Clustering by Mixing Flows

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We calculate the Lyapunov exponents for particles suspended in a random three-dimensional flow, concentrating on the limit where the viscous damping rate is small compared to the inverse correlation time. In this limit Lyapunov exponents are obtained as a power series in \(\epsilon\), a dimensionless measure of the particle inertia. Although the perturbation generates an asymptotic series, we obtain accurate results from a Padé-Borel summation. Our results prove that particles suspended in an incompressible random mixing flow can show pronounced clustering when the Stokes number is large and we characterize two distinct clustering effects which occur in that limit.

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This Letter describes the dynamics of particles suspended in a randomly moving incompressible fluid that we assume to be mixing: any given particle uniformly samples configuration space. At first sight, it seems as if the particles suspended in an incompressible mixing flow should become evenly distributed. This, indeed, happens if the particles are simply advected by the fluid. However, it has been noted [1] that when the finite inertia of the suspended particles is significant, the particles can show a tendency to cluster.

The current understanding of this remarkable phenomenon refers to a dimensionless parameter termed the Stokes number, \(St = 1/(\gamma \tau)\), where \(\gamma\) is the rate at which the particle velocity is damped relative to that of the fluid due to viscous drag, and \(\tau\) is the correlation time of the velocity of the fluid. There is a consensus [2–6] that clustering is most pronounced when \(St\) is of order unity.

In this Letter we argue that strong clustering can occur when \(St\) is large. We show that different clustering mechanisms compete at large values of \(St\) and quantify under which circumstances clustering occurs. Before describing our results and outlining how they are derived, we briefly summarize previous theoretical work on the clustering of inertial particles in turbulent flows.

This effect was first discussed by Maxey [1]: he approximated the inertial particle dynamics by advection in a “synthetic” velocity field that was obtained as a perturbation of the velocity field of the fluid, \(\mathbf{u}(\mathbf{r}, t)\). Maxey showed that this synthetic velocity field has positive divergence when the vorticity of \(\mathbf{u}(\mathbf{r}, t)\) is high or its strain rate low, and predicted that particles would have low concentrations in regions of high vorticity due to this “centrifuge effect.” This effect has been demonstrated in direct numerical simulation of particles suspended in a fully developed turbulent flow [3,7]. Experimental work [2] has also emphasized instantaneous correlations between vortices and particle-density fluctuations.

Later work has adapted results on the density statistics and Lyapunov exponents of purely advective flows obtained in [8,9]: Elperin [10] suggested combining these results with Maxey’s synthetic velocity field to obtain results for inertial particles; a similar approach was used in [11–13]. These results are not applicable at large \(St\), because the perturbation of the velocity field need not be small when inertial effects are important.

An alternative viewpoint arises from the work of Sommerer and Ott [14], who describe patterns formed by particles floating on a randomly moving fluid. They characterize the patterns in terms of their fractal dimension and suggest that the fractal dimension can be obtained from ratios of Lyapunov exponents of the particle trajectories using a formula proposed by Kaplan and Yorke [15].

The argument in [14] extends to particles suspended in turbulent three-dimensional incompressible flows (we consider this case, rather than floating particles). Consider the Lyapunov exponents \(\lambda_1 > \lambda_2 > \lambda_3\), They are rate constants defined in terms of the time dependence of, respectively, the length \(\delta r\) of a small separation between two trajectories, the area \(\delta A\) of a parallelogram spanned by two separation vectors and the volume \(\delta V\) of a parallelepiped spanned by a triad of separations:

\[
\begin{align*}
\lambda_1 &= \lim_{t \to \infty} r^{-1} \log_e(\delta r), & \lambda_1 + \lambda_2 &= \lim_{t \to \infty} r^{-1} \log_e(\delta A), \\
\lambda_1 + \lambda_2 + \lambda_3 &= \lim_{t \to \infty} r^{-1} \log_e(\delta V).
\end{align*}
\]

(1)

The Kaplan-Yorke estimate for the fractal dimension in a three-dimensional incompressible flow is determined by the dimensionless quantity (“dimension deficit”)

\[
\Delta = -(\lambda_1 + \lambda_2 + \lambda_3)/|\lambda_3|.
\]

(2)

When \(\Delta > 0\), the Kaplan-Yorke estimate of the dimension is \(d_H = 3 - \Delta\), and \(d_H = 3\) if \(\Delta \leq 0\). Clustering effects are significant if the fractal dimension is significantly lower than the dimension of space. This provides a strong motivation to study the Lyapunov exponents.

