Clustering of inertial particles in compressible chaotic flows

Vicente Pérez-Muñuzuri*

Group of Nonlinear Physics, Faculty of Physics, University of Santiago de Compostela, E-15782 Santiago de Compostela, Spain

(Received 24 October 2014; published 8 May 2015)

Clustering of inertial particles is analyzed in chaotic compressible flows. A simplified dynamical model for the motion of inertial particles in a compressible fluid at rest has been derived. Clustering enhancement has been observed for intermediate Stokes times and characterized in terms of the number of particles with negative finite-time Lyapunov exponents and the Lyapunov dimension of the model attractor. Cluster formation has been observed to depend on the nature of the flow; vortical or shear. The motion of heavy and light particles is analyzed in terms of the compressibility and correlation length of the density field.

DOI: 10.1103/PhysRevE.91.052906

PACS number(s): 89.75.Kd, 47.70.Fw, 47.70.Pq

I. INTRODUCTION

The well-known steady motion of a sphere in an incompressible flow at low Reynolds numbers was first studied by Stokes in 1851 [1]. He derived an equation for the drag on a sphere in the limit of creeping flow. Since then, the equation of motion of a small rigid sphere in an incompressible nonuniform flow has received some attention; Basset, Boussinesq, and Oseen (the BBO equation [2]) described its motion in an incompressible fluid at rest, and Maxey and Riley [3] and Gatignol [4] independently extended the BBO equation to a nonuniform incompressible flow, obtaining the following equation:

$$\frac{dV_i}{dt} = \rho_f \frac{Du_i}{Dt} + \left( \rho_p - \rho_f \right) g_i - \frac{9 \mu_f}{2 a^2} V_i - \frac{\rho_f}{2} \left( \frac{dV_i}{dt} - \frac{D}{Dt} \left[ u_i + \frac{a^2}{6} \nabla^2 u_i \right] \right) - \frac{9 \rho_f}{2a} \sqrt{\frac{v}{\pi}} \times \int_0^1 \frac{1}{\sqrt{1 - \xi}} \frac{d}{d\xi} \left( V_i - u_i - \frac{a^2}{6} \nabla^2 u_i \right) d\xi, \quad (1)$$

where $V_i$ is the velocity of the sphere, $u_i$ is that of the fluid, $\rho_p/\rho_f$ is the density of the particle or fluid that it displaces, $v = \mu/\rho_f$ is the kinematic viscosity, $a$ is the radius of the sphere, and $g_i$ is the gravity. The five terms on the right represent, respectively, the force exerted by the undisturbed flow, the buoyancy, the Stokes drag, the virtual-added mass, and the Basset history force. The terms in $a^2 \nabla^2 u_i$ are the Faxén corrections for the nonuniformity of the undisturbed fluid velocity field far from the sphere. The derivative $D/Dt$ is taken along the path of a fluid element, whereas the derivative $d/dt$ is taken along the trajectory of the particle. Some controversy about the use of these two derivatives in the added-mass term has been discussed over the last years [3–6]. In general, the values of these derivatives can differ substantially, but in the context of the low-Reynolds-number approximation used to derive Eq. (1) both derivatives are approximately the same. Further improvements to this equation have been published to take into account flows with a finite Reynolds number [6,7].

More recently, this equation has been used in a simplified form to describe the motion of inertial particles in turbulent incompressible flows [8]. For particles sufficiently small so that the Faxén corrections may be negligible, and excluding the Basset term, it is possible to obtain a minimal model for the particle trajectory in two dimensions:

$$\frac{d^2x_i}{dt^2} - \beta \frac{Du_i}{Dt} = - \frac{1}{\tau_p} \left( \frac{dV_i}{dt} - u_i \right), \quad (2)$$

with $\beta = 3 \rho_f/(2 \rho_p + \rho_f)$, $\tau_p = a^2/(3v\beta)$ is the Stokes time or particle viscous response time, and $V_i = dx_i/dt$. The dimensionless Stokes number $St = \tau_p/\tau_f$ characterizes the effect of particle inertia, and $\tau_f$ accounts for the characteristic timescale of the fluid. For intermediate values of $\tau_p \approx \tau_f$ (St ≈ 1) strong clusterization of the inertial particles on fractal-like structures has been observed [8]. Transport of noninteracting inertial particles in incompressible flows shows properties typical of compressible fluids. The most unexpected behavior is the formation of clusters of particles out of an initially homogeneous distribution. Some examples where clustering of inertial particles is of some importance are rain generation [9], composite materials [10], the advection of volcanic ash in the atmosphere [11], the formation of planetesimals in the early solar system [12], and other processes such as sediment transport in rivers, transport of dust from soil erosion, combustion or the mixing of sprays. In the limit of vanishing Stokes drag, inertial particles recover the motion of Lagrangian tracers and no clustering should be expected.

