) with each of the other \( x_j \)s. Hence, Voronoi regions are convex polyhedra (3D) with finite size according to definition (5). Each \( \Pi_i \) is called a Voronoi polyhedron. The complete set of \( \{ \Pi_i \} \) constitutes a tessellation of \( \mathbb{R}^d \), the Voronoi tessellation \( \mathcal{V}(\Phi) \) relative to \( \Phi \). A two-dimensional Voronoi tessellation of 25 cells is shown in Fig. 1 (right-hand frame), while an idea of a three-dimensional Voronoi tessellation can be obtained from the three Voronoi cells displayed in Fig. 2. The latter three cells are taken from a Voronoi network of 1000 cells, generated by Poissonian distributed nuclei, in a box with periodic boundary conditions.

As described above, given a field of velocities at a set of discrete particles a reasonable first assumption is that the velocity is constant within each Voronoi cell. The Voronoi method can therefore be regarded as the three- (or two-:) dimensional equivalent of approximating a one-dimensional function \( f(x) \) by a sequence of intervals wherein the function has a constant value. If the value of the function \( f(x) \) is known at \( M \) discrete points \( x_i \) (upper panel Fig. 3), this one-dimensional equivalent of the Voronoi method consists of adopting a constant value \( f(x_i) \) in the interval between \( (x_i + x_{i-1})/2 \) and \( (x_i + x_{i+1})/2 \) (see central panel of Fig. 3).

The first step of the Voronoi algorithm consists of calculating the Voronoi tessellation that is defined by the set of points at which the velocity field has been sampled. For this we use the three-dimensional geometrical Voronoi code that was developed by van de Weygaert (1991b, 1994). Starting from an input of points this code calculates the complete geometrical structure, i.e. the location of the walls, edges and vertices, of the corresponding Voronoi tessellation.

Subsequently, we proceed by determining the corresponding volume-averaged quantities. This is accomplished by a volume filtering of the resulting velocity field. By adopting a top-hat filter \( W_{\text{TH}} \) with radius \( R \) as the volume filter \( W_v \), the problem of determining the corresponding volume-averaged velocity gradient \( \tilde{v}_{ij} \) is that of determining the average value of \( v_{ij} \) within a sphere of radius \( R \),

\[
\tilde{v}_{ij}(x_0) = \frac{1}{R^3} \int_{R} dV W_{\text{TH}}(x,x_0) \cdot v_{ij}(x) \]

where the latter volume integral is over the part of space enclosed by the sphere with radius \( R \) centred on \( x_0 \). The constant value of the velocity \( v \) within each Voronoi cell automatically implies that the value of the velocity gradient \( v_{ij}(x) \) is equal to zero in their interior, so that the cells themselves have a contribution zero to the integral \( \int dV v_{ij} \). Only at the boundaries between the Voronoi cells will \( v_{ij} \) have a non-zero value. Moreover, the value of \( v_{ij} \) will be constant within each cell, as it corresponds to the change of that value of \( v \) between the two corresponding neighbour cells (see Fig. 4). The finite contribution by any Voronoi wall that lies within or intersects the filter sphere can be calculated by considering the volume defined by the surface of the wall and having an infinitesimal width \( \Delta s \) perpendicular to the wall. Imagine a Voronoi wall \( k \), being the boundary between two Voronoi cells \( k1 \) and \( k2 \) in whose interior the velocities are \( v_{k1} \) and \( v_{k2} \) (see Fig. 4), that intersects the top-hat sphere. The wall has a perpendicular width \( \Delta s_k \) and a surface area \( A_k \) within the sphere, while its orientation is determined by its normal vector \( n_k \). The velocity gradient \( v_{ij} \) can then be easily inferred from the velocity change \( \Delta v_{ij} = (v_{k2} - v_{k1}) \cdot e_i \) along the \( x \)-direction. Because this corresponds to an interval \( \Delta v = (n_k \cdot e_i) \Delta s_k \) in the \( y \)-direction, we find

\[
\frac{\partial v_{ij}}{\partial y} = \frac{\Delta v_{ij}}{\Delta s_k} = \frac{(n_k \cdot e_i)}{\Delta s_k} (v_{k2} - v_{k1}) \cdot e_x.
\]

This can be generalized directly to yield the following result for the volume-averaged value \( \tilde{v}_{ij} \) (with \( i,j \) = 1, 2, 3):

\[
\tilde{v}_{ij} = \frac{3}{4 \pi R^3} \sum_k A_k (n_k \cdot e_i) (v_{k1} - v_{k2}) \cdot e_j,
\]

where the sum is over all walls that intersect the sphere. In the specific case of the volume-averaged velocity divergence \( \theta \), this leads to the expression

\[
\tilde{\theta} = \frac{\nabla \cdot \tilde{v}}{H} = \frac{3}{4 \pi R^3} \sum_k A_k n_k \cdot (v_{k1} - v_{k2}) \cdot e_j.
\]

The problem of determining the volume-averaged velocity gradients (equation 8), or velocity divergence (equation 9), has therefore been reduced to determining the intersection of the walls in the Voronoi tessellations with spheres. This is a geometrical problem that can be solved with some effort (see Appendix A).

In practice we repeat this procedure of top-hat averaging at each point of a regular grid. From the values of \( \partial v_{ij}/\partial x_j \) at each grid point we can then easily evaluate the value of the velocity divergence \( \theta \), the shear \( \sigma_{ij} \) and the vorticity \( \omega \), where \( \omega = \nabla \times v = \epsilon^{ijk} \omega_{ij} \) and \( \epsilon^{ijk} \) is the completely antisymmetric tensor:

\[
\theta = \frac{1}{H} \left( \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \right),
\]

\[
\sigma_{ij} = \frac{1}{2} \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) - \frac{1}{3} (\nabla \cdot v) \delta_{ij},
\]

\[
\omega_{ij} = \frac{1}{2} \left( \frac{\partial v_j}{\partial x_i} - \frac{\partial v_i}{\partial x_j} \right).
\]

Summarizing, the end result of the operations described above consists of fields of top-hat averaged quantities like velocity divergence, shear and vorticity, sampled at regular grid intervals.
3.2 The Delaunay tessellation

A major characteristic of the Voronoi approach is that it leads to a discontinuous velocity field. This is evidently not the only unique way of defining the velocity field from a discrete set of sample points. Moreover, the Voronoi method may have problems in the case of small filter radii. Relevant non-zero values for the velocity gradients are only produced in the Voronoi walls. Many filter spheres remain empty when the filter scale is smaller than the average distance between Voronoi walls, i.e. when their scales are smaller than \( \L / N^{1/3} \) (with \( L \) the boxsize and \( N \) the number of Voronoi cells). This would yield many irrelevant and noisy filter velocity gradient averages. It may therefore be worthwhile to define another independent method based on a different interpolation scheme. In fact, this would give us the possibility of internally checking the results of the new methods that we have introduced here.

