Particle trapping in three-dimensional fully developed turbulence

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The statistical properties of fluid particles transported by a three-dimensional fully developed turbulent flow are investigated by means of high resolution direct numerical simulations. Single trajectory statistics are investigated in a time range spanning more than three decades, from less than a tenth of the Kolmogorov time scale, τ_η, up to one large-eddy turnover time. Our analysis reveals the existence of relatively rare trapping events in vortex filaments which give rise to enhanced intermittency on Lagrangian observables up to $10\tau_\eta$. Lagrangian velocity structure function attain scaling properties in agreement with the multifractal prediction only for time lags larger than those affected by trapping. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1846771]

The knowledge of the statistical properties of particle tracers advected by a fully developed turbulent flow is a key ingredient for the development of stochastic Lagrangian models in such diverse contexts as turbulent combustion, pollutant dispersion, cloud formation, and industrial mixing.[1–4] Given the importance of this problem, there are comparatively few experimental studies of turbulent Lagrangian dispersion. Progress in this direction has been hindered mainly by the presence of a wide range of dynamical time scales, an inherent property of fully developed turbulence. Indeed, in order to obtain an accurate description of the particles' statistics it is necessary to follow their paths with very high resolution, i.e., well below the Kolmogorov time scale τ_η, and for a long time lapse—of the order of an eddy turnover time T_L. The ratio of these time scales can be estimated as $T_L/\tau_\eta \sim R_\lambda$ where the microscale Reynolds number R_λ ranges in the hundreds for typical laboratory experiments. A recent breakthrough has been made by La Porta *et al.*[5,6] who, borrowing techniques from high-energy physics, were able to track three-dimensional trajectories with a resolution of $0.05\tau_\eta$ and thus to study the statistics of particle acceleration. However, owing to the small measurement volume, trajectories could be followed only up to a few τ_η, preventing any investigation of the long time correlations along particle paths. Conversely, the acoustical technique adopted by Mordant *et al.*[8] enabled them to successfully track particles for durations comparable to T_L but could not access time delays of the order of τ_η, and was restricted to one-dimensional measurements. More conventional techniques, e.g., based on CCD cameras,[9] reveal useful only for moderate Reynolds numbers ($R_\lambda \simeq 100$) due to their limitations in the acquisition rate. In addition, all laboratory techniques require a considerable amount of signal processing to get rid of experimental noise. Besides these drawbacks, increasing difficulties are met when attempting to deal with multiparticle tracking.

In light of the above remarks direct numerical simulation of fully developed turbulence represents a valuable alternative tool for the investigation of Lagrangian statistics[10–18] and its important contribution has been recently reviewed in Ref. 4. Nonetheless, computational approaches have to face three demanding requirements: (i) have the largest possible value of R_λ in order to maintain the flow in a fully developed turbulent state; (ii) resolve properly the dissipative scales with the aim of computing accurately small-scale observables; (iii) follow particle trajectories for times comparable to a large-eddy-turnover time. High resolution and huge computational resources are therefore needed to accomplish such a goal, making massive parallel computing by far and away the most appropriate tool. In this Letter we report the results of direct numerical simulations of Lagrangian transport in homogeneous and isotropic turbulence on the parallel computer IBM-SP4 at CINECA, on 512^3 and 1024^3 cubic lattices with Reynolds numbers up to $R_\lambda \sim 280$, a very accurate resolution of dissipative scales, and a long integration time $T \approx T_L$. The most important limitation with high-resolution DNS with respect to the experiments is the high computational cost that has to be paid to perform runs of a few large-eddy turnover times at such resolution. As a consequence large scale statistics cannot reach complete isot-

TABLE I. Parameters of the numerical simulations. Microscale Reynolds number R_λ, root-mean-square velocity $u_{\rm rms}$, energy dissipation ε, viscosity ν, Kolmogorov length scale $\eta=(\nu^3/\varepsilon)^{1/4}$, integral scale L, large-eddy turnover time $T_E=L/u_{\rm rms}$, Lagrangian velocity autocorrelation time T_L, Kolmogorov time scale $\tau_\eta=(\nu/\varepsilon)^{1/2}$, total integration time T, grid spacing δx, resolution N^3, and the number of Lagrangian tracers N_p. We also report the values of normalized acceleration variance a_0, and of C_0, the constant entering in the definition of the second order structure function, $\langle(\delta_\tau v)^2\rangle=C_0\varepsilon\tau$ (see text).