A third mechanism for clustering is the following: nothing prevents the infinitesimal volume element \(\delta V\) from collapsing to zero for an instant of time. These events correspond to “caustics,” where faster moving particles

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overtake slower ones. Caustics are associated with the density of particles on a surface becoming very high, facilitating the aggregation of suspended particles. This mechanism was recently proposed as a cause of clustering of inertial particles [16], and is also mentioned briefly in [13]. The significance of this effect is determined by the rate $J$ at which the infinitesimal volume element goes through zero for a given triplet of nearby trajectories.

Which of these three mechanisms is most important? Maxey’s centrifuge effect is weak at small $St$, where the particles are simply advected. There is a consensus that the Maxey’s centrifuge effect is weak at small $St$, where the particles may be neglected.

Two distinct mechanisms compete (clustering onto fractal sets versus clustering onto caustics in an otherwise homogeneous background) and dominate in different regions of the parameter space.

We model the particles suspended in the fluid flow by the equation of motion

$$\dot{r} = \gamma (u(r, t) - r),$$

where $r = (r_1, r_2, r_3)$ denotes the position of a particle. Equation (3) is appropriate for noninteracting spherical particles when the Reynolds number of the flow referred to the particle diameter is small and where the particle diameter is much smaller than the correlation length of the velocity field. Stokes’s formula gives the damping rate $\gamma = 6\pi \alpha \rho \omega / r$ where $\omega$ and $\alpha \rho$ are, respectively, the kinematic viscosity and density of the fluid, and $a$ and $m$ are the radius and mass of the particle. Effects due to the inertia of the displaced fluid are neglected. This is justified when the density of the suspended particles is large compared to that of the fluid. We assume that Brownian diffusion of the particles may be neglected.

We now discuss the dimensionless parameters of the problem: the velocity field is assumed to be characterized by its typical velocity $u = \sqrt{\alpha \rho}$, by a correlation length $\xi$, and by a correlation time $\tau$. In addition, the interaction of the fluid with the particles is determined by the damping rate $\gamma$. From these four quantities we can form two independent dimensionless groups: a dimensionless velocity, $\kappa = u \tau / \xi$, and the dimensionless damping $\nu = \gamma \tau$ (so that $St = \omega^{-1}$). The parameter $\kappa$ has been termed “Kubo number” [17]. It has not been considered before in this context. We argue that it cannot be large if $u(r, t)$ is to be a satisfactory model for a solution of the Navier-Stokes equations: $\tau \leq \xi / u$ since disturbances in the fluid velocity field $u(r, t)$ are transported by $u(r, t)$ itself.

In the case of fully developed turbulence the velocity field exhibits a power-law energy spectrum, with upper and lower cutoffs [18]. This raises the question of which length scale is associated with $\xi$. Below we show that when $St \gg 1$ the spectrum of the velocity field determines the Lyapunov exponents through one number, $D_1$, obtained from the correlation function of the strain rate [Eq. (11)]. There is no consensus in the literature as to how to evaluate (11). However, the magnitude of the strain rate is determined by the small-length cutoff (Kolmogorov length [18]). We therefore associate $\xi$ with the Kolmogorov length. We note that $\kappa \sim 1$ for fully developed turbulence. In other situations $\kappa$ can be small.

We now turn to a summary of our results and outline how they were derived (details will be published elsewhere). Linearizing the equations of motion (3) gives

$$\delta \dot{p} = -\gamma \delta p + F(t) \delta r, \quad \delta \dot{r} = \delta p / m,$$

where $p = m \dot{r}$ is the particle momentum and $F(t)$ is matrix of force gradients:

$$F_{\mu \nu}(t) = y m \frac{\partial H_{\mu \nu}}{\partial r_{\nu}} (r(t), t).$$
We take three trajectories displaced relative to a reference trajectory by small increments \((\delta r_{\mu}, \delta p_{\mu})\), with \(\mu = 1, 2, 3\). We introduce a triplet of orthogonal unit vectors \(\mathbf{n}_\mu(t)\) such that \(\mathbf{n}_\mu(t)\) is oriented along \(\delta r_{\mu}(t)\), and \(\mathbf{n}_\mu(t)\) lies in the plane spanned by \((\delta r_{\mu}(t), \delta r_{\mu}(t))\) [and \(\mathbf{n}_\mu(t)\) is continuous in \(t\)]. We write \(\mathbf{n}_\mu(t) = \mathbf{O}(t)\mathbf{n}_\mu(0)\) and \(\delta p_{\mu}(t) = \mathbf{R}(t)\delta r_{\mu}(t)\) where \(\mathbf{O}\) is an orthogonal and \(\mathbf{R}\) a general \(3 \times 3\) matrix. We define the elements of \(\mathbf{F}\) and \(\mathbf{R}\) transformed to the moving basis

\[
\begin{align*}
F'_{\mu\nu}(t) &= \mathbf{n}_{\mu}(t) \cdot \mathbf{F} \mathbf{n}_{\nu}(t), \\
R'_{\mu\nu}(t) &= \mathbf{n}_{\mu}(t) \cdot \mathbf{R} \mathbf{n}_{\nu}(t),
\end{align*}
\]

and find the following equation of motion for \(\mathbf{R}'\):

\[
\mathbf{R}' = -\gamma \mathbf{R}' - \mathbf{R}^{2}/m + \left[\mathbf{R}', \mathbf{O}^{+} \mathbf{O}\right] + \mathbf{F}'.
\]

(7)

The elements of \(\mathbf{O}^{+} \mathbf{O}\) are given by

\[
\mathbf{O}^{+} \mathbf{O} = \frac{1}{m} \begin{pmatrix}
0 & -R'_{21} & -R'_{31} \\
R'_{21} & 0 & -R'_{32} \\
R'_{31} & R'_{32} & 0
\end{pmatrix}.
\]

(8)

After a lengthy calculation we find that the Lyapunov exponents are obtained from averages of the diagonal elements of \(\mathbf{R}'\)

\[
\lambda_1 = \langle R'_{11} \rangle /m, \quad \lambda_2 = \langle R'_{22} \rangle /m, \quad \lambda_3 = \langle R'_{33} \rangle /m
\]

(9)

(analogous expressions are derived in [16,19]). Equations (7) and (8) for \(\mathbf{R}'\) can be simplified when the correlation time of the velocity field is sufficiently short, \(\omega \ll 1\), assuming that the amplitude of the random force is sufficiently small, \(\kappa \ll 1\). In this limit \(\mathbf{F}'\) behaves as a white-noise signal, and (7) reduces to a system of Langevin equations. We label the dynamical variables by a single index \(i = 3(\mu - 1) + \nu\) and scale the Langevin equations for \(R'_{i}\) to dimensionless form

\[
dx_i = \left(-x_i + \epsilon \sum_{j,k=1}^{9} \sum_{l=1}^{9} V_{j,k}^{l} x_j x_k \right) dt' + dw_i.
\]

(10)

Here \(t' = \gamma t\), \(x_i = \sqrt{\gamma/D_j} R'_{i}\), and \(\langle dw_idw_j \rangle = 2D_{ij} dt'\). The elements \(D_{ij}\) of the diffusion matrix \(\mathbf{D}\) are given by

\[
D_{ij} = \frac{1}{2} \int_{-\infty}^{\infty} dt \langle F'_{i}(t) F'_{j}(0) \rangle.
\]

(11)

The coefficients \(V_{j,k}^{l}\) are determined by the 2nd and 3rd terms on the right-hand side of (7). The dimensionless parameter

\[
\epsilon = D_{11}^{1/2}/(m \gamma^{3/2}) \sim \kappa \omega^{-1/2}
\]

(12)

is a measure of the inertia of the particles: it is proportional to \(a\) and therefore to \(m^{1/3}\). Thus we obtain all three Lyapunov exponents from the expectation values of variables in a system of Langevin equations. Earlier work has obtained the largest Lyapunov exponents for various problems using Langevin equations [19–21].

The elements of \(\mathbf{D}\) are determined by the fluctuations of the velocity field. We assume that the latter is incompressible, but for reasons explained below we add a small compressible component: \(u = \nabla \times A + \nabla \delta A_0\). The fields \(A_\mu(r, t), \mu = 1, 2, 3\) are taken to be Gaussian random functions, homogeneous in space and time, and isotropic in space. Their correlation functions are \(\langle A_\mu(r, t) A_\nu(r', t') \rangle = \delta_{\mu \nu} C(|r - r'|/\xi, |t - t'|/\tau)\). The field \(\delta A_0\) is statistically independent of \(A_\mu\) and has the same correlations, and in the end the limit \(\delta A_0 \rightarrow 0\) is taken.