Indeed, the Voronoi method can be viewed as an elementary zeroth-order interpolation scheme. However, it is possible to define a velocity field based on linear interpolation between the velocities of the sample points. This is the multidimensional equivalent of the one-dimensional situation where the approximation of a function by constant function values in bins centred on the sample points (central panel, Fig. 3) is replaced by linearly interpolated function values in between those sample points (lower panel, Fig. 3). For \( d = 1 \) linear interpolation simply consists of the approximation of a function \( f(r) \) by the value \( f(r) = \hat{a}_1 f(r_1) + \hat{a}_{d+1} f(r_{d+1}) \) in the interval \( r_1 \leq r \leq r_{d+1} \), where \( 0 \leq \alpha_1 \leq 1 \) and \( \alpha_1 + \alpha_{d+1} = 1 \). The natural extension to a space of arbitrary dimension \( d \) of the concept of the one-dimensional interpolation interval \( r_1 \leq r \leq r_{d+1} \) is a 'hyper-triangle' defined by \( d + 1 \) vectors \( r_k \), the vertices of that object. For \( d = 2 \) this is a triangle, for \( d = 3 \) a tetrahedron. Any vector \( r \) within the 'hyper-triangle' is a linear combination of the \( d + 1 \) vectors \( r_k \), \( r = \sum_{k=1}^{d+1} \alpha_k r_k \), with \( 0 \leq \alpha_k \leq 1 \) and \( \alpha_1 + \ldots + \alpha_{d+1} = 1 \). The linearity of the approximation of the function \( f(r) \) then implies that

\[
f(r) = f(r_1) + \alpha_2 V f (r_2 - r_1) + \ldots + \alpha_{d+1} V f (r_{d+1} - r_1)
= f(r_1) + \alpha_2 (f(r_2) - f(r_1)) + \ldots + \alpha_{d+1} (f(r_{d+1}) - f(r_1)) \tag{11}
\]

The choice of appropriate, and if possible optimal, interpolation 'hyper-triangles' is a critical issue that to a considerable extent determines the quality and accuracy of the multidimensional linear interpolation. An obvious minimal requirement is that the linear approximation of the function \( f \) leads to a unique value at every point in the subspace defined by the set \( \mathcal{P} \). In other words, we need a space-filling covering by mutual disjoint tetrahedra (for now we will restrict ourselves to \( d = 3 \), although it is trivial to follow the same argument for any other \( d \)). In the interior of each of these tetrahedra each of the velocity gradients \( \partial f / \partial r_j \) has one particular constant
A new method for accurate estimation of velocity field statistics

Figure 3. Illustration of the one-dimensional equivalents of the Voronoi and the Delaunay methods. The value of some function $f(x)$ has been determined at 20 randomly distributed positions $x_i$ along a line (top panel). The height of a star at position $x_i$ is proportional to the value $f(x_i)$. Central panel: 'Voronoi method'. The function $f$ in the whole bin centred on a point $x_i$, bounded by the points halfway in between $x_i$ and its neighbours $x_{i-1}$ and $x_{i+1}$, is assumed to have the constant value $f(x_i)$. Note that these bins are essentially one-dimensional Voronoi cells. Bottom panel: 'Delaunay method'. The function $f$ is approximated by linear interpolation from $f(x_i)$ to $f(x_i+1)$ in the interval $(x_i,x_{i+1})$, and similarly between $f(x_j)$ and $f(x_{j-1})$ in the interval $(x_{j-1},x_j)$. The intervals $(x_{i+1},x_{i-1})$ and $(x_{i-1},x_i)$ can be considered as the one-dimensional equivalents of Delaunay cells.

value, which is determined by the value of the function $f$ at the locations $x_k$ of its four vertices. A crucial requirement for an optimal accuracy of the linear approximation (equation 11) is that the tetrahedra in the space-filling network are as compact as possible, in the sense of having a size and elongation that are as small as possible. A uniquely defined solution for such an optimal 'triangulation' does not exist or, rather, is not really known. Here we argue that a Delaunay tessellation (Delaunay 1934) is at least a good approximation of such an optimal triangulation.

Formally, the Delaunay tessellation $\mathcal{D}(\mathcal{P})$ of a point set $\mathcal{P}$ is defined to be the tessellation consisting of all the tetrahedra defined by four nuclei whose circumscribing sphere is empty in the sense that no nucleus of the generating set of nuclei should be inside the circumsphere. A two-dimensional illustration of a Delaunay triangulation is given in Fig. 1 (left-hand frame). A principal characteristic of the circumsphere of a Delaunay tetrahedron is that the centre of the circumsphere (circum-centre) is a vertex of the Voronoi tessellation. This follows immediately from the extrapolation of the definition. After all, according to the definition of the Voronoi tessellation a vertex is defined by four nuclei that are equidistant from the vertex, i.e. the vertex is the circumcentre of the circumsphere of these four nuclei. If then there were a fifth nucleus within the sphere, it would be nearer to the circumcentre than are the four nuclei on the surface of the sphere. This would imply that the centre cannot be the common vertex of the Voronoi polyhedra of these four nuclei. Ergo, the four nuclei have to define a Delaunay tetrahedron. In other words, the Delaunay tessellation is the network that is obtained by joining all pairs of nuclei in $\mathcal{P}$ whose Voronoi polyhedra share a Voronoi wall. Such a pair of nuclei is called a contiguous pair. The close relationship between the Delaunay and the Voronoi tessellations can be quite well appreciated from the right-hand frame of Fig. 1, depicting the Voronoi tessellation of the same point set as the one in the left-hand frame.

Besides the fact that Delaunay tetrahedra fulfil the requirement of compactness, being objects of minimal size and elongation, an additional and equally important argument for the use of the Delaunay tetrahedra as the choice for linear interpolation intervals is provided by the duality between Delaunay and Voronoi tessellations. Linear interpolation requires the definition of neighbour intervals. An arguably natural definition of 'neighbour points' in the multidimensional situation is that the two points share a Voronoi wall, i.e. they should be contiguous to each other. Delaunay tetrahedra therefore seem to be a natural choice for linear interpolation intervals defined by four nuclei.

Moreover, by virtue of their duality, the Voronoi and the Delaunay tessellations for a given point set $\mathcal{P}$ are calculated...
by the same three-dimensional geometrical Voronoi tessellation code that was mentioned in the previous subsection (van de Weygaert 1991b, 1994). In this case the output is limited to a listing of all vertices of the Voronoi tessellations and the location of the four generating points that define the corresponding Delaunay tetrahedron.

To give a visual impression of the relationship between the Voronoi and the Delaunay approximation methods, Fig. 5 shows the resulting values of a function $f(r) = f(r_1, r_2)$ for $d = 2$. The Voronoi method (top frame, Fig. 5) yields a field that consists of regions where the function $f$ has a constant value, Voronoi cells in the $(r_1, r_2)$ plane. The resulting image is therefore one of a field of pillars of different height, with a Voronoi cell at the base of each of the pillars. The Delaunay method divides space into triangular regions, the Delaunay triangles in the $(r_1, r_2)$ plane, in which not the field value but the field gradients are constant. This yields a field of differently oriented triangles, connecting at their edges to the neighbouring triangles (bottom frame, Fig. 5).

Having defined the Delaunay tetrahedra as the interpolation intervals, we proceed by determining the (constant) values of each of the nine velocity gradient tensor components $\partial v_i/\partial x_j$ in each of these tetrahedra. These are determined from the location of each of the four vertices, $r_0, r_1, r_2$ and $r_3$, and the value of the velocity field at each of these locations, $v_0, v_1, v_2$ and $v_3$. Defining the quantities $\Delta x_n = x_n - x_0$, $\Delta y_n = y_n - y_0$ and $\Delta z_n = z_n - z_0$, for $n = 1, 2, 3$, as well as $\Delta v_{nx} = v_{nx} - v_{x0}$, $\Delta v_{ny} = v_{ny} - v_{y0}$, $\Delta v_{nz} = v_{nz} - v_{z0}$ and $\Delta v_{n} = v_{n} - v_{0}$, the following nine linear relations are obtained, with $n = 1, 2, 3$:

$$
\Delta v_{nx} = \frac{\partial v_x}{\partial x} \Delta x_n + \frac{\partial v_y}{\partial y} \Delta y_n + \frac{\partial v_z}{\partial z} \Delta z_n,
$$

$$
\Delta v_{ny} = \frac{\partial v_x}{\partial x} \Delta x_n + \frac{\partial v_y}{\partial y} \Delta y_n + \frac{\partial v_z}{\partial z} \Delta z_n,
$$

$$
\Delta v_{nz} = \frac{\partial v_x}{\partial x} \Delta x_n + \frac{\partial v_y}{\partial y} \Delta y_n + \frac{\partial v_z}{\partial z} \Delta z_n.
$$