R_λ	$u_{\rm rms}$	ε	ν	η	L	T_E	T_L	τ_η	T	δx	N^3	N_p	a_0	C_0
183	1.5	0.886	0.00205	0.01	3.14	2.1	1.3	0.048	5	0.012	512^3	$0.96\cdot10^6$	3.3 ± 0.3	5.0 ± 0.8
284	1.7	0.81	0.00088	0.005	3.14	1.8	1.2	0.033	4.4	0.006	1024^3	$1.92\cdot10^6$	3.5 ± 0.3	5.2 ± 0.8

ropy even with a nominally fully isotropic forcing. The fluctuations of total energy among the three velocity components is of the order of 10%. Isotropy is restored at small scales, due to the faster eddy turn over times and to the "return-to-isotropy" induced by the energy cascade. For example, we find that distortions from a perfectly isotropic statistics for the acceleration are smaller than 1%.

The Navier–Stokes equations

$$\partial_t \boldsymbol{u} + \boldsymbol{u}\cdot\boldsymbol{\nabla}\,\boldsymbol{u} = -\boldsymbol{\nabla}\,p + \nu\boldsymbol{\Delta u}, \tag{1}$$

are integrated on a triply periodic box by means of a fully dealiased pseudospectral code (the numerical parameters are listed in Table I). Energy is injected at an average rate ϵ by keeping constant the total energy in each of the first two wave number shells.[19] With the present choice of parameters the dissipative range of length scales is extremely well resolved. With regard to the Eulerian scaling properties of the velocity field, our results are in perfect numerical agreement with previous numerical simulations at comparable R_λ (see, e.g., Ref. 20). Upon having reached statistically stationary conditions for the velocity field, millions of Lagrangian tracers have been seeded into the flow and their trajectories integrated according to $d\boldsymbol{X}/dt=\boldsymbol{u}(\boldsymbol{X}(t),t)$, over a time lapse of the order of T_L. Particle positions $\boldsymbol{X}(t)$ and velocities $\boldsymbol{v}(t)=\dot{\boldsymbol{X}}(t)$ have been stored at a sampling rate $0.07\tau_\eta$. The forces acting on the particle—pressure gradients $\boldsymbol{\nabla}p(\boldsymbol{X}(t),t)$, viscous forces $\nu\boldsymbol{\Delta u}(\boldsymbol{X}(t),t)$ and external input—and the resulting particle acceleration $\boldsymbol{a}(t)=\dot{\boldsymbol{v}}(t)$ have been recorded along the particle paths every $0.14\tau_\eta$. The resulting database permits detailed study of the statistics of Lagrangian velocity and acceleration over a range of time scales spanning more than three decades. In what follows, we will focus on the description of the statistics of single-particle trajectories, deferring the discussion of multiparticle statistics to a forthcoming publication. The analysis reveals the presence of frequent entrapment events within vortical structures (see Fig. 1), first observed in Ref. 6. The characteristic frequency of these helical paths is comparable to τ_η^{-1} and their duration can be as long as $10\tau_\eta$. The velocity experienced during these events can attain $5u_{\rm rms}$ with an ensuing acceleration $5u_{\rm rms}/\tau_\eta$ as large as $80a_{\rm rms}$. As we will show below, these events have a significant impact on time correlations up to $10\tau_\eta$. The probability density function (PDF) of the acceleration $a(t)$ is strongly intermittent with stretched exponential tails (a more focused analysis of the PDF of the acceleration including a comparison with multifractal prediction can be found in Ref. 7). Classical Kolmogorov scaling arguments (see, e.g., Ref. 21) yield for the acceleration variance the prediction: $\langle a^2\rangle=a_0\varepsilon^{3/2}\nu^{-1/2}$. We measure the values $a_0=3.5\pm0.3$ and $a_0=3.3\pm0.3$ for $R_\lambda=284$ and $R_\lambda=183$, respectively, in agreement with the results of Ref. 14 at comparable R_λ. The dependence on Reynolds number may be interpreted as a consequence of intermittency.[6,7] The acceleration kurtosis, $\kappa=\langle a^4\rangle/\langle a^2\rangle^2$ shows a weak dependence on R_λ as well; we measure $\kappa=35\pm4$ and $\kappa=40\pm3$ for $R_\lambda=183$ and $R_\lambda=284$, respectively.