The Langevin equations (10) are equivalent to a Fokker-Planck equation with stationary solution \(P(x)\). In the limit of \(\epsilon \rightarrow 0\) the latter is Gaussian

\[
P_0(x) \propto \exp(-\frac{1}{2} x \cdot \mathbf{D}^{-1} x) \equiv \exp[-\Phi_0(x)].
\]

(13)

This suggests transforming the Fokker-Planck operator so that its \(\epsilon = 0\) limit is a harmonic oscillator. Introducing \(Q(x) = \exp(\Phi_0(x)/2) P(x)\), the steady-state Fokker-Planck equation can be written as \((\hat{H}_0 + \epsilon \hat{H}_1) |Q\rangle = 0\), where we have represented the function \(Q(x)\) by a "ket vector" \(|Q\rangle\). The operator \(\hat{H}_0\) is the Hamiltonian for nine uncoupled harmonic oscillators

\[
\hat{H}_0 = \sum_{i=1}^{9} \hat{a}_i^+ \hat{a}_i,
\]

(14)

where \(\hat{a}_i^+\) and \(\hat{a}_i\) are, respectively, the creation and annihilation operators for the degree of freedom labeled by \(i\) (satisfying \([\hat{a}_i, \hat{a}_j^+] = \delta_{ij}\). The non-Hermitian perturbation \(\hat{H}_1\) can be expressed in terms of the eigenvalues \(\omega_i\) of \(\mathbf{D}\) and the elements \(J_{ij}\) of an orthogonal matrix \(\mathbf{J}\) satisfying \(\mathbf{D} = \mathbf{J} \omega \mathbf{J}^{-1}\), with \(\omega = \text{diag}(\omega_i)\):

\[
\hat{H}_1 = \sum_{i,j,k} H_{ij}^{(1)} \hat{a}_i^+ \hat{a}_j \hat{a}_k^+ + \hat{a}_j^+ \hat{a}_k
\]

(15)

\[
H_{ij}^{(1)} = \int \omega_j \omega_k / \omega \sum_{lmn} V_{ij} \omega_j \omega_k \omega_n J_{i lm} J_{j mn} J_{k mn}.
\]

Regularity is needed since one eigenvalue vanishes in the limit of \(\delta A_0 \rightarrow 0\). We determine \(|Q\rangle\) by perturbation theory in \(\epsilon\). Given \(|Q\rangle\), the Lyapunov exponents are obtained as \(\lambda_1 = \gamma \epsilon (x_1), \lambda_2 = \gamma \epsilon (x_3), \lambda_3 = \gamma \epsilon (x_9)\), and

\[
\langle x_i \rangle = \langle \Phi_0 | Q \rangle \sum_{ij} J_{ij} \omega_i \langle \Phi_0 | \hat{a}_j + \hat{a}_j^+ | Q \rangle.
\]

(16)

where \(\langle \Phi_0 | \rangle\) denotes the null eigenvector of \(\hat{H}_0\). From (16) we obtain series expansions in the form

\[
\lambda_1 / \gamma = 3 \epsilon^2 - 29 \epsilon^4 + 564 \epsilon^6 - 14 977 \epsilon^8 + 488 784 \epsilon^{10} - 18 670 570 \epsilon^{12} + \ldots,
\]

\[
\lambda_2 / \gamma = 8 \epsilon^4 - 459 / 2 \epsilon^6 + 14 281 / 2 \epsilon^8 - 757 273 \epsilon^{10} + 361 653 709 / 36 \epsilon^{12} + \ldots,
\]

\[
\lambda_3 / \gamma = -3 \epsilon^2 - 9 \epsilon^4 - 789 / 2 \epsilon^6 - 5787 / 2 \epsilon^8 - 895 169 / 3 \epsilon^{10} - 101 637 719 / 36 \epsilon^{12} + \ldots.
\]
Note that only even powers of $\varepsilon$ contribute, and that all coefficients are rational numbers. Equation (17) is the main result of this Letter. The expansion is valid in the underdamped limit $\omega \ll 1$ when $\kappa \ll 1$.