(12)

From these equations we can easily infer that the components of $\partial v_i/\partial x_j$ can be calculated from

$$
\frac{\partial v_i}{\partial x} = A^{-1} \begin{pmatrix} \Delta v_{i1} \\ \Delta v_{i2} \\ \Delta v_{i3} \end{pmatrix},
$$

$$
\frac{\partial v_i}{\partial y} = A^{-1} \begin{pmatrix} \Delta v_{i1} \\ \Delta v_{i2} \\ \Delta v_{i3} \end{pmatrix},
$$

$$
\frac{\partial v_i}{\partial z} = A^{-1} \begin{pmatrix} \Delta v_{i1} \\ \Delta v_{i2} \\ \Delta v_{i3} \end{pmatrix},
$$

(13)

where $A^{-1}$ is the inverse of the matrix

$$
A = \begin{pmatrix} \Delta x_1 & \Delta y_1 & \Delta z_1 \\ \Delta x_2 & \Delta y_2 & \Delta z_2 \\ \Delta x_3 & \Delta y_3 & \Delta z_3 \end{pmatrix}.
$$

(14)

Note that the four points of the interpolation tetrahedron are both necessary and sufficient to fix the value of each of the nine velocity gradients. While in the linear regime only six of these quantities would be needed, by virtue of the absence of vorticity, all nine quantities are necessary in the non-linear regime. From the values of $\partial v_i/\partial x_j$ we can then easily evaluate the value of the velocity divergence $\partial_0$, the shear $\sigma_{ij}$ and the vorticity $\omega$ (see equation 10) in each Delaunay tetrahedron.

Subsequently we have to determine the corresponding volume-averaged quantities. As described in the previous section we accomplish this by top-hat filtering with a filter $W_{TH}$ that has a characteristic radius $R$. The problem has therefore been reduced to determining the average value of $\partial_0$, $\sigma_{ij}$ and $\omega$ in a sphere of radius $R$, centred on some location $x_0$. For example, for the volume-averaged velocity divergence, $\overline{\partial_0}(x)$, we have

$$
\overline{\partial_0}(x_0) = \frac{\int dV \partial_0(x)W_V(x, x_0)}{\int dV W_V(x, x_0)}.
$$

(15)

As the value of $\partial_0$ is constant within each cell of the space-filling Delaunay tessellation, the problem reduces to simply determining the intersection of the Delaunay tetrahedra with the filter sphere (Appendix B), and using the intersection volume as the weighting value of $\partial_0$ in the integral of equation (15). In other words, $\overline{\partial_0}$ follows from

$$
\overline{\partial_0}(x_0) = \frac{3}{4\pi R^3} \sum_k \theta_k V_{k,r},
$$

(16)

where the sum is over all Delaunay tetrahedra $k$ that intersect with the filter sphere, and $V_{k,r}$ is the volume of the corresponding intersection, while $\theta_k$ is the value of $\partial_0$ in $k$. It is good to note that the geometrical issue of determining the intersection between a tetrahedron and a sphere is far from trivial. A description of our algorithm is provided in Appendix B, but we should note that more efficient evaluations are probably possible. Evidently, the discussion is exactly analogous for the volume-averaged values of the shear tensor components $\sigma_{ij}$ and of the vorticity $\omega_{ij}$.

As with the Voronoi method, the final end result of the operations described above consists of a field of top-hat averaged quantities at regular grid intervals.

4 COMPUTATIONAL CONSIDERATIONS

In the previous section we developed the theoretical groundwork for the use of the Voronoi and the Delaunay tessellations as optimal tools for determining the velocity divergence field, as well as the vorticity and shear fields, from the value of the velocity field at a discrete number of locations. The practical implementation of both methods consists of a two-phase approach. (1) In the first step, the algorithm calculates the Voronoi or Delaunay tessellation for the set of points at which
4.1 The tessellation algorithm

On the basis of the duality between Voronoi and Delaunay tessellations we can then define the values of the velocity divergence, vorticity and/or shear throughout the whole of the sample volume. (2) The subsequent second phase is the volume filtering of the resulting tessellation-defined field. In essence, volume filtering consists of the determination of the average value of the velocity gradient field, produced by the tessellation algorithm, within the filter volume. Usually, the filtering averages are determined for a set of regular grid positions.

The central operation of the geometric Voronoi algorithm is the calculation of all the Delaunay tetrahedra of the point distribution. Evidently, this simultaneously yields all Voronoi vertices, the centres of the corresponding circumscribing spheres. Finding the appropriate connections between the vertices, such that they define the edges, the polygonal Voronoi walls and finally the complete polyhedral Voronoi cells, is the major and most cumbersome part of the work. Our algorithm is an elaboration on the work of Tanemura, Ogawa & Ogita (1983), who gave a sketch of the basic algorithm for finding a Delaunay tetrahedron and a Voronoi polyhedron, in combination with four underlying geometric theorems. Through efficient administrative, data storage and searching procedures our algorithm manages to restrict itself to calculating every Delaunay tetrahedron and Voronoi cell only once during the construction of the complete tessellation. In a brute force construction procedure wherein each Voronoi cell is completely calculated without use of prior information, this would be repeated three times and once time respectively. This has the additional advantage that it allows one to discard a point \( i \) from any further consideration once its Voronoi cell \( \Pi_i \) has been calculated.

For the sake of clarity it is good to recapitulate some basic properties of Voronoi tessellations (also see Fig. 2). A nucleus \( i \) defines a complete polyhedral Voronoi cell. The boundary of the cell consists of a set of polygonal walls, each of which is shared with a nucleus \( j \) that is contiguous to \( i \). A Voronoi wall is the part of space that is as close to \( i \) as to \( j \), and closer to these two nuclei than to any of the other nuclei. On average there are \( \approx 15.54 \) walls per Voronoi cell if the generating point distribution is Poissonian, an average number that can vary from realization to realization (unlike the 2D case, where the average number of edges is always 6). The boundary of a polygonal wall is formed by a number of edges, with a Voronoi vertex at the two tips of each edge. In other words, the structure of a wall is completely determined by listing the locations of the Voronoi vertices along its edge.
in the right geometrical order. Note that each edge is shared by three contiguous nuclei $i$, $j$, and $k$, to which every point on the edge is equidistant while being closer to any of these three than to any of the other nuclei. Likewise, a Voronoi vertex is equidistant to its closest four nuclei in the generating point process. For a Poisson point process there are $\approx 27.07$ vertices per Voronoi cell, and some 5,228 per Voronoi wall.

Our code assumes that the generating point processes, and consequently also the tessellations themselves, have periodic boundary conditions. This assumption, however, can be relaxed with some additional effort. Usually the points are distributed within a box of equally sized edges, although any rectangular parallelepiped is feasible. The first step of the algorithm is the storage of the set of generating nuclei in a multidimensional binary tree. This data structure, on average, stores points that are close together in space at nearby positions of a binary tree structure (see e.g. Bentley 1986). Nearby points in space can then be tracked efficiently by means of a recursive searching procedure. Building this tree is an $N \log N$ procedure; finding the nearest $M$ points is a task that requires a limited effort proportional to $M \log N$ (see appendix F in van de Weygaert 1994).