However, few efforts have been carried out to include the effects of compressibility on the motion of inertial particles in a fluid [13]. Time-varying density effects were investigated previously [14] and found to be of importance. Only recently, Parmar et al. [15,16] obtained an explicit equation for the time-dependent force on a small sphere for nonuniform compressible flows. This equation can be conveniently written as follows [see Eqs. (8.1)–(8.6) in Ref. [16] for further details]:

$$\rho_p \frac{dV_i}{dt} = \frac{\rho_f}{\tau_p} \frac{Du_i}{Dt} - \frac{9 \mu}{2a^2} (V_i - \overline{V_i})$$

$$+ \frac{1}{2} \left( \frac{D}{Dt} \rho_f \overline{u_i} - \frac{d}{dt} \rho_f V_i \right), \quad (3)$$

where the overlines mean volume and surface averages, respectively. The buoyancy or gravity, the Faxén corrections,
and the Basset or viscous unsteady forces have been neglected for simplicity. Besides, flow variations and particle-acceleration timescales have been considered to be much larger than the acoustic timescale. The form of the above equation is quite similar to Maxey and Riley equation (1) but incorporates the effects of the nonuniform density field $\rho_f(x,t)$.

The motion of passive or Lagrangian tracers in compressible turbulent [17] or chaotic flows [18,19] has attracted some attention during the last years, both theoretically and experimentally, but few studies have been performed with inertial particles to my knowledge. Among other techniques, finite-time Lyapunov exponents (FTLE) have been used extensively to quantify mixing and especially to extract persisting transport patterns in the flow, so-called Lagrangian coherent structures (LCSs) [20–23]. FTLE analysis is directly linked to the dynamical systems approach to transport that analyzes the phase space of the dynamical system driving the trajectories in a flow. LCSs are locally the strongest repelling or attracting material lines and represent the cores of Lagrangian patterns. Being material lines, i.e., a line of fluid particles, they cannot be crossed by ideal tracers. Therefore, they are transport barriers separating the flow into different fluid masses, a fundamental and very useful property that may be used to define clusters of fluid particles. However, few studies have used these techniques to identify geometric separatrices from trajectories of inertial particles [24]. The purpose of this paper is to address the process of inertial tracers clustering in a chaotic compressible flow in terms of the FTLE field.

II. MODELS

We investigate the effects of compressibility on the inertial particle motion in two chaotic flows; the chaotic shear flow and the periodically varying double-gyre flow (see Appendix for equations). The dynamics of both flows are completely different. In the first model, the flow is the combination of two orthogonal motions, each with a sinusoidal velocity profile, capable of producing repeated stretching and folding of the fluid parcels. On the other hand, the double-gyre model consists of two vortices rotating in opposite directions that conversely expand and contract periodically in the x direction such that the rectangle enclosing the gyres remains invariant. The periodic perturbation leads to mixing between both gyres.

Here we consider flow velocities of the form

$$u_i = u_i^0/\rho_f, \quad \partial_i u_i \neq 0, \quad \partial_i u_i^0 = 0,$$

that trivially satisfy the continuity equation $\partial_i (\rho_f u_i) = 0$. The spatial dependence of the flow density is modeled [18,19] as

$$\rho_f(x) = 1 + \epsilon \sin (2\pi x_1/\lambda) \sin (2\pi x_2/\lambda),$$

where $\epsilon$ and $\lambda$ are the compressibility of the flow and wavelength, respectively. For any periodic function $\rho_f(x)$, similar results to those presented here are expected.