For the shortest time delay, the velocity increment PDF $P(\delta_\tau v)$ approaches the acceleration distribution, while at larger time separations the PDFs are decreasingly intermittent and eventually become slightly sub-Gaussian for $\tau\approx T_L$, with a kurtosis $\langle(\delta_\tau v)^4\rangle/\langle(\delta_\tau v)^2\rangle^2\approx2.8$. The intermittency in the PDFs of $\delta_\tau v$ can be conveniently quantified in terms of the Lagrangian velocity structure functions $S_p(\tau)=\langle(\delta_\tau v)^p\rangle$, that are expected to behave as power laws τ^{ξ_p}. The scaling exponents ξ_p can be evaluated by looking at the logarithmic slope $d\log S_p(\tau)/d\log\tau$ that should display a plateau in the range $\tau_\eta\ll\tau\ll T_L$. From Fig. 2 it is clear that it is very difficult to extract the values for ξ_p. However, by means of the extended self-similarity procedure,[22] it is possible to estimate the relative exponents $\xi_4/\xi_2=1.7\pm0.05$, $\xi_5/\xi_2=2.0\pm0.05$, $\xi_6/\xi_2=2.2\pm0.07$, in fair agreement with those obtained in Ref. 8 (see Table II). Let us notice that the values measured here also show good agreement with the prediction obtained by translating the classical Eulerian multifractal formalism to the Lagrangian case.[7,24,25] The range of time delays over which relative scaling occurs is $10\tau_\eta$ to $50\tau_\eta$. In this range anisotropic contributions induced by the large scale flow appear to influence the scaling properties. The only way to reduce them would be to repeat many Lagrang-

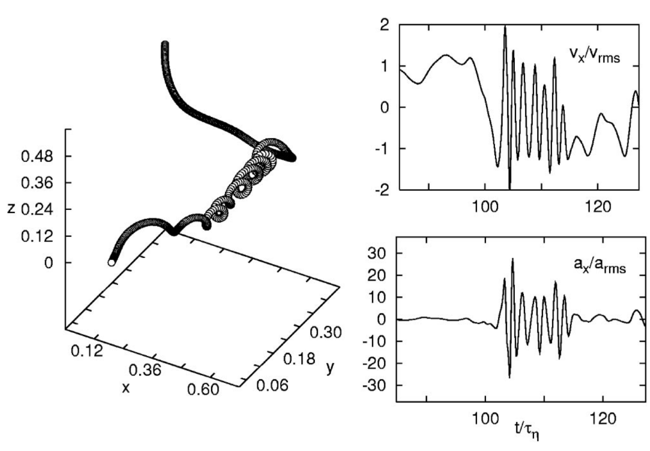

FIG. 1. Trajectory and time series. Left panel: 3D trajectory of a trapping event in vortex filament. Acceleration and velocity fluctuations here reach about 30 and 2 r.m.s. values, respectively (right panels).