The algorithm then proceeds with the sequential computation of each Voronoi cell $\Pi$. In turn, the construction of a cell $\Pi_i$ consists of the determination of the structure of each of its Voronoi walls. A slight complication is of course that beforehand it is unknown which and with how many nuclei $i$ shares a wall. The identity of these contiguous nuclei can be revealed in different ways. First, a subsample $S_i$ of $M \approx 50$ nearest nuclei is selected. As contiguous points are likely to be close in physical space, the subset $S_i$ is considered to be the primary sample of contiguity candidates. Initially any search for a new contiguous nucleus is restricted to $S_i$. If $i$ is not yet part of a Delaunay tetrahedron, the first contiguous nucleus is the nucleus $i_1$ that is closest to $i$. Evidently, $i_1$ belongs to $S_i$. A subsequent second contiguous nucleus $i_2$ is found by looking for the nucleus that together with $i$ and $i_1$ yields the triangle of minimal circumradius. Although almost always $i_2 \in S_i$, there are occasional exceptions, and an appropriate correction procedure for this has to be included. A subsequent third contiguous nucleus $i_3$ is the one that together with $i$, $i_1$, and $i_2$ defines a Delaunay tetrahedron. As in the case of $i_2$, the search for $i_3$ is initially restricted to $S_i$, but occasionally corrective action is needed and the search extended to a limited set of nuclei outside $S_i$. This corrective procedure is efficiently performed via the multidimensional binary tree. On the other hand, $i$ can have been one of the four defining nuclei of one or more previously determined Delaunay tetrahedra. If so, we know that the other three nuclei of any of these tetrahedra are contiguous to $i$. In both situations an initial set $C_i$ of contiguous nuclei is produced. Subsequently, we work our way through the list $C_i$, calculating one by one the corresponding walls. For each nucleus $i_k$ in $C_i$ at least one Delaunay tetrahedron is known. These tetrahedra are the starting point of any further search. They are ordered in the appropriate geometrical order, and the gaps are filled in. Within the wall around $\{i, i_k\}$ a tetrahedron $\mathcal{D}_{\beta,i} = \{i, i_k, i_p, i_q\}$ should connect to a tetrahedron $\mathcal{D}_{\beta,i} = \{i, i_k, i_p, i_q\}$. If such a tetrahedron $\mathcal{D}_{\beta,i}$ already exists, its centre will be the Voronoi vertex connecting to the one of $\mathcal{D}_{\beta,i}$. If not, we have to search for the nucleus $i_k$ - first in the subset $S_i$, if necessary followed by a corrective procedure. In this way new Delaunay tetrahedra are computed not at random, but always starting from previous knowledge of three of the four defining nuclei. This searching procedure will automatically yield a new contiguous nucleus, and $i_k$ is added to the list $C_i$. Continuing along the same direction, the polygonal wall gets progressively mapped by the connecting Voronoi vertices, a process which is completed once a tetrahedron connects to $\mathcal{D}_{\beta,i}$ on the side $\{i, i_k, i_p\}$. Meanwhile newly determined Delaunay tetrahedra have produced new contiguous nuclei for the set $C_i$. After completion of the wall around $\{i, i_k\}$ the process proceeds with the next contiguous nucleus in the list $C_i$. The construction of the Voronoi polyhedron $\Pi_i$ has been completed once the walls around all the nuclei in the constantly updated list $C_i$ have been determined.

In the construction procedure that we sketched in the previous paragraph each Delaunay tetrahedron, and its corresponding Voronoi vertex, is computed only once. When four nuclei $i, i_k, i_p, i_q$ are found to constitute a Delaunay tetrahedron, this information is passed on to all four of these nuclei – likewise with the Voronoi wall shared by the nuclei $i$ and $j$. During construction of the Voronoi cell $\Pi_i$ the elaborate wall construction procedure described above is skipped when the wall with $j$ has been computed earlier during the construction of $\Pi_j$. Instead, construction proceeds with the next nucleus in the contiguity list $C_i$ for which such a wall has not yet been determined, naturally only after having notified the cell $\Pi_i$ of the existence of the wall it shares with $j$. Besides selection of the subset $S_i$ of $M$ closest neighbours, one of the first steps in the computation of a Voronoi cell $\Pi_i$ is therefore processing of the information on the walls and vertices that were obtained previously during the computation of other cells. This also implies that the nucleus $i$ can be discarded from any further considerations once the cell $\Pi_i$ has been determined, all of the Delaunay tetrahedra in which it participates already having been calculated. This results in a progressive pruning of the multidimensional tree during the tessellation construction procedure.

4.2 The filtering algorithms

The tessellation algorithms lead to constant values of the velocity gradients within either the Voronoi walls, for the Voronoi method, or the Delaunay tetrahedra, for the Delaunay method. Subsequently, this field is filtered (see Sections 3.1 and 3.2). The operation of filtering is basically equivalent to determining a weighted average of the field within the filter volume. In the application of the Voronoi and the Delaunay methods we restrict ourselves to determining top-hat filtered fields, which have the virtue that their filter values consist of bounded spheres of radius $R$.

Because in the Voronoi method the value of the velocity gradients differs from zero only in the walls of the Voronoi tessellations, the filtering consists of determining the surface area of the intersections of the polygonal Voronoi walls with spheres of radius $R$. The technicalities of this procedure are treated in Appendix A.

In the Delaunay method we end up with the more complicated situation of constant non-zero values of the velocity gradients in the Delaunay tetrahedra. The basic operation of top-hat filtering is therefore determining the volume of the intersections of tetrahedra with a sphere. This turns out to be a far from trivial geometrical problem. In Appendix B we describe a provisional recipe to accomplish this operation.
However, it is quite likely that considerably more efficient ways are feasible, which would lead to a substantial gain in efficiency of the Delaunay method.

4.3 Computational effort

In practice, the amount of CPU time for the calculation of a Voronoi cell in the Voronoi tessellation construction procedure is almost independent of the number $N$ of generating nuclei, so that the total tessellation construction time is almost linearly proportional to $N$. The CPU effort required for the construction of the multidimensional binary tree is of the order of $kN \log N$. In addition, we use a time $\propto M \log N$ for the selection of each subset $S_i$ of $M$ closest neighbours, so that a total time $\mathcal{O}(NM \log N)$ is spent on the selection of all neighbour sets $S_i$. It is the subsequent step for the actual construction of each polyhedral Voronoi cell $\Pi_i$ that dominates the CPU consumption. It is almost independent of $N$, due to the fact that it takes place in subsets $S_i$ that contain approximately the same number of $M \approx 50$ nuclei. Its total CPU requirement is therefore something like $\mu N$, where $\mu \gg \alpha \times k$.

To illustrate the above, we quote some CPU tests on an IBM 7011/2ST Power PC. For a range of 100 to 50 000 generating nuclei the CPU time per cell is indeed constant, $\approx 0.010$ s. For a tessellation of 40 000 nuclei the tessellation computation time is $\approx 407.28$ s, while the corresponding tree building time is $\approx 28.03$ s. For comparison, in the case of a tessellation of 10 000 Voronoi cells these are 10.05 s and 0.25 s respectively.

The construction of the Voronoi and Delaunay tessellations is considerably less time consuming than the ensuing Voronoi wall or Delaunay tetrahedron intersection procedures. The major share of the effort lies in the computation of the intersections between the spheres and either the Voronoi walls or Delaunay tetrahedra. The CPU time per intersection is basically constant. Here we quote some numbers for a top-hat filter of $R = 15.0h^{-1}$ Mpc; where the filtered quantities were determined at 20$^3$ grid positions in a box with an edge size of $200h^{-1}$ Mpc, containing a tessellation generated by $N = 40 000$ nuclei. The number of intersection evaluations is proportional to $R^3$, as well as linearly proportional to $N$. With respect to the latter it is worthwhile to realize that a Voronoi tessellation generated by $N$ nuclei has approximately 7 768$N$ Voronoi walls and 6 768$N$ Delaunay tetrahedra (i.e. $\approx 310720$ walls and $\approx 270720$ Delaunay tetrahedra for a Voronoi tessellation of 40 000 cells).

