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 Pade-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 characterise 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 which 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 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 field. There is a consensus 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 summarise previous theoretical work on the clustering of inertial particles in turbulent flows.

This effect was first discussed by Maxey: he approximated the inertial particle dynamics by advection in a ‘synthetic’ velocity field which was obtained as a perturbation of the velocity field of the fluid, $u(r,t)$. Maxey showed that this synthetic velocity field has negative divergence when the vorticity of $u(r,t)$ 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. The theoretical work of Maxey and experimental work on turbulent flows has emphasised 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: Elperin suggested combining these results with Maxey’s synthetic velocity field to obtain results for inertial particles; a similar approach was used in. 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 work of Sommerer and Ott, who describe patterns formed by particles floating on a randomly moving fluid. They characterise 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.

The argument in extends to particles suspended in turbulent three-dimensional incompressible flows. 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 parallelepiped spanned by two separation vectors and the volume $\delta V$ of a parallelepiped spanned by a triad of separations:

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

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

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

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 proposition provides a strong motivation to study the Lyapunov exponents of the problem.
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 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 $\text{St}$, where the vortices do not persist for a sufficiently long time to be effective, implying that significant clustering is only observed when $\text{St} \sim 1$. However, there is at present no understanding of what happens at large values of $\text{St}$. In the following we describe quantitative results for the Lyapunov exponents $\lambda_j$, for the dimension deficit $\Delta$ and for the rate of caustic formation $J$; these are summarised in Fig. 1 a - c.

Our results show that in order to understand the clustering effect it is necessary to consider not only the Stokes number, but an additional dimensionless parameter, $\kappa$, defined below. We infer that strong clustering can occur at large Stokes numbers. 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

$$\ddot{r} = \gamma (u(r, t) - \dot{r})$$  \hspace{1cm} (3)$$

where $r = (r_1, r_2, r_3)$ denotes the position of a particle. Eq. 3 is appropriate for non-interacting spherical particles when the Reynolds number of the flow referred to the particle diameter is small. It is assumed that the radius of the particle and the molecular mean free path of the fluid are sufficiently small. Stokes’s formula gives the damping rate $\gamma = 6 \pi \rho a u / m$ where $\rho$, $p_1$ are respectively the kinematic viscosity and density of the fluid, and $a$, $m$ 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 also assume that Brownian diffusion of the particles is negligible.

We now discuss the dimensionless parameters of the problem: the velocity field is assumed to be characterised by its typical velocity $u = \sqrt{\langle u^2 \rangle}$, by a correlation length $\xi$ and 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 $\omega = \gamma \tau$ (so that $\text{St} = \omega^{-1}$). 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.

Consider now the particular case of fully-developed turbulence. In this case, the velocity field exhibits a power-law energy spectrum, with upper and lower cut-offs [18]. The smaller length scale is the Kolmogorov length, which is the size of the smallest vortices generated by the turbulence. It is given by $(\nu^3 / \varepsilon)^{1/4}$, where $\varepsilon$ is the rate of dissipation per unit mass of fluid. The Kolmogorov length corresponds to the correlation length $\xi$ in our theory. The corresponding typical velocity $u$ and correlation time $\tau$ are also determined solely by the same two parameters, $\varepsilon$ and $\nu$, implying 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). Linearising the equations of motion 3 gives

$$\delta \dot{p} = -\gamma \delta p + F(t) \delta r ; \quad \delta \dot{r} = \delta p / m$$  \hspace{1cm} (4)$$

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

\[ F_{\mu \nu}(t) = \gamma m \frac{\partial u_{\mu}}{\partial r_{\nu}}(r(t), t) \, . \]  

(5)