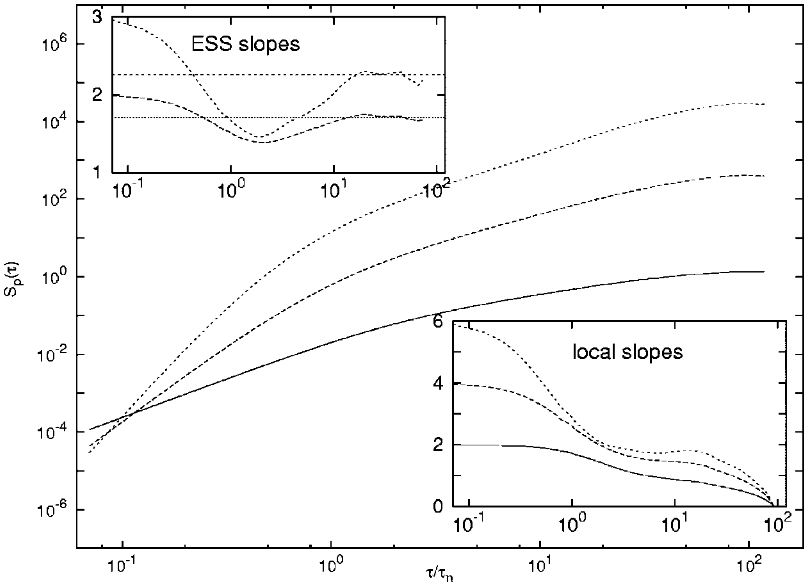

FIG. 2. Log–log plot of Lagrangian structure functions of orders $p=2$, 4, 6 (bottom to top) vs τ. Bottom right: logarithmic local slopes $d \log S_p(\tau)/d \log \tau$ (same line styles). Top left: ESS local slopes with respect to the second order structure function $d \log S_p(\tau)/d \log S_2(\tau)$, for $p=4$, 6 bottom and top, respectively. Straight lines correspond to the Lagrangian multifractal prediction with the same set of fractal dimensions used to fit the Eulerian statistics (Refs. 7 and 25). Data refer to the v_x component. The two other velocity components exhibit slightly worse scaling due to anisotropy effects. Relative scaling exponents and error bars are estimated from the mean and standard deviations of local slopes in the interval $[10\tau_\eta, 50\tau_\eta]$. Data refer to $R_\lambda=284$.

ian experiments with different initial conditions for the velocity field and perform ensemble averages. Unfortunately, this is an unfeasible task with the state-of-the-art computational resources.

It is interesting to remark that for values of τ in the range from τ_η to $10\tau_\eta$, the local slopes are significantly smaller and tend to accumulate around the value 2 for all orders. This relevant correction to scaling cannot be attributed to the influence of the dissipative range $\tau < \tau_\eta$, since the latter would increase the value of the local slope, rather than decreasing it. A similar effect can be detected in Eulerian structure functions as well, yet the intensity in the latter case is much less pronounced. These strong deviations in the Lagrangian scaling laws are most likely due to the trapping events depicted in Fig. 1. Indeed, the long residence time within small-scale vortical structures introduces an additional weighting factor that enhances the effect with respect to Eulerian measurements. This could possibly be the reason of the systematic small underestimate of the relative scaling exponents, ξ_p/ξ_2, measured in the experiment of Ref. 8 with respect to our estimate (see Table II). In other words, the experimental estimate of the scaling exponents might be partially flawed by contributions from time intervals affected by trapping events.

TABLE II. Summary of the relative scaling exponents measured in our DNS (first line), and in the experimental data of Ref. 8 (second line). In the third line we also show the theoretical values predicted by the Lagrangian multifractal formalism, $\xi_p=\min_h[(ph+3-D(h))/(1-h)]$ where the fractal dimension $D(h)$ is extracted from the analysis of Eulerian scaling properties (Ref. 7). The fourth line shows the values predicted by the classical dimensional scaling $\langle(\delta_\tau v)^p\rangle \sim (\varepsilon\tau)^{p/2}$.

	ξ_4/ξ_2	ξ_5/ξ_2	ξ_6/ξ_2
DNS	1.7 ± 0.05	2.0 ± 0.05	2.2 ± 0.07
Expt.	1.56 ± 0.06	1.8 ± 0.2	
LM Theory	1.71	2.00	2.26
Dim. Scal.	2	2.5	3