In the case of the Voronoi method we need on average 0.126 ms per intersection. The surface area of approximately 5 759 500 intersections had to be calculated, which resulted in a total CPU time of 1 454 s. As expected, an intersection between a sphere and a Delaunay tetrahedron is more time demanding, taking $\approx 1.32$ ms, while the subsequent determination of the velocity gradient tensor (equation 13) takes on average another $\approx 0.157$ ms. Our code needed 12 882 264 intersection determinations, so that some 17 034 CPU seconds ($\approx 4.7$ CPU hours) were spent on this part of the procedure, with an additional 1235 s for the velocity gradient tensor calculations. Here we should add the remark that, due to the way the code selects the spheres and tetrahedra that are likely to intersect, some 39 per cent of the intersections actually turned out to be empty.

An additional important computational consideration concerns memory space. Here the Delaunay method has a clear advantage over the Voronoi method. For the Voronoi method we need to store all the available information on the Voronoi tessellation. In this way we are able to reconstruct the Voronoi walls, in particular the links between and locations of the vertices that delineate those walls. As yet we still use the output of the general Voronoi code, although we intend to make a special-purpose version of the Voronoi code. The latter should reduce the memory allocation considerably. For example, the structure of the complete Voronoi tessellation of 40 000 cells is contained in seven files of in total 105 Mbyte. By contrast, the Voronoi code was adapted for the Delaunay method so that only the information on the Delaunay tetrahedra is stored, comprising two files of in total 14.3 Mbyte.

In practice the limitations of memory space are considerably more restrictive than the required CPU time for the number of data points that can be handled by the Voronoi and the Delaunay tessellation methods. For example, in the case of a data set of 128$^3$ particles, the Delaunay method would require a feasible 750 Mbyte of memory space. However, the more than 5.5 Gbyte needed by the Voronoi method probably prohibit this method from becoming applicable to data sets comprising more than $\approx 100 000$ points.

5 APPLICATION: VELOCITY STATISTICS OF AN N-BODY SIMULATION

In order to compare the new ‘Voronoi tessellation method’ (Section 3.1), the new ‘Delaunay tessellation method’ (Section 3.2) and the old ‘two-step method’, which we briefly described in Section 2 (see e.g. Juszkiewicz et al. 1995; Bernardeau 1994b), we have applied the new methods to the result of an $N$-body simulation. This simulation, kindly provided by H. Couchman, follows the evolution, in a $\Omega = 1$ universe with Hubble parameter $H_0 = 50$ km s$^{-1}$ Mpc$^{-1}$, of a system of 128$^3$ particles within a cubic simulation box of 200$h^{-1}$ Mpc size and with periodic boundary conditions. The simulation started from standard cold dark matter initial conditions, and was followed until the epoch when the rms linear density fluctuations reach unity in a spherical top-hat box of radius $8h^{-1}$ Mpc.

As it was not feasible for us to apply the Voronoi method for a particle sample of 128$^3$ points (see discussion at the end of Section 4), we needed to reduce the number of particles used in the analysis. To do so we take advantage of the fact that the filtered velocity field at the radius corresponding to the quasi-linear regime is not sensitive to the details of the small-scale velocity field in the very dense regions. Therefore, the statistical quantities we are interested in are not affected if we sample the data set in such a way that it does not reduce the number density of particles in the underdense regions while it does so in the very dense areas. To achieve this goal we have constructed an algorithm in which eight different grids are superposed, all with the same grid size but shifted by half of the grid size in each of the possible directions. Subsequently, we perform a sequential operation on the set of simulation particles, whereby we consider the location of each particle, rejecting those whose locations in all of the shifted grids would be in a grid cell that has already been occupied by a previously considered particle. For a grid size of $10h^{-1}$ Mpc the final number of points is about 40 000. It corresponds to a mean distance between points of...
about $6h^{-1}$Mpc. We constructed the Voronoi and Delaunay tessellations of these particle samples, in order to derive the statistical properties of the velocity field in the way that was described in detail in the previous section. In addition, we checked the robustness of the results by repeating the same analysis for a grid size of $7.5h^{-1}$Mpc and double the number of points.

5.1 Results for the velocity divergence

In order to illustrate the substantial improvements that are obtained by the Voronoi tessellation method and the Delaunay tessellation method, in comparison with older methods like the two-step one, and to compare the results with known theoretical predictions, we will in particular focus our analysis on the velocity divergence. The same simulation was tentatively analysed with the two-step method by Bernardeau (1994b, also see Juszkiewicz et al. 1995). In the scatter plot of Fig. 6 we compare the estimates of $\theta$ that we obtained with the Delaunay method at 203 locations on a regular grid, with those obtained by the two-step method (left-hand frame) and the Voronoi method (right-hand frame), both at the same grid locations. The scatter plot clearly shows the good agreement between the Voronoi and the Delaunay tessellation methods. Given the fact that both methods are quite different, this provides considerable confidence in them. On the other hand, the old two-step method yields very noisy estimates. Moreover, it tends to underestimate the value of $\theta$ by a factor of about 1.2. This effect is probably due to the fact that the effective smoothing radius is slightly larger because of the combination of the two smoothing procedures.

In Fig. 7 we present similar scatter plots, for three different smoothing radii, to show the correlation between the divergences measured by the Voronoi and the Delaunay methods. The noise becomes very important for radii smaller than $5h^{-1}$Mpc, that is when the radius becomes smaller than the mean distance of the sampled particles. The results obtained for a smoothing length of $2.5h^{-1}$Mpc are obviously not reliable and show specific features associated with the methods that have been used. For example, at these small radii a large fraction of the smoothing spheres do not intersect any of the walls of the Voronoi tessellation. The Voronoi method therefore yields values of zero for $\theta$ in these spheres. This situation is actually rather similar to the case of Poisson noise, with the velocity divergence only having a non-zero value at some discrete locations. For the Delaunay method the effect is less dramatic. However, the measured velocity divergence gets affected by the fact that information from larger scales, i.e. from the mean separation scale, leaks into the local velocity. This effect can also be traced in the other scatter plots. In the latter we note that the measured values of the velocity divergence tend to be smaller in the case of the Delaunay method than in the case of the Voronoi method. Overall, however, at a scale of $10-15h^{-1}$Mpc we expect all measured quantities to be free of systematic errors, so that they can be analysed with confidence.

In Table 1 we summarize the resulting values of the moments of the velocity divergence obtained with the Delaunay method (with superscript Del.) and the Voronoi method (with superscript Vor.), from an analysis in which the velocity divergence has been measured at 503 different grid points. The error bars have been obtained by dividing the simulation into four equal subsamples, and performing the same analysis for each of the subsamples. The results on the variance clearly show that the rms of the velocity divergence, $\sigma_\theta$, is lower than the rms density fluctuations, $\sigma_\delta$. This effect was also noticed by Juszkiewicz et al. (1995), and is an indication for the departure of the dynamics from the linear approximation, since in the linear regime $\sigma_\delta$ and $\sigma_\theta$ are expected to be equal.