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 triplod of orthogonal unit vectors \(n_\nu(t)\) such that \(n_1(t)\) is oriented along \(\delta r_1(t)\), and \(n_2(t)\) lies in the plane spanned by \((\delta r_1(t), \delta r_2(t))\). This determines \(n_3(t)\) up to a sign which is fixed by requiring continuity. We write \(n_\nu(t) = O(t)n_\nu(0)\) and \(\delta p_\mu(t) = R(t) \delta r_\mu(t)\) where \(O\) is an orthogonal and \(R\) a general \(3 \times 3\) matrix. We define the elements of \(F\) and \(R\) transformed to the moving basis:

\[ F'_{\mu \nu}(t) = n_\mu(t) \cdot F(t) n_\nu(t), \quad R'_{\mu \nu}(t) = n_\mu(t) \cdot R(t) n_\nu(t) \]  

(6)

and find the following equation of motion for \(R'\)

\[ \dot{R}' = -\gamma R' - \frac{1}{m} R'^2 + [R', O^+ \dot{O}] + F'. \]  

(7)

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

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

(8)

We find that the Lyapunov exponents are equal to the long-time average of the diagonal elements of \(R'\)

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

(9)

Eqs. (4) and (5) for \(R'\) 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 \(F'\) behaves as a white-noise signal, and (5) 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 \(R'\) to dimensionless form

\[ dx_i = -(x_i + \epsilon \sum_{j=1}^9 \sum_{k=1}^9 V_{jk}^{(i)} x_j x_k) dt' + dw_i \]  

(10)

Here \(t' = \gamma t\), \(x_i = \sqrt{\gamma / D_i} R_{ii}'\), and \langle \text{dw}_i \text{dw}_j \rangle = 2 D_{ij} dt'. The elements \(D_{ij}\) of the diffusion matrix \(D\) are given by

\[ D_{ij} = \frac{1}{2} \int_{-\infty}^{\infty} dt \langle F_{\mu}^i(t) F_{\nu}^j(0) \rangle . \]  

(11)

The coefficients \(V_{jk}^{(i)}\) are determined by the 2nd and 3rd terms on the rhs of (4). The dimensionless parameter

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

(12)

is a measure of the inertia of the particles: it is proportional to \(a\) and therefore to \(m^{1/2}\). 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 [14,20,21].

The elements of \(D\) 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: \(u = \nabla \cdot A + \nabla \delta A_0\). The fields \(A_\mu(r, t), \mu = 1, 2, 3\) are taken to be homogeneous in space and time, and isotropic in space. Their correlations are determined by \((A_\mu(r + R, t + t) A_\nu(r_0, t_0) = \delta_{\mu \nu} C(|r - r'|/\xi, |t - t'|/\tau)\). The field \(\delta A_0\) is statistically independent of \(A_\mu\), has the same correlation function, and in the end the limit \(\delta A_0 \to 0\) is taken.

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

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

(13)

This suggests transforming the Fokker-Planck operator so that its \(\epsilon = 0\) limit is transformed into a harmonic oscillator. This is achieved by 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

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

(14)

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

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

(15)

\[ H^{(1)}_{ijk} = \sqrt{\omega_j \omega_k / \omega_i} \sum_{l,m} V_{j}^{(i)l} J_{il} J_{jm} J_{nk} . \]

Regularisation is needed since one eigenvalue vanishes in the limit of \(\delta A_0 \to 0\). We determine \(|Q\rangle\) by perturbation theory in \(\epsilon\). Given \(|Q\rangle\), the Lyapunov exponents are obtained as \(\lambda_1 = \gamma \langle x_1 \rangle, \lambda_2 = \gamma \epsilon \langle x_2 \rangle, \lambda_3 = \gamma \epsilon \langle x_3 \rangle\), and

\[ \langle x_i \rangle = \frac{1}{|\Phi_0(Q)|} \sum_j J_{ij} \sqrt{\omega_j} \langle \Phi_0 | \hat{a}_j + \hat{a}^+_j | Q \rangle \]  

(16)

