Preferential Sampling of Elastic Chains in Turbulent Flows

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The development of Lagrangian techniques, in experiments and theory, have lead to major advances in our understanding of the complexity of turbulent flows, especially at small scales [1–3]. What makes this possible is the use of tracer particles which uniformly sample the flow and hence access the complete phase space in which the dynamics resides. This feature of tracers depends, crucially, on the assumption that the particles remain inertia-less and point-like. When some of these assumptions are relaxed, it may lead to dissipative particle dynamics and preferential sampling of the structures in a flow [4–10]. This is, for instance, the case for heavy, inertial particles, which show small-scale clustering and concentrate away from vortical regions. Various phenomena can influence the properties of inertial clustering in turbulence, such as gravity [11, 12], turbophoresis [13, 14], or the non-Newtonian nature of the fluid [15]. Preferential sampling in turbulent flows may also emerge as a result of the motility of particles, as in the case of gyrotactic [16], interacting [17], or jumping [18] micro-swimmers.

We now propose a novel mechanism for preferential sampling in turbulent flows which is induced by extensibility. A simple model of an extensible object which retains enough internal structure is a chain of tracers with an elastic coupling between the nearest neighbours. We show, remarkably, that turning on such elastic interactions amongst tracers leads to very different dynamics: unlike the case of non-interacting tracers, an elastic chain preferentially samples vortical regions of the flow.

We perform a systematic study of this phenomenon and quantify, via the Okubo-Weiss parameter, the level of preferential sampling and its dependence on the elasticity and deformability of the chain.

Harmonic chains have been at the heart of several important problems in the areas of equilibrium and non-equilibrium statistical physics. These have ranged from crystalline to amorphous transitions [19], electrical and thermal transport both in and out-of-equilibrium [20], as well as understanding structural properties of disordered and random systems [21]. Given the ubiquity and usefulness of the elastic chain, it is surprising that the effect of a turbulent medium on long chains has not been studied as extensively as in other areas of non-equilibrium statistical physics.

There is another reason why this study is important. The last decade or more has seen tremendous advances in our understanding of heavy inertial particles and their dynamics. These were helped primarily by the pioneering results on the issue of preferential concentration, which plays a dominant role in every aspect of turbulent transport. In contrast, similar studies of extended objects such as fibers are recent [22–25], even though they are just as important and common place in nature and industry. However, the effect of elasticity, which is intrinsic to extensible objects (just as inertia is to finite-sized particles), in determining their dynamics in a turbulent flow is an open question. In this paper, we settle this question through a model which is amenable to detailed numerical simulations.

We consider a chain of $N_b$ identical beads, with negligible inertia, connected through (phantom) elastic links with its nearest left and right neighbours; the two end beads are free. If $x_1, \ldots, x_{N_b}$ denote the positions of the beads, the position of the center of mass of the chain is $X_c = (x_1 + \cdots + x_{N_b})/N_b$, and $r_i = x_{i+1} - x_i$ ($i = 1, \ldots, N_b - 1$) are the vector displacements between the $i$-th and $(i+1)$-th bead. Then the equations of motion for the chain in a velocity field $u(x, t)$ are:

\begin{equation}
\dot{X}_c = \frac{1}{N_b} \sum_{i=1}^{N_b} u(x_i, t) + \frac{\sqrt{\tau_0}}{2\tau} \sum_{i=1}^{N_b} \xi_i(t) \tag{1a}
\end{equation}

\begin{equation}
\ddot{r}_j = u(x_{j+1}, t) - u(x_j, t) + \frac{\sqrt{\tau_0}}{2\tau} [\xi_{j+1}(t) - \xi_j(t)] - \frac{1}{4\tau} (2f_jr_j - f_{j+1}r_{j+1} - f_{j-1}r_{j-1}) \tag{1b}
\end{equation}

with $f_j = (1 - |r_j|^2/r_m^2)^{-1}$ and $j = 1, \ldots, N_b - 1$. The nonlinear elastic links are characterised by their relaxation time $\tau$ and maximum length $r_m$, which, in turn, determines the maximum or contour chain length $L_m = N_tr_m$ ($N_t = N_b - 1$ is the number of links). Thus, at any given instant in time, the length of the...
chain \( R = \sum_{j}^{N_b} r_j < L_m \). The thermal fluctuations on each bead are modelled by independent white noises \( \xi_i(t) \) \( (i = 1, \ldots, N_b) \), whose amplitude \( r_0 \) sets the equilibrium length of the chain in the absence of flow. Although the effect of thermal fluctuations on the motion of the center of mass is negligible in a turbulent flow, their effect on the separation vectors is essential: thermal fluctuations prevent the chain from collapsing into a point-like particle and hence a tracer. Finally, inter-bead hydrodynamic interactions are ignored.