However, our main interest concerns higher order moments. In recent years a lot of theoretical results on the statistical properties of the velocity divergence have been obtained. Bernardeau (1994a) derived the following results on the third- and fourth-order moments for cosmological models with Gaussian initial conditions, $\Omega = 1$ and $\Lambda = 0$. For the condition of a small $\sigma_\theta$, the following expressions were found:

$$\langle \theta^2 \rangle = T_3 + O(\sigma_\theta^2(R))$$

with

$$T_3 = \frac{26}{7} + \gamma_1,$$

and

$$\frac{\langle \theta^3 \rangle - 3\langle \theta^2 \rangle^2}{\langle \theta^2 \rangle^3} = T_4 + O(\sigma_\theta^2(R))$$

with

$$T_4 = \frac{12088}{441} + \frac{338}{21} \gamma_1 + \frac{7}{3} \gamma_2^2 + \frac{2}{3} \gamma_2,$$

where the parameters $\gamma_1$ and $\gamma_2$ are the successive logarithmic derivatives of $\sigma_\theta^2(R)$ with respect to $R$,

$$\gamma_1 = \frac{d \log \sigma_\theta^2(R)}{d \log R} = -(n + 3),$$

$$\gamma_2 = -\frac{d^2 \log \sigma_\theta^2(R)}{d \log^2 R}.$$

For a CDM spectrum, Table 1 lists the values of the parameters $n$ and $\gamma_2$ for different smoothing radii. The corresponding theoretical values of $T_3$ and $T_4$ can be determined from equations (18) and (20). The values for $T_3$ measured from the simulation by both the Voronoi and the Delaunay methods are found to be in remarkable agreement with these theoretical predictions in the cases of all four different radii. While it was not possible to determine $T_4$ as accurately in the case of the largest radius, it was found to agree reasonably well with the theoretical predictions for radii $R \leq 10h^{-1}$Mpc, i.e. at radii for which this quantity could be measured sufficiently accurately. This solves the issue raised by Lokas et al. (1995), who questioned the validity of the perturbation theory for the divergence of the velocity field. From our results we can conclude that the departure they observed in their work was due to the systematic errors introduced by the smoothing schemes they used.

5.2 The probability distribution function (PDF) of the velocity divergence

Although it is interesting to study the individual moments, as they highlight different features of the total distribution, a more complete picture is obtained by looking at the global shape of the PDF of the velocity divergence. In Fig. 8 we present,
A new method for accurate estimation of velocity field statistics

Figure 6. Comparison of the estimated values of the velocity divergence $\theta$ at the present epoch, top-hat filtered with a filter radius $R = 15 h^{-1}$ Mpc, at $2^d$ grid positions. The simulation consists of $128^3$ particles in a periodic box of $200 h^{-1}$ Mpc size, and concerns an $\Omega = 1$ universe with CDM initial conditions (see text). The left-hand panel is a scatter plot of the value of $\theta$ at each of the grid positions obtained with the two-step method against the value at the same position for the Delaunay method. The right-hand panel is a similar scatter plot, but then for the values obtained with the Voronoi method and the Delaunay method.

Figure 7. Scatter plots of the value of the top-hat filtered velocity divergence $\theta$ determined by the Voronoi method against the value determined by the Delaunay method, for $2^d$ grid positions. The plot concerns the same $128^3$ CDM N-body simulation as in Fig. 6. Each frame represents a different top-hat filter radius. Left-hand panel: $R = 2.5 h^{-1}$ Mpc. Central panel: $R = 5.0 h^{-1}$ Mpc. Right-hand panel: $R = 10.0 h^{-1}$ Mpc.

for two different radii, the measured velocity divergence PDF. These measures are compared with the theoretical predictions of Bernardeau (1994b) obtained from the re-summation of the series of the cumulants (solid curves). For $n = -1$ there is a simple analytical expression that can be used for the PDF of $\theta$ (given here for $\Omega = 1$),

$$p(\theta)d\theta = \frac{(2\kappa - 1)/\kappa^{3/2} + \lambda^2/\lambda_0^{3/2})^{-3/2}}{\kappa^{3/4}(2\pi)^{1/2}\sigma_0} \exp\left[-\frac{\theta^2}{2\lambda^2}\right] d\theta,$$

with

$$\kappa = 1 + \frac{\theta^2}{9\lambda^2},$$

$$\lambda = 1 - \frac{2\theta}{3}.$$

This expression was used in the plot for $R = 10h^{-1}$ Mpc. For $R = 15h^{-1}$ Mpc, however, the solid curve was obtained by numerical integration of the inverse Laplace transform (similar to equation 18 of Bernardeau 1994b).

The PDFs measured by both the Voronoi and the Delaunay methods are clearly in remarkably good agreement with the theoretical predictions, down to probabilities of about $10^{-4}$. On the other hand, previous methods, like the two-step method (open squares in Fig. 8), produce PDFs that deviate substantially from the theoretical curves, producing spurious tails at both the low- and high-value ends of the PDF. Particularly noteworthy is the fact that the new tessellation methods manage to reproduce the expected sharp cutoff at the positive values of $\theta$, which corresponds to voids.

The accuracy of the perturbation theory calculations is therefore confirmed for the shape of the PDF of the velocity divergence. This is clearly of great importance, as the shape of the PDF can be potentially used to measure $\Omega$ (Bernardeau et al. 1995).

5.3 Vorticity and shear

When introducing the Voronoi and Delaunay methods in Section 3, we made the observation that both methods can actually be used to study the statistical properties of any quantity related to the velocity deformation tensor, such as the vorticity and the shear. In Fig. 9 we compare by means of scatter plots the results that have been found with our two methods for the norms of these quantities, $\omega$ (left-hand frame) and $\sigma$. 

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Table 1. Statistical parameters for the density and the velocity field at different radii.

<table>
<thead>
<tr>
<th>Radius/(h^{-1} Mpc)</th>
<th>7.5</th>
<th>10.0</th>
<th>12.5</th>
<th>15.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>n</td>
<td>-1.16</td>
<td>-0.98</td>
<td>-0.86</td>
<td>-0.73</td>
</tr>
<tr>
<td>\gamma</td>
<td>-0.51</td>
<td>-0.57</td>
<td>-0.60</td>
<td>-0.64</td>
</tr>
<tr>
<td>\sigma_\delta</td>
<td>0.99</td>
<td>0.74</td>
<td>0.57</td>
<td>0.47</td>
</tr>
<tr>
<td>\sigma_\theta^\text{Del}</td>
<td>0.63 ± 0.02</td>
<td>0.53 ± 0.02</td>
<td>0.45 ± 0.015</td>
<td>0.38 ± 0.015</td>
</tr>
<tr>
<td>\sigma_\theta^\text{Vor}</td>
<td>0.67 ± 0.02</td>
<td>0.55 ± 0.02</td>
<td>0.46 ± 0.015</td>
<td>0.39 ± 0.015</td>
</tr>
<tr>
<td>-T_3</td>
<td>1.87</td>
<td>1.69</td>
<td>1.57</td>
<td>1.44</td>
</tr>
<tr>
<td>-T_3^\text{Del}</td>
<td>1.74 ± 0.06</td>
<td>1.66 ± 0.06</td>
<td>1.58 ± 0.10</td>
<td>1.50 ± 0.12</td>
</tr>
<tr>
<td>-T_3^\text{Vor}</td>
<td>1.70 ± 0.05</td>
<td>1.64 ± 0.07</td>
<td>1.56 ± 0.09</td>
<td>1.48 ± 0.12</td>
</tr>
<tr>
<td>T_4</td>
<td>5.35</td>
<td>4.04</td>
<td>3.25</td>
<td>2.47</td>
</tr>
<tr>
<td>T_4^\text{Del}</td>
<td>4.9 ± 0.6</td>
<td>4.6 ± 0.6</td>
<td>4.5 ± 1.5</td>
<td>4.5 ± 2</td>
</tr>
<tr>
<td>T_4^\text{Vor}</td>
<td>4.6 ± 0.4</td>
<td>4.3 ± 0.9</td>
<td>4.2 ± 1.5</td>
<td>4.3 ± 2</td>
</tr>
</tbody>
</table>

Table 2. The relative magnitudes of the divergence \( \theta \), vorticity \( \omega \) and shear \( \sigma \) (in units of \( H \)).

