Geometry of Lagrangian Dispersion in Turbulence

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(Received 13 April 2000)

Turbulent flows disperse Lagrangian particles resulting in the growth of pairwise separations and, for sets of three or more particles, in a nontrivial dynamics of their configuration. The shape of such clusters is controlled by the competition between coherent straining of the cluster and the independent random motion of the particles due to small scale velocity fluctuations. We introduce a statistical description of the geometry of the Lagrangian clusters and predict a self-similar distribution of shapes, which should be observable in the inertial range of scales in high Reynolds numbers flows.

PACS numbers: 47.11.+j, 47.27.–i

One of the defining attributes of turbulent flow is the effective mixing that it produces thanks to the chaotic motion of the material points of the fluid and consequently, that of any advected particles. According to Taylor, a single material point (or advected particle) on time scales much longer than the turnover of the largest eddy exercises a Brownian motion with effective diffusivity set by the characteristic scale and time of the flow. On the other hand, a pair of points separated by the scale smaller than that of the largest eddy separates superdiffusively according to the Richardson law $\langle R^2(t)\rangle \sim \varepsilon t^3$ (where ε is the rate of energy dissipation) [1,2]. The difficulty of tracking particles has been a serious impediment to direct experimental verification, yet recent observations in a two-dimensional flow are compatible with Richardson's prediction [3]. Newly developed methods of particle tracking [4,5] should allow further direct tests of the Richardson law. They will also allow one to follow more than one or two particles making it possible to study not only the statistics of pair separations but also the geometry of particle configurations. The latter is interesting because it provides information about the dispersion process which goes beyond Richardson scaling and probes the effect of transiently coherent turbulent fluctuations.

Indeed, there is much more to turbulent mixing than the random meander of particles. The complexity of the process is evident in the structure of an advected scalar field which tends to organize into fronts of high gradient observed in experiment [6–9]. Recent work on the passive scalar problem [10–12] has attributed the breakdown of the Kolmogorov-Obukhov-Corrsin scaling theory to the appearance of such structures. Formation of "fronts" is associated with transient domains of hyperbolic flow which because of the volume preservation distort and necessarily "flatten" blobs of fluid. The same mechanism would result in a relatively high probability for multipoint ($n > 3$) clusters to become nearly coplanar. The distortion of the cluster due to larger scales of the flow is opposed by the independent and uncorrelated random motion of its constituent points due to small scale turbulence. The average degree of this distortion is a measure of relative importance of the correlated and incoherent relative Lagrangian motion of particles and provides insight into the geometric structure of turbulent fluctuations. It can be measured by following three or more material points in the flow and is the main subject of the present work.

In this work we investigate the geometrical aspects of Lagrangian dispersion, and, in particular, the dynamics of small $n = 3, 4$ clusters of material points via (1) direct numerical simulations (DNS) of the Navier-Stokes equations at moderate Reynolds numbers ($R_\lambda \approx 82$), and (2) a simple phenomenological model of the Lagrangian kinematics (first advanced in the context of passive scalar [10]) which describes the combined action of coherent and incoherent random strain. The DNS demonstrate that initially regular clusters of points, whose scale R_0, at $t = 0$, lies in the dissipation range rapidly evolve into very strongly distorted configurations, while clusters of larger size, comparable with the integral scale, relax towards a uniform shape distribution. The phenomenological model allows us to qualitatively extrapolate the DNS measurements to the high Reynold's number regime. We argue here in favor of the existence, within the inertial range of scales, of a self-similar state where the average size of the cluster increases, but the statistical distribution of shapes is stationary and nonuniform, so that most likely clusters are strongly distorted. Finally, we discuss the nontrivial relation between the kinematics of Lagrangian clusters and the anomalous scaling established for the multipoint correlators of the advected scalar [10,12–16].