An interesting consequence of Eq. (3) is that it can be reduced to Eq. (1) by applying the Reynolds transport theorem and then assuming the terms inside the volume and surface integrals are nearly uniform over the sphere. This assumption is valid if the size of the sphere is small compared to the length scale of variations in the undisturbed flow. Thus, the minimal model (2) is also valid for compressible fluids and can be written as

$$\frac{dx_i}{dt} = V_i,$$
$$\frac{dV_i}{dt} = -\frac{\beta}{\rho_f} (V_i - u_i) + \frac{\beta}{\tau} \frac{Du_i}{Dt},$$

where $x(t)$ stands for the position of the particle, $\beta = \beta(x)$, and $\phi_i = a^2/\mu$. The last set of equations incorporates the influence of the nonuniform density field (5) through the $\beta$ coefficient and the flow field $u$. The term $\overline{\rho_f} \phi_i$ is the mean dissipative timescale of the compressible flow, equivalent to the Stokes time defined above for incompressible flows. As the spatial mean $\overline{\rho_f} = 1$, $\phi_i$ will be considered the Stokes time from now on.

In order to characterize the transport of inertial particles, the finite-time Lyapunov exponents $\sigma$ are computed along their trajectories in the flow [25] as

$$\sigma(x_0, V_0, t_0, \tau) = \frac{1}{\tau} \int_0^{\tau} \ln \sqrt{\mu_{\text{max}}[C(x(t))]},$$

where $\mu_{\text{max}}$ is the maximum eigenvalue of the right Cauchy–Green deformation tensor $C = F^T F$. $F$ is defined by $F(x_0) = V[x(t_0 + \tau)]$, and $x(t_0 + \tau)$ is the final position of the tracer. Initially, the position of the tracers $x_0$ must be defined and their velocity set equal to the flow $V_0 = u(x_0, t_0)$. For the computation of FTLE fields the integration time $\tau$ must be predefined. Basically, the time $\tau$ has to be long enough to allow trajectories to explore the coherent structures present in the flow. The FTLE at a given location measures the maximum stretching rate of an infinitesimal fluid parcel over the interval $[t_0, t_0 + \tau]$ starting at the point $x_0$ at time $t_0$. Repelling (attracting) coherent structures for $\tau > 0$ ($\tau < 0$) can be thought of as finite-time generalizations of the stable (unstable) manifolds of the system. These structures govern the stretching and folding mechanism that control flow mixing.

III. RESULTS

We analyze the role of the Stokes time $\phi_i$ defined in Eq. (6), at constant compressibility $\epsilon$, on the FTLE fields for the shear flow model in Fig. 1. For intermediate $\phi_i$ values, coherent structures are strongly affected by the density field (5) and the formation of clusters with a grid configuration is clearly visible. Ridges of the FTLE field enclose regions with negative values of the FTLE. As time evolves, this configuration remains approximately constant. For larger $\phi_i$ values, the grid-type configuration disappears and particles evolve freely. For $\epsilon = 0$, FTLE fields do not depend on the Stokes time. For the double-gyre flow, Fig. 2, for any value of $\epsilon$, FTLE fields change with $\phi_i$. For the Lagrangian limit $\phi_i \to 0$, results described in Ref. [19] are recovered. For intermediate values of the Stokes time $\phi_i^{\text{max}}$, a grid-type configuration develops inside the vortexes as $\epsilon$ increases. However, this configuration changes for larger values of $\phi_i$ as multiple and folded coherent structures develop.

Due to the specific characteristics of the flows, inertial particles behave differently in both flows. The chaotic shear flow is a combination of two orthogonal motions, each with sinusoidal velocity and density profiles. Each motion acts alternatively for one-half of the flow period favoring the
clustering of the particles in the interstices of a net where \( \rho_f < 1 \) and wavelength \( \lambda \) for some intermediate value of \( \phi_s \). The upper row of Fig. 3 shows this behavior for three \( \phi_s \) values. Increasing the compressibility favors trapping of the particles. For the double-gyre flow, for \( \epsilon = 0 \), vortex cores are expected to be regions of high concentration of light particles, while high-strain areas should concentrate heavy particles. The lower row of Fig. 3 shows the increasing accumulation of particles for some intermediate value of \( \phi_s \). However, contrary to the shear flow results, the presence of a nonuniform density field favors that as compressibility increases, trapping of inertial particles decreases. The density field disturbs particle trapping inside the gyres cores favoring that particles may be expelled out of the cores and eventually all particles may reach the boundaries. A more detailed discussion on the role of particle density and the clustering behavior will be given later. In both flows, trapping of particles by the density field is characterized by negative values of the FTLE.