When the separations between the beads are small enough for the velocity differences to be approximated as \( u(x_{i+1}, t) - u(x_j, t) \approx \nabla u(t) \cdot r_j \), Eqs. (1) reduce to one of the most common bead-spring models in polymer physics, namely the Rouse model with FENE (finitely extensible nonlinear elastic) springs \([26, 27]\). Such a model is thus appropriate when the carrier flow is linear and in space; in a turbulent flow this requires the size of the links to be smaller than the viscous scale at all times \([28–31]\). By considering the full velocity difference between adjacent beads, Eqs. (1) generalize the usual bead-spring models and describe an elastic chain that may extend into the inertial range of turbulence or even beyond the integral scale (see Refs. \([32–35]\) for an analogous generalization of the dumbbell \( (N_b = 2) \) model).

What is the effect of a turbulent velocity field \( u \) on the motion of such chains? To answer this, we solve, by using a pseudo-spectral method with a \( 2/3 \) de-aliasing rule, the two-dimensional Navier-Stokes equation on a square grid with \( 1024^2 \) collocation points and \( 2\pi \) periodic boundary conditions. We drive the system to a homogeneous and isotropic, turbulent, statistically steady state through an external, deterministic force \( f = -F_0 k_f \cos(k_f x) \) \( (F_0 \) is the amplitude and \( k_f \) the energy-injection scale in Fourier space, which sets the typical size of the vortices \( \ell_f = 2\pi k_f^{-1} \)). Forcing at small wavenumbers ensures that the vortices are fairly large: this allows us to clearly illustrate the issues of preferential sampling which are central to this work. We use a small Ekman-friction coefficient \( \mu \) (in addition to a coefficient of kinematic viscosity \( \nu \)) to prevent pile-up of energy at the large scales due to inverse cascade. Consequently the turbulent flow is in the direct-cascade regime. The definition of \( \ell_f \) also allows us to characterise the stretching ability of the flow in terms of the dimension-less Weissenberg number \( Wi = \tau / \ell_f \), where \( \ell_f = \ell_f / \sqrt{2E} \) is the turnover time scale of the large vortices (\( E \) is the mean kinetic energy of the flow).

The temporal evolution of the chain (Eqs. (1)) is done by a second-order Runge-Kutta scheme, augmented by a rejection algorithm \([27]\) to avoid numerical instabilities due to the divergence of the nonlinear force for \( |r_j| \) approaching \( r_m \). A bilinear scheme is used to interpolate, from the Eulerian grid, the fluid velocity at the typically off-grid positions of the beads \([36, 37]\). In order to observe the regime of preferential sampling, we choose parameters for the chain which ensure that its equilibrium length in a quiescent flow is similar to the enstrophy dissipation scale, while \( \ell_f < L_m < 2\pi \).

This model of an elastic chain in a turbulent flow is the ideal setting, theoretically and numerically, to investigate the natural interplay between the relative importance of Lagrangian (uniform) mixing and the elasticity of the links. It is this competing effect that leads to a surprising preferential sampling of the flow by the chain, hitherto not observed.

To illustrate this phenomenon, we begin by randomly seeding \( 5 \times 10^4 \) chains into the flow and study their evolution in time for different \( Wi \). (We evolve a large number of chains simultaneously for the purpose of visualizing their sampling behaviour and for obtaining good statistics of the chain dynamics; we do not describe the collective motion of an ensemble of chains, which would interact with each other hydrodynamically or by direct
FIG. 2. Lagrangian pdfs of (a) the Okubo-Weiss parameter $\Lambda$ and (b) the scaled lengths of the chains $R/\ell_f$ for different values of $Wi$. Parameter values: $\ell_f = 1.25, t_f = 1.35, L_m = 3.75, N_L = 9, \nu = 10^{-6}, \mu = 10^{-2}$, and $F_0 = 0.2$.

contact.) In Fig. 1 we show the center-of-mass positions at an instant of time overlaid on the vorticity field of the turbulent flow for $Wi = 0.04$ and $Wi = 0.9$. It is immediately apparent that for the case of small elasticity the chains behave like tracers and distribute evenly (Fig. 1(a)). However, for larger $Wi$ there is a preferential sampling of the vortical regions (Fig. 1(b)).