To describe a cluster of n particles, located at $\vec{x}_i$ ($i = 1, n$), we define $n - 1$ vectors involving position differences only. A convenient choice is $\vec{\rho}_1 = (\vec{x}_2 - \vec{x}_1)/\sqrt{2}$, $\vec{\rho}_2 = (2\vec{x}_3 - \vec{x}_1 - \vec{x}_2)/\sqrt{6}$, $\vec{\rho}_3 = (3\vec{x}_4 - \vec{x}_1 - \vec{x}_2 - \vec{x}_3)/\sqrt{12}$ (the center of mass has no influence on the shape of the cluster). The radius of gyration, defined by $R^2 = \sum_{i=1}^{n-1} \vec{\rho}_i^{\,2}$ measures the spatial extent of the swarm of particles. To characterize the shape of the object, we introduce a "moment of inertia-like" tensor by

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$$g^{ab} \equiv \sum_{i=1}^{n-1} \rho_i^a \rho_i^b , \tag{1}$$

where ρ_i^a is the a component of the vector $\vec{\rho}_i$. The eigenvalues of this tensor g_i ($g_1 \geq g_2 \geq g_3 = R^2$) provide a way of quantifying the shapes of the set of points. For example, for $n \geq 4$, $g_1 = g_2 = g_3$ corresponds to an isotropic object. The case $g_1 \approx g_2 \gg g_3$ corresponds to a pancakelike object and $g_1 \gg g_2, g_3$ to a needlelike object. The same considerations apply for a triangle, $n = 3$, with the restriction that $g_3 = 0$. A convenient way to describe the overall shape of the swarm consists of monitoring the ratio $I_2 = g_2/R^2$ ($0 \leq I_2 \leq 1/2$). Alternatively, for $n = 3$, the area of a triangle, $\mathcal{A} = |\vec{\rho}_1 \times \vec{\rho}_2|$, and, for $n = 4$, the volume of a tetrahedron, $V = |\det(\vec{\rho}_1, \vec{\rho}_2, \vec{\rho}_3)|$ may also be used to construct dimensionless measures of the cluster shape; e.g., for the triangle, $\omega \equiv 2\mathcal{A}/R^2 = 2\sqrt{I_2(1 - I_2)}$. Statistically, the geometry of the evolving Lagrangian cluster is characterized by a (time dependent) probability distribution function (pdf) of these invariants. Their pdf should be compared with the case of the isotropic Gaussian distribution $P_G(\vec{\rho}_1, \ldots, \vec{\rho}_{n-1}) = \mathcal{N} \exp(-\sum_i \vec{\rho}_i^2)$. In the triangle case, one can explicitly compute the pdfs of I_2:$p_G(I_2) = 4(1 - 2I_2)$ ($\langle I_2 \rangle_{G,3} = 1/6$), and of area $\mathcal{A}$:$p_G(\mathcal{A}) = 4\mathcal{A} \exp(-2\mathcal{A})$ (see also [17]). For $n = 4$ the pdfs of volume and of I_2 may be determined by a straightforward Monte Carlo (MC) calculation ($\langle I_2 \rangle_{G,4} \approx 0.222$).

Numerically, we consider a turbulent flow in a periodic box, forced at large scale. The Navier-Stokes equations are integrated with a standard pseudospectral code, with 128^3 resolution. The Reynolds number is $R_\lambda \approx 82$. Regular tetrahedra with an edge of size r_0 are initiated at the vertices of a regular sublattice of size $(27)^3$ of the full domain. The initial radius of gyration is $R_0 = \sqrt{3/2}\, r_0$. The integration of the advection equation for the particles requires a precise interpolation of the velocity field; we use a third order interpolation algorithm [18]. The results discussed below do not depend qualitatively on the Reynolds number in the range $21 \leq R_\lambda \leq 82$.

The evolution of $\langle I_2 \rangle$ as a function of time for initially regular tetrahedra with $r_0 = q\eta$ with $q = 1/4$, 1, 4, 16, 32, and 64 is shown in Fig. 1(a). A rapid decrease of I_2 corresponding to strong initial growth of distortion is observed, more so as the initial size of the swarm gets smaller. At very short times, all the curves corresponding to the dissipative scale ($r_0 \lesssim 5\eta$) superpose. A systematic comparison with data at a lower Reynolds number demonstrates that the characteristic distortion time in the dissipation range is the Kolmogorov time, $\tau_K = (\nu/\epsilon)^{1/2}$. For $R \gtrsim 10\eta$, the characteristic time of distortion is $\tau(r_0) = r_0^{2/3}\epsilon^{-1/3}$. When $r_0 = \eta/4$, the shape distortion is maximum when $\langle R \rangle \approx 10\eta$, at the low end of the inertial range. At larger scales/times, the distributions of I_2, V, and R all appear to approach asymptotically the Gaussian distribution: $\langle I_2 \rangle_{G,4} \approx 0.222$. For values of R_0 close to L, the integral scale, the dip of $\langle I_2 \rangle$ preceding the relaxation to the uniform distribution is very weak. The results obtained for triangles are qualitatively completely similar. Figure 1(b) shows the mean value of the volume of the tetrahedra. At short times, and for $r_0 \lesssim 4\eta$, the volume is approximately conserved, as expected, since the velocity field in the dissipative range is well approximated locally