<table>
<thead>
<tr>
<th>Radius/(h^{-1} Mpc)</th>
<th>7.5</th>
<th>10.0</th>
<th>12.5</th>
<th>15.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>\sigma_\theta^\text{Del}</td>
<td>0.63 ± 0.02</td>
<td>0.53 ± 0.02</td>
<td>0.45 ± 0.015</td>
<td>0.38 ± 0.015</td>
</tr>
<tr>
<td>\sigma_\theta^\text{Vor}</td>
<td>0.67 ± 0.02</td>
<td>0.55 ± 0.02</td>
<td>0.46 ± 0.015</td>
<td>0.39 ± 0.015</td>
</tr>
<tr>
<td>\omega^\text{Del}</td>
<td>0.183 ± 0.003</td>
<td>0.118 ± 0.001</td>
<td>0.081 ± 0.001</td>
<td>0.059 ± 0.001</td>
</tr>
<tr>
<td>\omega^\text{Vor}</td>
<td>0.243 ± 0.004</td>
<td>0.147 ± 0.002</td>
<td>0.098 ± 0.0015</td>
<td>0.070 ± 0.001</td>
</tr>
<tr>
<td>\sigma^\text{Del}</td>
<td>0.50 ± 0.01</td>
<td>0.41 ± 0.01</td>
<td>0.347 ± 0.009</td>
<td>0.297 ± 0.008</td>
</tr>
<tr>
<td>\sigma^\text{Vor}</td>
<td>0.55 ± 0.01</td>
<td>0.45 ± 0.01</td>
<td>0.366 ± 0.009</td>
<td>0.310 ± 0.008</td>
</tr>
</tbody>
</table>

\[ \omega^2 = \sum_k \omega_k^2 \]  
\[ \sigma^2 = \sum_{ij} \sigma_{ij} \sigma_{ij} \]  

These plots should be compared with the similar plot of the velocity divergence in the right-hand frame of Fig. 6. Because the mean vorticity is small its statistics are quite sensitive to noise. Even for a radius as large as 15h^{-1} Mpc the resulting measured value of the mean vorticity can be significantly affected by systematic errors. Since it does not vanish in the linear regime, such a sensitivity does not exist for the velocity shear. A summary of the expectation values of \( \omega \) and \( \sigma \) is given in Table 2, which also contains the values obtained for the rms of \( \theta \).

We find that the amount of shear is slightly smaller than the amount of divergence. In fact, the value for \( \sigma \) found with both methods is almost exactly consistent with the magnitude of the shear expected in the linear regime,

\[ \frac{1}{H^2} \langle \sigma^2 \rangle = \frac{2}{3} \langle \theta^2 \rangle. \]

As far as the amount of vorticity is concerned, we see that it shows the expected rapid decrease with scale. For \( R \gtrsim 10h^{-1} \) Mpc it seems fair to assume that the vorticity is small compared with the divergence. To give a crude idea of them, Fig. 10 shows the PDFs of \( \omega \) and \( \sigma \), for \( R = 15h^{-1} \) Mpc, obtained with the two new methods.

5.4 The local density–velocity relationship

In addition to the analysis of the statistical properties of the velocity field, it is also possible to use the Voronoi and the Delaunay methods to study the joint distributions of the density and the velocity field. Fig. 11 displays scatter plots of the local density contrast \( \delta \) against respectively divergence (left-hand frame), vorticity (central frame) and shear (right-hand frame). The strong correlation between the density and the divergence is as expected, although there is quite a large amount of scatter. For comparison, the solid line shows the prediction by Bernardeau (1992). From the scatter plot against the vorticity we can infer that the mean vorticity increases slightly with the density. A similar conclusion can be made for the shear. It confirms the idea that voids tend to be regular spherically expanding regions, whereas dense matter concentrations tend to have non-radial motion.
A new method for accurate estimation of velocity field statistics

The velocity field in the local Universe is an important and essential source of information on structure formation. Particularly interesting for an understanding of the evolution and dynamics of the structures in the Universe are the various components of the gradient of the velocity field, the velocity divergence, shear and vorticity. One approach is to study the statistical properties, both moments and the full probability distribution function (PDF), of the divergence, shear and vorticity of the local smoothed velocity field. Considerable effort has been directed to obtaining analytical results for the statistics of the velocity divergence in the linear and quasi-linear regimes in the case of structure formation scenarios based on Gaussian initial density and velocity fields.

To study more advanced stages of structure evolution we often have to resort to N-body simulations, yielding discretely sampled velocity fields. The discrete nature of the velocity sampling complicates the determination of the statistical properties of the velocity field. In this paper we have introduced and developed two numerical methods, the Voronoi tessellation method and the Delaunay tessellation method, that yield reliable and accurate estimators of volume-averaged quantities in the case of discretely sampled velocity fields. The fact that they concern volume-averaged quantities is of crucial importance. Almost all analytical results concern volume-averaged quantities while in essence all available numerical estimators only yield mass-averaged quantities. The latter considerably obscured the comparison between statistical results from analytical models and N-body studies, and even led to false conclusions regarding e.g. the validity of perturbation theory.

The availability of estimators of volume-averaged velocity statistics is important for several reasons. First, it allows us to check independently whether the perturbation calculations that yield the quasi-linear results are indeed valid. Secondly, if so, we can apply the new estimators with confidence to highly non-linear circumstances. And finally it may be feasible to apply them, in adapted form, to the available catalogues of measured galaxy peculiar velocities.

Both the Voronoi tessellation method and the Delaunay tessellation method are based on important objects in stochastic geometry, the Voronoi and the Delaunay tessellations of a point set. A Voronoi tessellation of a set of nuclei is a space-filling network of polyhedral cells, each of which delimits the part of space that is closer to its nucleus than to any of the other nuclei. The Delaunay tessellation is also a space-filling network of mutual disjoint objects, tetrahedra in 3D. The four vertices of each Delaunay tetrahedron are nuclei from the point set, such that the corresponding circumscribing sphere does not have any of the other nuclei inside. The Voronoi and the Delaunay tessellations are closely related, and are dual in the sense that one can be obtained from the other.

In a first evaluation of the two new methods we calculated, on a regular grid, the volume-averaged velocity divergence, shear and vorticity of an 128³-particle N-body simulation of structure formation in an Ω = 1 CDM universe. Computer memory space limitations in the case of the Voronoi method forced us to sample some 40 000 particles from the total sample of 128³ particles. This sampling was performed such that the number density in underdense regions was not reduced. A comparison study between the Voronoi method, the Delaunay method, the conventional 'two-step' method and analytical theoretical predictions yields encouraging results for our new methods. The comparison study consists of comparison of scatter plots, and third- and fourth-order moments as well as the global PDFs. The Voronoi and the Delaunay methods show remarkably good agreement with each other, as well as with theoretical predictions. On the other hand, considerable differences with the conventional 'two-step' method were found.

We may therefore conclude that the Voronoi and the Delaunay methods represent optimal estimators for determining the probability distribution function of volume-averaged quantities.
velocity field quantities. As yet it is difficult to judge which of the two methods is the preferable one. The results produced by both methods agree very well for a considerable range of situations. However, the Delaunay method is clearly the better one for small filter radii, as it provides a reasonable estimate of the velocity gradients throughout the whole of space. The Voronoi method, on the other hand, only does so in the Voronoi walls. Consequently, irrelevant and noisy filter averages are produced by the latter if the filter scale is smaller than the average wall distance because the small filter spheres frequently end up being empty. Another advantage of the Delaunay method is its approximately 8 times lower memory space requirement. However, this may be a mere practical issue, as a more efficient Voronoi method implementation is certainly feasible. A clear disadvantage of the Delaunay method is the fact that it is almost 12 times more CPU-time consuming than the Voronoi method. This is largely due to the inefficient calculation of the intersection between a tetrahedron and a sphere. We expect that better and faster prescriptions are possible, which may possibly lead to a five- to tenfold acceleration of this algorithm.