Figure 1(c) demonstrates the coupling between the translational and the extensional dynamics of the chain by showing a snapshot in which the entire chains, and not just the centers of mass, are overlaid on the vorticity field. This figure emphasizes the strong correlation between the positions of elongated chains with regions of low vorticity, where the straining flow stretches out the chains. In contrast, the chains that encounter vortices tend to curl up and contract to a much smaller size. These strikingly different phenomena are best seen in a video of the time evolution of the chains [38]. All of this suggests the following picture: a stretched chain is more likely to leave straining zones and coil up in vortical regions.

The above observations can be quantified via a Lagrangian approach by measuring the statistics of the extension $R$ and the Okubo-Weiss parameter $\Lambda$ along the trajectories of the centers of mass of the chains. We recall that $\Lambda = (\omega^2 - \sigma^2)/4\langle \omega^2 \rangle$, where $\omega$ is the vorticity and $\sigma$ is the strain rate, is the discriminant of the characteristic equation for $\nabla u$ and is here rescaled with the mean enstrophy. The sign of $\Lambda$ uniquely determines the local flow geometry: For positive $\Lambda$, the flow is vortical; for negative $\Lambda$ it is extensional [36, 39]. Values of $\Lambda$ near zero correspond to either a weak amplitude of $\nabla u$ or to a shearing flow, which has comparable amounts of vorticity and straining.

In Fig. 2 we show the Lagrangian probability distribution function (pdf) of (a) $\Lambda$ and (b) $R$ for different values of $Wi$. The $\Lambda$ distribution for tracers ($Wi = 0$) is also shown for comparison (its positive skewness is a consequence of the strongest velocity gradients occurring in intense vortical zones [40, 42]). We find strong quantitative evidence that increasing elasticity leads to a chain preferentially sampling vortical regions of the flow (Fig. 2(a)). This is accompanied by an increase in the probability of highly stretched configurations (Fig. 2(b)).

The key to understanding the phenomenon of preferential sampling lies in the correlation between the translational and the extensional dynamics of a chain. This is quantified through the joint pdf $P(R, \Lambda)$, which shows that when its center of mass is in vortical regions, a chain is in a contracted state (Fig. 3). The velocity terms in Eq. (1a) can therefore be Taylor-expanded about $X_c(t)$, and Eq. (1a) reduces to the equation of motion of a tracer. Thence, the center of mass follows the flow and remains trapped in the vortex. Contrastingly, away from vortical
regions, i.e., in straining or shearing regions, an extensible chain is highly stretched (Fig. 3). As time proceeds, a large-$Wi$ chain stretches to lengths so long that eventually it is unable to follow the rapidly evolving straining zones. On departing from these zones, such a chain is likely to encounter a vortex and begin to coil up (seen clearly in the video [25]). The links of the chain that enter the vortex shrink and follow the rotational flow, eventually leading to the entrainment of the entire chain within the vortex. A stiff chain (small-$Wi$), which remains short in straining zones, samples the negative values of $\Lambda$ more, leading to annular contours (Fig. 3 inset).

The stretching out of a chain in straining zones may thus be seen as a precursor to its entrainment inside vortices. This explains why strong preferential sampling of vortices occurs only when $Wi$ is so large that there is a significant probability for chains to be stretched beyond $\ell_f$ (see Fig. 2 for $Wi = 0.49, 1.22$). On the other hand, if the maximum length $L_m < \ell_f$, then one would expect this mechanism to fail and the chain to uniformly sample the flow for all $Wi$. We have confirmed this hypothesis in our simulations but do not show the results for brevity.

The results, so far, suggest a complete picture for the dynamics of an elastic chain in a turbulent flow: A chain with a sufficient degree of elasticity—defined as the ratio of elastic and fluid time scales—preferentially samples the flow. But is this effect truly independent of the characteristic fluid length scale $\ell_n$?