To assess quantitatively the compressibility effects on the FTLE, we perform systematic simulations for different values of the Stokes time \( \phi_s \) and compressibility \( \epsilon \). To characterize the resulting FTLE fields, it is convenient to calculate the mean FTLE value \( \overline{\sigma} \), the standard deviation of spatial FTLE variability and the percentage of inertial particles with \( \sigma < 0 \). Results are shown for both flows in Fig. 4.

For any value of \( \epsilon \), for intermediate values of the Stokes time \( \phi_s \), the number of tracers with negative Lyapunov exponents reaches a maximum value \( N_{\text{max}} \) at \( \phi_{s}^{\text{max}} \approx 1 \). At this value, a maximum of clustering of the inertial particles is obtained. Note that, for the shear flow, clustering enhancement monotonically increases with the compressibility and the Stokes time \( (N_{\text{max}} = 0 \text{ for } \epsilon = 0) \). On the other hand, for the double-gyre flow the opposite situation occurs; the peak maximum decreases with increasing compressibility and with decreasing Stokes times \( \phi_s \). In this case, for the incompressible case \( \epsilon = 0 \), maximum clustering is observed for intermediate Stokes times. For both flows, for \( \phi_s \to 0 \) and \( \phi_s \to \infty \), clustering diminishes and the number of tracers with \( \sigma < 0 \) goes to zero. This nonlinear behavior is also observed in the spatial mean value of the FTLE and its standard deviation [Figs. 4(a), 4(b) and 4(d), 4(e)]. Note that, for
The rest of the parameters are as in Figs. 1 and 2.

These variables, for Stokes times larger than the maximum clustering enhancement, the mean FTLE and its variability do not recover their values at $\phi_l \to 0$. The larger mean FTLE values correspond to an increase in variability as the flow becomes more turbulent and less coherent. For the limit of vanishing Stokes times, the dynamics of Lagrangian tracers in a compressible flow is recovered [19]. For very large Stokes times, particles tend to follow ballistic trajectories, are less influenced by the flow and no clustering is expected.

The clustering behavior of the inertial particles on the correlation length $\lambda$ of the density field depends on the characteristics of the flow model as is shown in Fig. 5. Increasing $\lambda$ avoids dispersion and favors concentration of particles inside the cores of the vortices, thus enhancing clustering. However, for the shear flow, as $\lambda$ increases, the number of interstices with low compressibility $\rho_f < 1$ diminishes, so less particles can be trapped. Note that for both flows, as $\lambda \to L$, $N_{\text{max}} \to N_{\text{max}}(\epsilon = 0)$.

Another common feature shared by both flows is the clustering enhancement ($N_{\text{max}}$ increases) with increasing flow amplitude $A$. For the same integration time, enclosing of particles within the streamlines of the double-gyre flow is favored as $A$ increases, while for the chaotic shear flow more particles are attracted towards areas of low compressibility. On the other hand, varying the flow period $T$ does not contribute significantly to cluster enhancement.

### A. Lyapunov dimension and flow compressibility

Compressibility effects in turbulent incompressible flows have been described by the Lyapunov spectrum $\chi_1 > \cdots > \chi_{2d}$ ($d = 2$) for inertial particles [8]. Fractal geometry theory shows that Hausdorff dimensions $d_H$ lower than $d = 2$ indicate the presence of fractal sets, while for $d_H > 2$ particles fill the whole $d$-dimensional space. Following these results, we investigate the formation of clusters in terms of the Lyapunov dimension which is an upper bound for the Hausdorff dimension and can be easily calculated [26] as