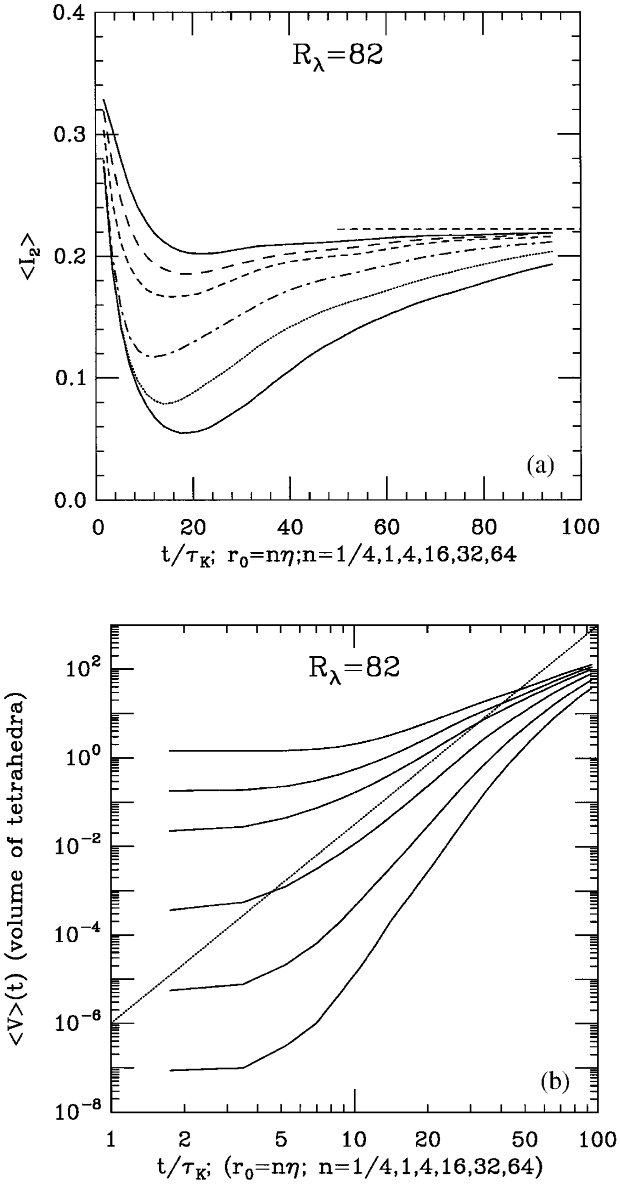

FIG. 1. Evolution of the ratio $\langle I_2 \rangle$ (a) and of $\langle V \rangle$ (b) for a set of $(27)^3$ initially regular tetrahedra, with an edge size of $r_0 = n\eta$, $n = 1/4$, 1, 4, 16, 32, and 64. The integral size is $L \sim 64\eta$; $R_\lambda \approx 82$. In (a), the dashed horizontal line shows the Gaussian value, $\langle I_2 \rangle_{G,4} \approx 0.222$. Time has been scaled by the Kolmogorov time scale. The smaller the value of r_0, the lower the minimal value of $\langle I_2 \rangle$. (b) shows the growth of the averaged value of the volume, $\langle |V| \rangle$ of the tetrahedra. No convincing Richardson scaling is seen ($\langle |V| \rangle \propto \epsilon^{3/2} t^{9/2}$; compare with the dashed line). The results obtained for triangles are qualitatively very similar.

by $v_a(r,t) = M_{ab}(t) r_b$ with tr$M = 0$ due to incompressibility. Because of this constraint, the growth of R is due to shape distortions. Once R reaches inertial scale values, the contribution of small scale fluctuations becomes important and Lagrangian dynamics deviates from the linear volume preserving map which it was in the dissipative range: the average volume begins to grow. The pdf of volumes corresponding to a value of r_0 in the dissipative range shows very wide tails. The number of tetrahedra followed (27^3) was not large enough to obtain a reliable estimate of the second moment of the distribution.