In forthcoming work we will apply the newly developed tool to a plethora of structure formation scenarios, based on both Gaussian and non-Gaussian initial conditions. The reliability of the results obtained with both the Voronoi and the Delaunay methods allows us to study to what extent the velocity field PDFs are sensitive discriminators that highlight physical differences between the scenarios. In particular, we are interested in the possibility of extracting the value of \( g \) from these velocity statistics. The availability of the reliable numerical estimators that we developed here is a crucial step in making this a practical possibility. We therefore also wish to develop our methods for the even less ideal circumstances of observational data. To see whether this is feasible, one of the first steps is to see to what extent our methods are sensitive to substantial amounts of noise in the data. These issues will be addressed in a forthcoming study. Also, we intend to make the software that we developed for both the Voronoi and the
A new method for accurate estimation of velocity field statistics

Figure 11. Scatter plots of the value of the local density contrast \( \delta \) against the velocity divergence \( \theta \) (left-hand frame), vorticity \( \omega \) (central frame) and shear \( \sigma \) (right-hand frame), at \( 2^1 \) grid positions, for the same \( 128^3 \)-particle CDM N-body simulations as in Figs 6-10. All quantities are top-hat filtered with a top-hat radius \( R_{TH} = 15h^{-1} \) Mpc. The solid line in the left-hand panel indicates the prediction of the \( \delta - \theta \) relation by Bernardeau (1992).

Delaunay methods publicly available once it has been made user-friendly.

In addition, we feel that variations of the two numerical tools that we have introduced here can be applied to a variety of other applications in astrophysical situations. In many situations the value of a particular physical quantity is only known at a limited number of discrete points in space. The optimal adaptive nature of both the Voronoi and the Delaunay tessellations to the point distribution makes methods based on them promising estimators of the general run of quantities over the whole of the sample space.

ACKNOWLEDGMENTS

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APPENDIX A: THE INTERSECTION OF A SPHERE AND A POLYGON

For the implementation of the Voronoi method we need to calculate the surface of the intersection of a polygon and a sphere.

Fig. A1 sketches the geometrical situation we encounter. The problem naturally reduces to a planar problem in the plane of the polygon (bottom panel) where one has to calculate the...
1996MNRAS.279..693B F. Bernardeau and R. van de Weygaert

Figure A1. The intersection of a sphere and a polygon. The dashed disc is the intersection of the sphere with the plane supporting the polygon. The points I, J are the intersecting points of the polygon with the small circle.

surface of the intersection of the polygon with the disc. This figure corresponds to the generic case where the circle intersects the polygons at two different points I, J. The surface is then given by the sum of the surface of the polygon (I, A, B, C, D, J) and the surface of the segment defined by the points I, J, given by π(θ - sin(θ))R_J^2/2, where R_J is the radius of the disc.

There are in fact other possible cases: the disc may be entirely contained in the polygon (the surface is then that of the disc), may contain the whole polygon (the surface is the surface of the polygon) or may have more than two intersection points with the polygon. In the latter case the surface is obtained by a combination of polygons and segments.

APPENDIX B: THE INTERSECTION BETWEEN A SPHERE AND A TETRAHEDRON

For the implementation of the Delaunay method we need to calculate the volume of the intersection of a sphere and a tetrahedron. In the following we use (A, B, C, D) to indicate the four points that define the tetrahedron. The letters I, J, K and L represent any arbitrary order of these four points.

The volume of the intersection is calculated by a sequence of complementary volume calculations. To be specific, the intersection volume follows by taking the volume of the whole sphere as a start. From that volume we then extract the volumes cut out by each of the planes defined by three points (I, J, K). In total there are four such planes, the possible permutations of (A, B, C, D). Subsequently, we have to correct by adding each of the volumes contained in the six spherical segments defined by two planes (I, J, K) and (I, J, L). Finally, we should subtract the volumes of the four cones defined by the three planes containing I, J, K, or L. In short,

\[ V_{\text{intersection}} = V_{\text{sphere}} - \sum_{\text{perm.}} V_{I,J,K} + \sum_{\text{perm.}} V_{I,J,L} - \sum_{\text{perm.}} V_{SI}, \]

where the summations are made over the possible permutations for I, J, K, L, and

(i) \( V_{\text{sphere}} \) is the volume of the sphere;
(ii) \( V_{I,J,K} \) is the volume of the sphere segment delineated by the plane (I, J, K) on the side opposite to the point L.
(iii) \( V_{I,J,L} \) is the volume of intersection of the sphere segments carved out by the planes (I, J, K), opposite to the point L, and (I, J, L), opposite to the point L;
(iv) \( V_{SI} \) is the volume of the intersection of the sphere segments defined by the planes (I, K, L), opposite to J, (I, J, L), opposite to K, and (I, J, K), opposite to L.
The calculation of $V_P$ is quite straightforward. It is given either by the expression

$$V_P = \pi R^3 \left( \frac{2}{3} - x - x^3/3 \right),$$

where $x$ is the distance of the centre of the sphere to the plane in units of the radius $R$, or by the volume of the complementary part in the sphere.

The calculation of $V_{A \perp J}$ is intrinsically more complicated. The geometrical problem is illustrated in Fig. B1 in the plane orthogonal to the planes $(I,J,K)$ and $(I,J,L)$. The edge $(I,J)$ is indicated by the point $I$. The distance $x$ is the distance of the centre of the sphere to this line (expressed in units of the radius). The volume to be calculated, $V_A$, is indicated by the cross-hatched area. It depends on $x$ and the angle $\theta$, and for $x \tan \theta < 1$ is given by

$$V_A = \frac{1}{3} \left\{ -dx^2 \sin \theta \cos \theta ight. \\
+ x(3 + (3 - x^2) \tan^2 \theta) \sin \theta \cos^2 \theta \arctan \left( -\frac{x \cos \theta}{d} \right) \\
+ \arctan \left[ \frac{x - d^2 \tan \theta}{d(1 - x \tan \theta)} \right] \\
- \arctan \left[ \frac{x + d^2 \tan \theta}{d(1 + x \tan \theta)} \right] \\
+ x \pi \left( 3 \sin^3 \theta + 3 \cos^2 \theta \sin \theta - x^2 \sin^3 \theta \right)/2 \left\}$$

and by the same expression plus $\pi/3$ otherwise. In this expression, the parameter $d$ is defined by

$$d = (1 - x^2)^{1/2}.$$  

This expression is strictly valid only when $0 < \theta < \pi$. Otherwise equations (B2) and (B3) have to be combined to get the proper answer.

The calculation of the volumes $V_S$ is even more cumbersome in its practical implementation, but is given by a combination of equations (B2) and (B3). The typical geometrical situation is presented in Fig. B2. By default we assume the tip $I$ to be located within the sphere. If this is not the case the situation is simpler and can be reduced quite straightforwardly to previously discussed situations and equations.

The volume $V_S$ can also be calculated by the determination of a sequence of complementary volumes,

$$V_S = V_{\text{tetra.}} - \sum_{\text{perm.}} V_{P_j} + \sum_{\text{perm.}} V_{A_{\perp J,K,L}'},$$  

where $V_{\text{tetra.}}$ is the volume of the tetrahedron defined by $I$ and the intersection points $J',K',L'$ of the three half-lines $[I,J)$, $[I,K)$ and $[I,L)$ with the spheres. The volume $V_P$ is that of the fraction of the sphere above the plane $(J',K',L')$ (obtained with equation B2), and $V_{A_{\perp J,K,L}'}$ are the three volumes of the fractions of the sphere that are bounded by $(J',K',L')$ and respectively $(I,J',K')$, $(I,J',L')$, $(I,K',L')$, and that do not contain $I$ or, respectively, $L'$, $K'$, $J'$. These volumes are given by a proper use of expression (B3).

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