$$d_L = j + \sum_{i=1}^{j} \frac{|\chi_j|}{|\chi_{j+1}|},$$

where $j$ satisfies $\sum_{i=1}^{j} \chi_i \geq 0$ and $\sum_{i=1}^{j+1} \chi_i < 0$. Figure 6 shows the Lyapunov dimension calculated for the chaotic shear flow from Eq. (6) as a function of the Stokes time $\phi_l$ for different compressibility values. Similar results were obtained for the double-gyre flow, although they are not shown here. Note that $d_L < 2$ for intermediate values of the Stokes time, and $d_L \to 2$ for the Lagrangian-tracers limit ($\phi_l \to 0$). For large Stokes times, particles fill the whole space and $d_L > 2$. The presence of a minimum was already discussed [8] for turbulent flows and indicates a value for which compressibility effects are maximum. Particles concentrate onto fractal sets ($d_L < 2$) and very dense and almost empty regions develop. At the minimum of $d_L$, the concentration of particles into the clusters is a maximum. For the shear flow, clustering

This is a representative text that describes the behavior of inertial particles in compressible flows, focusing on the clustering enhancement and the influence of flow parameters on this behavior. The text also introduces the concept of Lyapunov dimension to quantify the compressibility effects and shows how these effects are reflected in the clustering behavior of particles. The figures and equations provided illustrate these concepts, showing how the clustering evolves with different parameters and flow conditions.
enhancement increases with $\epsilon$ [Fig. 4(c)], and $d_L$ → 0, as most of the particles are located in a network. For $\epsilon = 0$ there are $d_L$ values smaller than $d = 2$ that, however, were not appreciated in terms of particles with $\sigma < 0$.

B. Particle density effects in gyre flow

The vortical behavior of the double-gyre flow offers the possibility to study the cluster formation of inertial particles with different density values $\rho_p$. Figure 7 shows the time evolution of the number of particles with $\sigma < 0$ for different Stokes times and particle density $\rho_p$ values for the double-gyre flow. The peak value at $\phi_p^{\text{max}}$ increases with time monotonically, while for very large Stokes times the amount of cluster particles decreases to zero. Initially, the number of cluster particles shows little change, indicating that a certain time is needed for the particles to adjust their initial velocity to the local field. This is more evident as $\rho_p$ increases. Finally, after some time, the number of particles within the clusters reaches their asymptotic values: 100% for $\phi_p^{\text{max}}$ and zero for $\phi_p \rightarrow \infty$. Note that it takes longer to reach these values as $\rho_p$ increases.

For a constant integration time, clustering diminishes with increasing $\rho_p$, as heavy particles are less influenced by the flow (move slowly) and they have less probabilities to be displaced towards trapping areas. On the other hand, for the shear flow, similar results were observed although not shown here. For both flows, for the Lagrangian limit $\phi_p \rightarrow 0$, the number of cluster particles goes quickly to zero for any value of $\rho_p$.

The spatial distribution of the cluster particles is shown in Fig. 8 for different compressibility and particle-density values at a given instant of time. For any $\epsilon$, light particles concentrate inside the inner cores of the vortices as they are driven inward due to the lesser inertial, while heavy particles tend to move away and concentrate in regions of flow characterized by low values of the vorticity (high strain) near the fixed points of the flow. Such a phenomenon is known as preferential concentration [27]. Note for $\rho_p = 1$ the spiraling effect as particles are expelled from the vortices via the slingshot effect. This is not the case for the shear flow where particles, independently of their density, tend to concentrate in areas with low values of flow density.

As compressibility increases, the presence of the density field makes difficult the motion of particles towards their final destinations because they are also trapped by the field. This interaction is more visible for heavy particles (right panels in Fig. 8).

IV. CONCLUSIONS

I studied the motion of inert particles in two chaotic compressible flows, namely: the shear and double-gyre flows. For the equation of motion of inertial particles we used a simplified model (6) derived from a recently proposed model for compressible nonuniform flows [15,16]. For the compressible flows analyzed in this paper, our simplified model is equivalent to Eq. (2) [8] but incorporates the nonuniform effects of the density field through the flow field. In the considered flows, clustering of inertial particles is strongly affected by compressibility and the Stokes time $\phi_s$. Clustering enhancement has been observed for intermediate Stokes times $\phi_s \approx \tau_f$. $St \approx 1$ and characterized in terms of the number of particles with negative FTLE and the Lyapunov dimension. However, two different behaviors have been described in terms of the compressibility $\epsilon$ and the type of flow, due to the interaction between the density field and the specific dynamics of the flows.