The coefficients in (17) exhibit rapid growth typical of an asymptotic series. We have attempted to sum (17) using Borel summation, explained in [22], which improves convergence by dividing coefficients by a factorial

$$
\lambda_j/\gamma \sim \text{Re} \int_c dt e^{-t} \sum_{l=1}^{l_{\text{max}}} c^{(l)}_j (e^2 t)^l,
$$

where $c^{(l)}_j$ are the coefficients of (17) and $l_{\text{max}} = 7$ is the number of nonzero coefficients available for each $\lambda_j$. The sum in the integrand is approximated by Padé approximants [22] of order $n$, namely, $P_n$ or $P_n^{*}$ with $n \leq l_{\text{max}}/2$. The integration path in (18) is taken to be a ray in the upper right quadrant in the complex plane.

Results of Padé-Borel summations of the series for $\lambda_j$ are shown in Fig. 1(a) and converge to results of numerical simulations provided $\varepsilon$ is not too large. For $\lambda_i$ numerical evidence indicates the presence of additional nonanalytical contributions not captured by the Padé-Borel summation. The results of Fig. 1(a) allow us to determine the quantity $\Delta$ defined in Eq. (2). The result is shown in Fig. 1(b). We find that $\Delta$ is maximal for $\varepsilon = 0.21$ and positive (indicating clustering onto a fractal set) for $0 < \varepsilon < 0.33$. The red solid line in Fig. 1(d), $\varepsilon \sim \kappa \omega^{-1/2}$, always positive, but tends to zero for small $\varepsilon$ as $\Delta = 10\varepsilon^2 \sim \kappa^2/\omega$. In the limit of $\varepsilon \rightarrow 0$ the dynamics becomes advective (despite being underdamped): to lowest order in $\varepsilon$ our results coincide with those for purely advective flow [8].

We now turn to the rate $J$ of caustic formation. It is the rate at which $\delta V(t) = (\delta r_1(t) \wedge \delta r_2(t)) \cdot \delta r_3(t)$ goes through zero. Since $\delta p_3$ typically remain bounded, caustics correspond to instances where the elements of the third column of $\mathbf{R}'$ go to $-\infty$ and reappear at $\infty$. The rate for these events to occur is the rate of escape of the Langevin process (10) to infinity. It is expected [16] to have a nonanalytic dependence on $\varepsilon$, of the form $C \exp(-S/\varepsilon^2)$, as demonstrated in Fig. 1(c). In this panel, $J/\gamma$ is compared to $-(\lambda_1 + \lambda_2 + \lambda_j)/\gamma$. Caustics are very rare when $\varepsilon \ll 1$ but frequent when $\varepsilon$ is large, and they are the only clustering mechanism when $\varepsilon > 0.33$.

Finally, we comment on the relation between our results and earlier works (cited above), which suggest that clustering occurs only for $\omega = 1$ (with the value of $\kappa$ unspecified). It must be emphasized that the earlier quantitative theoretical results on clustering are confined to the overdamped limit $\omega \gg 1$, where inertial effects are small: for purely advective flow there is no clustering ($\Delta = 0$ and $J = 0$). Inertial effects were incorporated by Elperin and others [10–12], using Maxey’s perturbative correction to the velocity. Their results are valid only for the limit $\omega \gg 1$, and are distinct from our series expansions (17): this is most easily seen by calculating corrections to $\Delta$ in this overdamped limit. We find that $\Delta \sim \kappa^2/\omega^2$, implying that clustering effects are small in this regime. In the underdamped regime, by contrast, we obtained $\Delta \sim \kappa^2/\omega$ which can be of order unity.

Our results are summarized schematically in Fig. 1(d). First, at small $\kappa$, strong clustering occurs in the region indicated, above the line $\varepsilon \sim \kappa \omega^{-1/2} = 0.33$. Second, since the dimension deficit $\Delta$ is positive in this regime, the reasoning of Sommerer and Ott [14] indicates that the particles cluster on a fractal. Third, as $\varepsilon \rightarrow 0$ the dynamics becomes advective. In this limit the dimension deficit $\Delta$ and the rate of caustic formation $J$ vanish: particles advected in an incompressible flow remain uniformly distributed. Fourth, when $\varepsilon > 0.33$ we find that the dimension deficit $\Delta$ is negative, implying that the particles do not lie on a fractal. They are, however, not homogeneously distributed: in this regime particles cluster because they are brought into close contact by caustics.

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