The kinematics of Lagrangian dispersion may be modeled by the following equation for the evolution of $\vec{\rho}$ [10,11,19]:

$$\frac{d\rho_i^a}{dt} = \rho_i^b M_{ba} + u_i^a\,, \tag{2}$$

where $M_{ba} = (\partial_b V_a)$ with tr$M = 0$ represents the smooth velocity gradient due to the components of velocity at wave numbers of order $\sim 1/R$ (in a Fourier decomposition) which coherently strains and shears the cluster, whereas u_i^a denotes the incoherent random velocity component arising from Fourier modes with wave number $> R^{-1}$. The long wavelength part of the velocity field is irrelevant as it simply advects the cluster as a whole. Dimensionally, the strain is $M \sim \epsilon^{1/3} R^{-2/3}$, and should evolve on a time scale $\tau(R) \sim \epsilon^{-1/3} R^{2/3}$. Similarly, the small scale velocity fluctuations are of order $u \sim \epsilon^{1/3} R^{1/3}$, and evolve with a characteristic time smaller than $\tau(R)$. For our purely kinematic purpose, let us consider a simple Gaussian model of the inertial range:

$$\frac{dM_{ab}}{dt} = -\frac{M_{ab}}{\tau(R)} + \eta_{ab}, \tag{3}$$

$$\langle \eta_{ab}(t)\eta_{cd}(t')\rangle = C_\eta^2 \delta(t - t') \times \left(\delta_{ab}\delta_{cd} - \frac{1}{d}\,\delta_{ac}\delta_{bd}\right)\Big/\tau(R)\,, \tag{4}$$

$$\langle u_i^a(t) u_j^b(t')\rangle = \left(\frac{C_v}{3}\right)^2 \delta(t - t')\delta_{ij}\delta_{ab} R^2/\tau(R)\,. \tag{5}$$

The growth of distortion is clearly due to the action of the coherent strain [20], while the incoherent, small scale term (u_i^a) acting by itself would produce a uniform distribution of shapes. The two dimensionless factors C_v and C_η describe the relative importance of the two terms with the ratio C_v/C_η, *a priori* of order 1 in the inertial range. For R comparable to the integral scale however, most of the velocity field becomes effectively "small scale" (compared to R), so relaxation towards the Gaussian shape distribution is expected.

We have studied Eqs. (2)–(5) numerically using the MC approach. As expected dimensionally, the scale R eventually grows as $t^{3/2}$. More importantly for our purpose, the ratio $\langle I_2\rangle$ reaches a finite value when $t \to \infty$. This corresponds to the appearance of a dynamical self-similar state with stationary distribution of shapes: $P(\rho, t) \to P(R/t^{3/2}, g/R^2)$. Indeed, all the distributions we have computed numerically converge to a time independent limit when t is large. In the self-similar state the "coherent" distortion generated by scales comparable to R is balanced by the randomizing effect of small scale fluctuations. Thus the limiting value of $\langle I_2\rangle$ depends monotonically on the ratio C_v/C_η, as Fig. 2 demonstrates, in the case of tetrahedra. The Gaussian value is recovered when $C_v/C_\eta \to \infty$, whereas the distortion increases without limit ($\langle I_2\rangle \to 0$) when $C_v/C_\eta \to 0$. For the case of triangles the "shape" tensor g is parametrized by a single variable $\omega \equiv 2\mathcal{A}/R^2$ ($w \le 1$). Figure 3 presents the pdf of w, as well as the pdf of w conditioned on several values of $R/\langle R\rangle$. We observe that the clusters with the radius of gyration larger than average are more distorted, as evidenced by the shift of the maximum of P towards smaller values of w. A systematic variation of the pdfs of radii of gyration/pair separation as a function of C_v/C_η ratio is observed: when C_v/C_η decreases as the coherent straining term becomes larger, the pdfs develop wider tails. We expect a similar nontrivial distribution of pair separation/radius of gyration to appear in real turbulent flows with large enough inertial ranges. It would be interesting to determine the effective C_v/C_η ratio by fitting the data.