For $\epsilon = 0$ the shear flow clustering is not observed, independently of the particle density or the Stokes time, while for the gyre flow, clustering is observed to depend on the particle density. For the last flow, light particles concentrate in the inner cores, while heavy particles move to high strain areas (preferential concentration). It is interesting to note that for the gyre flow, the transport of inertial particles in compressible flows ($\epsilon = 0$) shows properties typical of compressible fluids. The formation of clusters of particles out of an initially homogeneous distribution was also described in the literature [8,28,29]. For $\epsilon > 0$, for the shear flow, inertial particles cluster on network-like structures where $\rho_f < 1$ and clustering is enhanced with increasing $\epsilon$. However, for the gyre flow, the density field interacts with the vortical motion of the gyres not favoring the motion of particles towards their natural final destinations: inner cores (light particles) or high-strain areas (heavy particles). This interaction leads to a diminishing of cluster particles for any Stokes time.
The effect of the density correlation length $\lambda$ on the clustering of inert particles has also been analyzed for both flows in terms of the FTLE field attaining different results. While clustering enhancement has been observed for the double-gyre flow, the opposite behavior occurs for the shear flow. This is also a consequence of the different flow dynamics, vortical and shear, as described above.

Finally, an interesting field of research will be the study of cluster formation of drops or bubbles in nonuniform compressible flows. Although some attempt has been made to model the motion of these objects in compressible flows [30], the exchange of matter or thermodynamic properties between the drop and the flow, not yet considered, could contribute to the study of the aggregation of radiosonde balloons [31], or the transport of water vapor in the atmosphere, where the presence of large eddies and shear stresses determine their dynamics, among other examples in geophysical flows.

ACKNOWLEDGMENTS

This work was supported by Xunta de Galicia and Ministerio de Economía y Competitividad under Research Grants CN2012/315 and CGL2013-45932-R, respectively. Computational part of this work was done in the Supercomputing Center of Galicia, CESGA. The author gratefully acknowledges the helpful comments of D. Garaboa and the anonymous reviewers.

APPENDIX

The chaotic shear flow model [22,32,33] is described by the equations

$$(u_1,u_2) = \frac{1}{\rho_f}(A \sin(2\pi x_2/L + \varphi_0),0),$$

$$nT \leq t < (n + \frac{1}{2})T,$$

over the domain $[-20,20] \times [-20,20]$, $L = 40$. $T$ and $A$ are the period and shear amplitude of the flow, respectively, and $n$ is the period number [34].

On the other hand, the periodically varying double-gyre flow [20,35] is used as a standard test case for LCSs and can be considered a local view of a gulf stream ocean front. In this case, the flow is described by the velocity field,

$$u_1 = -\frac{\pi A}{\rho_f} \sin(\pi f(x_1,t)) \cos(\pi x_2),$$

$$u_2 = \frac{\pi A}{\rho_f} \frac{\partial f}{\partial x_1} \cos(\pi f(x_1,t)) \sin(\pi x_2),$$

where

$$f(x_1,t) = a(t)x_1^2 + b(t)x_1,$$

$$a(t) = \psi \sin \omega t,$$

$$b(t) = 1 - 2\psi \sin \omega t,$$

over the domain $[0,2] \times [0,1]$. As in the previous model, $T = 2\pi/\omega$ and $A$ are the period and amplitude of the flow, respectively. For $\psi = 0$ the system can be thought of as a time-independent two-dimensional Hamiltonian system. For this case there is a heteroclinic connection of the unstable manifold of the fixed point $(1,1)$ with the stable manifold of the fixed point $(1,0)$.

For the numerical experiments, initially a cluster of 400 × 400 (shear flow) and 600 × 300 (gyre flow) particles were regularly spaced in the domains. Then, the trajectories of these particles are calculated by integrating the equations above using a fourth-order Runge–Kutta scheme and a fixed time step of $\Delta t = 10^{-3}$.

[34] Transport barriers due to Kolmogorov–Arnold–Moser (KAM) tori, typically present in periodically driven conservative flows, can be avoided by breaking the periodicity using a random phase $\phi$, that is selected independently and uniformly from $[0,2\pi)$ in each half of the period.