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

\[
\begin{align*}
\lambda_1/\gamma &= 3\epsilon^2 - 29\epsilon^4 + 564\epsilon^6 \\
&
-14977\epsilon^8 + 488784\epsilon^{10} - 18670570\epsilon^{12} + \cdots \\
\lambda_2/\gamma &= 8\epsilon^4 - 459/2\epsilon^6 + 14281/2\epsilon^8 \\
&
-757273/3\epsilon^{10} + 361563709/36\epsilon^{12} + \cdots \\
\lambda_3/\gamma &= -3\epsilon^2 - 9\epsilon^4 - 789/2\epsilon^6 - 5787/2\epsilon^8 \\
&
-895169/3\epsilon^{10} - 101637719/36\epsilon^{12} + \cdots .
\end{align*}
\]

Note that only even powers of \(\epsilon\) contribute, and that all coefficients are rational numbers. Eq. (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 \[22\]. We have attempted to sum the series (17) using Padé-Borel summation \[22\]. We have attempted to sum the series (17) using Padé-Borel summation \[22\]. We have attempted to sum the series (17) using Padé-Borel summation \[22\]. We have attempted to sum the series (17) using Padé-Borel summation \[22\]. We have attempted to sum the series (17) using Padé-Borel summation \[22\].

\[
\lambda_j/\gamma \sim \text{Re} \int dt \, e^{-t} \sum_{l=1}^{l_{\text{max}}} c_l^{(j)} t^{-l} e^{2t} \quad \text{(18)}
\]

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 \[23\] of order \(n\), namely \(P_n^m\) or \(P_{n+1}^m\) 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. 1a and converge to results of numerical simulations provided \(\epsilon\) is not too large. For \(\lambda_2\) numerical evidence indicates the presence of additional non-analytical contributions not captured by the Padé-Borel summation. The results of Fig. 1a allow us to determine the quantity \(\Delta\) defined in eq. (2). The result is shown in Fig. 1b. We find that \(\Delta\) is maximal for \(\epsilon \approx 0.21\) and positive (indicating clustering onto a fractal set) for \(0 < \epsilon < 0.33\). The red line in Fig. 1a, \(\epsilon \sim \kappa \omega^{-1/2} = \text{const.}\), indicates schematically where \(\Delta\) is zero. Above the red line \(\Delta\) is always positive, but tends to zero for small \(\epsilon\) as \(\Delta = 10\epsilon^2 \sim \kappa^2/\omega\). In the limit of \(\epsilon \rightarrow 0\) the dynamics becomes advective (despite being underdamped): to lowest order in \(\epsilon\) 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 \(\delta W(t) = (\delta r_1(t) \wedge \delta r_2(t)) \cdot \delta r_3(t)\) goes through zero. Since \(\delta p_n\) typically remain bounded, caustics correspond to instances where the elements of the third column of \(R'\) go to \(-\infty\) and reappear at \(+\infty\). The rate at which these events occur is given by the escape rate of the Langevin process \[10\] to infinity. It is expected \[10\] to have a non-analytic dependence on \(\epsilon\), of the form \(C \exp(-S/\epsilon^2)\), as demonstrated in Fig. 1c. In this panel, \(J/\gamma\) is compared to \(-(\lambda_1 + \lambda_2 + \lambda_3)/\gamma\). We see that caustics are very rare when \(\epsilon \ll 1\), but frequent when \(\epsilon\) is large and they are the only clustering mechanism when \(\epsilon > 0.33\).

Finally, we comment on the relation between our results and earlier works (cited above), which suggest that clustering only occurs for \(\omega \approx 1\) (with the value of \(\kappa\) unspecified). It must be emphasised 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 \[10, 11, 12\], 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.

The results of this letter are summarised schematically in figure 1d. First, at small \(\kappa\), strong clustering occurs in the region indicated, above the line \(\epsilon \sim \kappa \omega^{-1/2} = 0.33\). 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 \(\epsilon \rightarrow 0\) 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 \(\epsilon > 0.33\) we find that the dimension deficit \(\Delta\) is negative implying that 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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