For large values of $Wi$, as we have seen, the typical inter-bead separation approaches $L_m/N_b$. For the results reported so far, $N_b$ was such that $L_m/N_b < \ell_f$. As $N_b$ decreases, however, we will eventually obtain characteristic inter-bead separations of the order of $L_m/N_b > \ell_f$. In this setting, typically, no two neighboring beads will be able to reside in a vortex simultaneously. Hence the mechanism for preferential sampling will fail, and the chain will start sampling the flow uniformly once more. This suggests that, apart from the role of elasticity, the dynamics of a chain for large values of $Wi$ ought to depend on a second dimensionless number $\Phi \equiv L_m/(N_b \ell_f)$, such that for $\Phi > 1$ there should be uniform sampling, while for $\Phi < 1$ preferential sampling.

Direct evidence for this is presented in Fig. 4 which shows the mean value of the Okubo-Weiss parameter, $\langle \Lambda \rangle$, as a function of $Wi$, for different values of $\Phi$. For smaller $\Phi$, there is an increase in $\langle \Lambda \rangle$ that eventually saturates for $Wi \gtrsim 5$. However, for larger values of $\Phi$, $\langle \Lambda \rangle$ increases initially $[-1]$—indicating preferential sampling of the vortical regions of the flow—before decreasing again to reflect uniform sampling (see video [44]). The chain, however, continues to stretch as the elasticity increases for all values of $\Phi$, and its mean square extension does not show any non-monotonic behavior (inset of Fig. 4).

At large $Wi$ a chain is indeed typically longer for larger values of $\Phi$ owing to the reduced level of preferential sampling of vortices and correspondingly lower probability of being in a contracted state.

Figure 4 lends itself to an intuitively appealing picture of the motion of a chain. For a given turbulent flow (characterised by $t_f$ and $\ell_f$), whether or not a chain of a given elasticity and maximum length $L_m$ may coil—and hence preferentially sample—depends on the number of links which form the chain. In particular, for a highly extended chain (large $Wi$), decreasing the number of links limits the ability of the chain to coil up into vortices. This result highlights the importance of deformability of extensible chains. In our study, we have considered a freely-jointed chain. However, the bending stiffness of the chain may be modeled by introducing a potential force that is a function of the internal angle between neighboring links and restores them to an anti-parallel configuration $[26]$. Such stiffness would prevent the chain from coiling up and, therefore, would reduce preferential sampling in a manner analogous to that of increasing $\Phi$ in our freely-jointed model.

The elastic chain is a simplified model for various physical systems, which include, inter alia, fibers, microtubules, and algae in marine environments. Such systems of course present additional properties that were not taken into account here, such as the inertia and the stiffness of the system, hydrodynamic and excluded-volume interactions between different portions of it, and the modification of the flow generated by the motion of the system. These effects will certainly change quantita-
tive details of the dynamics, but the mechanism at the origin of preferential sampling identified here is of general validity. It indeed relies on a few basic ingredients: the system must be extensible, its equilibrium size should be smaller than $\ell_f$ and its contour length greater than $\ell_f$.

Before we conclude, it is also important to stress that we chose two-dimensional turbulent flows to take advantage of their long-lived vortical structures, which help to convincingly illustrate these new phenomena of preferential sampling; needless to say the mechanism itself is independent of whether the flow is two- or three-dimensional. Finally, we cannot avoid mentioning that the preferential concentration of inertial particles through dissipative dynamics is completely different from the mechanism that we report here. Hence it is tempting to investigate the interplay between the competing effects of inertia and elasticity in future studies of inertial extensible objects in turbulent flows.

We thank Abhishek Dhar, Anupam Kundu, and Rahul Pandit for useful suggestions and discussions. We acknowledge the support of the Indo-French Centre for Applied Mathematics (IFCAM). SSR acknowledges DST (India) project ECR/2015/000361 for financial support. JRP acknowledges travel support from the ICTS Infosys Collaboration grant. The simulations were performed on the ICTS clusters Mougli and Mario, as well as the work stations from the project ECR/2015/000361: Goopy and Bagha.
[42] D. Mitra and P. Perlekar, Phys. Rev. Fluids 3, 044303 (2018)
[43] See also Refs. 32, 33 for dumbbells in cellular flows.

[44] Online movie showing uniform sampling of highly stretched dumbbells: https://youtu.be/YdFXMFFU1qU