The saturation of local slopes to the value 2 around τ_η can be interpreted as the signature of trapping in vortical quasi-one-dimensional structures with almost discontinuous tangential velocity. Indeed inside these structures we have $\delta_\tau v \sim v_{\rm rms}$ with the probability of being inside a filament scaling as τ^2. In order to quantify this effect we computed the statistics over a velocity signal filtered out of the trapping events. A trapping event is defined when the mean acceleration amplitude, averaged over a time window of Δ_t is larger than $7a_{\rm rms}$. We have used two different time windows with $\Delta_t=2\tau_\eta$, $4\tau_\eta$. We have found that such events are relatively rare, covering approximately 1% of the whole statistics for the shorter window. The computation of the filtered velocity structure functions is then done by removing the contributions of increments $\delta_\tau v$ if one or both extremes of the time interval fall into a coherent event. The comparison between filtered and unfiltered structure functions is drawn in Fig. 3 for the sixth order. The analysis reveals that the effect of long-lasting coherent acceleration events associated to trapping is twofold: first, the conditioned structure functions $S_p^{(f)}(\tau)$ are much smoother at small time increments than the unconditioned $S_p(\tau)$; second, the local slopes now do not show any saturation effect and the "bottleneck" for $\tau \sim \tau_\eta$ is almost absent (see inset of Fig. 3). The large-time behavior is left unchanged upon filtering, indicating that trapping events influence the statistics in a neighborhood of τ_η only. Let us notice also that doubling the window length does not affect much the curves, an indication that coherence inside the vortex persists for time lags larger than τ_η. Similar results are obtained with different threshold values and for the run at lower resolution (not shown). These results point to the conclusion that trapping in coherent vortical regions is responsible for the corrections to scaling behavior observed for time increments of the order of the Kolmogorov time scale. These findings suggest that stochastic models for particle dispersion based on dimensional arguments might be inherently inadequate to describe the short-time behavior of real trajectories. In summary, we have presented the analysis of

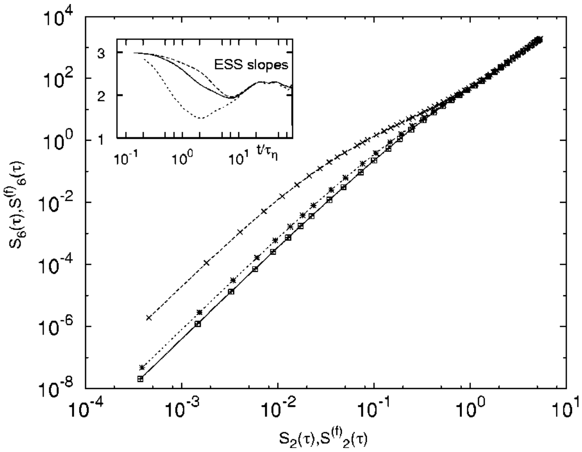

FIG. 3. ESS plots. Sixth-order structure functions vs the second-order one, with and without filtering of trapping events. Symbols refer to: $\times$ structure functions without any filtering, $S_p(r)$; $*$ structure function with filtering, $S_p^{(f)}(r)$, defined on a $\Delta_t = 2\tau_\eta$ window; $\square$ with filtering on $\Delta_t = 4\tau_\eta$. Inset: ESS local slopes of the curve in the body of the figure vs $\log(\tau/\tau_\eta)$. Upon filtering (two upper curves in the inset), the "bottleneck" effect on structure functions, i.e., the shallower slope observed in the neighborhood of τ_η, is suppressed. The behavior for time lags longer than $10\tau_\eta$ is unchanged. Data refer to $R_\lambda = 284$. Similar results are obtained for structure function of order $p=4$ (not shown).

single-particle statistics in high Reynolds number flows. At variance with experiments, we can investigate the statistical properties of millions of particles on a wide range of time intervals, from a small fraction of the Kolmogorov time up to the integral correlation time. We found clear indications that velocity fluctuations along Lagrangian trajectories are affected by multiple-time dynamics. Only in the interval $10\tau_\eta < \tau < T_L$ we observed anomalous scaling for Lagrangian velocity structure functions in agreement with the multifractal prediction.[7,24,25] For frequencies of the order of τ_η^{-1} we noticed that velocity fluctuations are affected by events where particles are trapped in vortex filaments. Events with trapping times much longer than expected on the basis of simple dimensional analysis appear frequently. The main novelty of Lagrangian single-particle statistics with respect to the Eulerian one is the importance of particle trapping by small-scale vortical structures. Indeed, the event analyzed in Fig. 1 would have a much smaller weight in an Eulerian analysis because of large-scale sweeping past the fixed probe. The strong "bottleneck" induced by particle entrapments on Lagrangian structure functions can be removed by filtering out the contribution of coherent, intense acceleration events. One of the most challenging open problems arising from our analysis is how to incorporate such dynamical processes in stochastic modelization of particle diffusion[3] and in the Lagrangian multifractal description.[23–25]

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