In summary, we have investigated the statistical geometry of Lagrangian trajectories of $n = 3, 4$ particles. We find that Lagrangian shapes are strongly distorted by the coherent action of larger scale flow and on the basis of a phenomenological model predict that in flows with wide

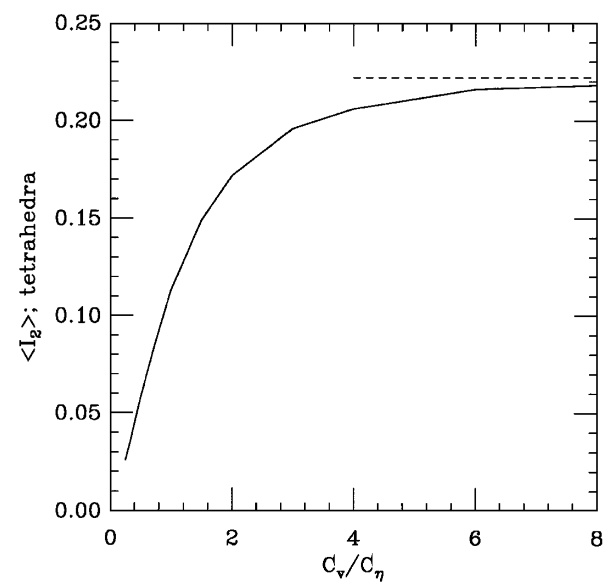

FIG. 2. The value of the anisotropy of the tetrahedra reached asymptotically evolving according to the stochastic model Eqs. (2)–(5) at long times, as a function of the ratio C_v/C_η. The dotted line is the Gaussian ensemble value. Qualitatively very similar results are obtained for the triangles.

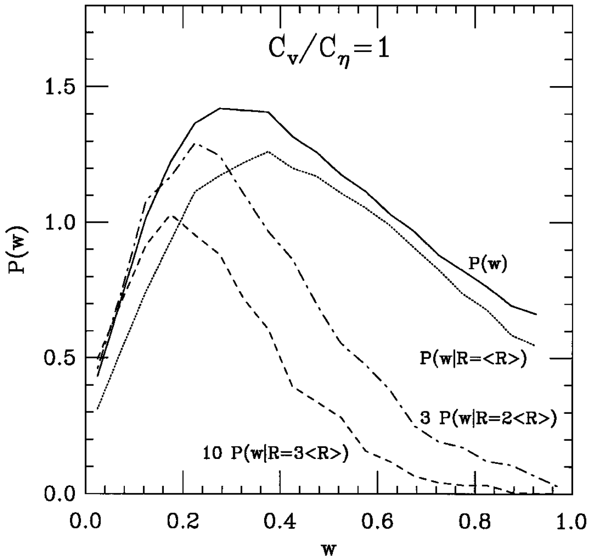

FIG. 3. The pdf of w [$w = 2\sqrt{I_2(1 - I_2)}$], and the pdf of w conditioned on R characterizing the self-similar state solution of Eqs. (2)–(5) ($C_v/C_\eta = 1$). The total distribution of w is different from the distribution in the Gaussian ensemble [$P_G(w) = 2w$]. The maximum probability shifts towards low values of w, implying a higher degree of distortion when conditioning on a higher value of $R/\langle R \rangle$.

inertial range (in contrast to our DNS) multipoint configurations should achieve a nontrivial statistically self-similar shape distribution. We also observe a correlation between the rate of dispersion (defined as growth of the average interparticle distance) and the degree of distortion which indicates the importance of high strain events. Recent work on the passive scalar problem [10,12–16] has related the appearance of anomalous scaling with zero modes of the evolution operator governing multipoint correlators. Configurational degrees of freedom proved essential since without them there would not be zero modes. The nontrivial configurational statistics of a dispersing Lagrangian cluster which we discussed above is intimately, but not directly, related to the zero modes dominating static correlators. Both are governed by the same evolution operator H, but whereas the zero modes are annihilated by it, the inertial range self-similar state that we described satisfies $d/dt = \alpha R^{1/3} d/dR = H$. Further interest in multipoint Lagrangian statistics is justified as it extends beyond kinematics and into "dynamics" of turbulent fluctuation [21] and quantifies the intermittent nature of turbulent dispersion. Finally, Lagrangian statistics is becoming accessible experimentally and is offering a possibility of a novel and insightful comparison of observation and theory.

A. P. and B. I. S. wish to acknowledge the hospitality of the Isaac Newton Institute for Mathematical Sciences, in Cambridge, U.K., where part of this work has been done. A grant of computer time from IDRIS (France) is gratefully acknowledged.

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