The dynamics of small spherical particles immersed in a fluid flow have received considerable attention in the past few years from both theoretical and experimental points of view. On one hand, these particles are the simplest models for impurities whose transport in flows is of practical interest, and, on the other, their motion is governed by dynamical systems that even in the most minimal approximations display a rich and complex variety of behavior. When the density of the particles does not match that of the fluid, it is intuitively clear that the trajectories of a particle and of a fluid parcel will in general differ. This has been demonstrated in two-dimensional flows in which particles with density higher than the basic flow tend to migrate away from the parts of the flow dominated by rotation—in the case of chaotic flows, the KAM (Kolmogorov-Arnold-Moser) islands—while particles lighter than the fluid display the opposite tendency [1–3]. A more surprising result, however, is that neutrally buoyant particles may also detach from the fluid-parcel trajectories in the regions in which the flow is dominated by strain, to settle in the KAM islands [4]. The subtle dynamical mechanism responsible for the latter phenomenon has suggested a method to target KAM islands in Hamiltonian flows, and a recent generalization named a bailout embedding permits its extension to Hamiltonian maps as well [5].

Despite its obvious importance from the point of view of applications, the case in which the base flow is three dimensional has been much less investigated. The probable reason for this is that very few simple realistic three-dimensional incompressible flow models exist. The few that are simple are not realistic—e.g., the ABC (Arnold-Beltrami-Childress) flow [6]—and those that are realistic are far more complex. In the study of the Lagrangian structure of three-dimensional incompressible time-periodic flows, where this difficulty is already present, the alternative approach of qualitatively modeling the flows by iterated three-dimensional volume-preserving (Liouvillian) maps has been successful in predicting fundamental structures later found both in more realistic theoretical flows and in experiments [7–10]. However, no similar approach has been followed to describe the motion of impurities in this kind of flow.

This Letter introduces the idea of bailout embeddings to non-Hamiltonian systems. Two fundamentally unexplored problems are attacked with this new technique: first the investigation of generic structures of the dynamics of small particles in three-dimensional time-periodic flows, and second the study of the effects of noise and fluctuations on the dynamics of such particles, as well as the practical use of this analysis to reveal structures in three-dimensional flows that would be largely hidden to other methods. Regarding the former, we produce qualitative predictions using the bailout approach for maps that we confirm for flows. For the latter, we show that intricate but well-defined structures may arise in a surprising way in the distribution of particles driven by extremely chaotic flows and the presence of noise. Bailout embedding is amenable to theoretical and experimental analysis in fluid dynamics, but the technique has many potential uses in the much broader community of physicists dealing in one way or another with nonlinear dynamical systems.

Let us first recall the equation of motion for a small, neutrally buoyant, spherical tracer in an incompressible fluid (the Maxey-Riley equation) [11,12]. Under assumptions allowing us to retain just the Bernoulli, Stokes drag, and Taylor added mass contributions to the force exerted by the fluid on the sphere (the particle radius and its Reynolds number are small, as are the velocity gradients around it [4]), the equation of motion for the particle at position $x$ is

$$\frac{d}{dt}(\dot{x} - u(x)) = - (\lambda + \nabla u) \cdot (\dot{x} - u(x)), \quad (1)$$

where $\dot{x}$ represents the velocity of the particle, $u$ that of the fluid, $\lambda$ a number inversely proportional to the Stokes number of the particle—the ratio of the relaxation time of the particle back onto the fluid trajectories to the time scale of the flow—and $\nabla u$ the Jacobian derivative matrix of the flow. The difference between the particle velocity and the velocity of the surrounding fluid is exponentially damped with negative damping term $- (\lambda + \nabla u)$. In the
case in which the flow gradients reach the magnitude of
the viscous drag coefficient, there is the possibility that
the Jacobian matrix $\nabla u$ may acquire an eigenvalue of
positive real part in excess of the drag coefficient. If in
these instances we can discard the time dependence of the
eigenvectors it is clear that the trajectories, instead of
converging exponentially onto those defined by $x = u$,
may detach from them.

For incompressible two-dimensional flows, since the
Jacobian matrix is traceless, the two eigenvalues must add
up to zero, which implies that they are either both purely
imaginary or both purely real, equal in absolute value and
opposite in sign. The result is that the particles can
abandon the fluid trajectories in the neighborhood of the
saddle points and other unstable orbits, where the
Jacobian eigenvalues are real, and eventually overcome
the Stokes drag, to finally end up in a regular region of the
flow on a KAM torus dominated by the imaginary
eigenvalues. From a more physical point of view, this effect
implies that the particles tend to stay away from the
regions of strongest strain. In contrast to the two-
dimensional case, in time-dependent three-dimensional
flows the incompressibility condition implies only that the
sum of the three independent eigenvalues must be zero. This
less restrictive condition allows for many more combinations. Triplets of real eigenvalues, two posi-
tive and one negative or vice versa, as well as one real
eigenvalue of either sign together with a complex-
conjugate pair whose real part is of the opposite sign,
are possible. Accordingly, chaotic trajectories may have
one or two positive Lyapunov numbers, and a richer range
of dynamical situations may be expected.

Instead of investigating all these in terms of a given
fully fledged three-dimensional time-periodic model
flow, we follow a qualitative approach based on iterated
maps that roughly reproduces the properties of the impu-
ritvity dynamics in a generic flow of this kind. In order to
construct the map we first note that the dynamical system
governing the behavior of neutrally buoyant particles is
composed of some dynamics within another larger set of
dynamics. Equation (1) can be seen as an equation for a
variable $\delta = x - u$ which in turn will define the equation of
motion $x = u$ of a fluid element whenever the solution of
the former be zero. In this sense we may say that the
fluid-parcel dynamics is embedded in the particle dy-
namics. In reference to the fact that some of the embedding
trajectories abandon some of those of the embedded
dynamics, the generalization of this process is dubbed a
bailout embedding [5].

It is rather easy to construct this type of embedding for
map dynamics. Given a map $X_{n+1} = T(X_n)$, a general
bailout embedding is given by

$$X_{n+2} - T(X_{n+1}) = K(X_n) \cdot (X_{n+1} - T(X_n)),$$

(2)

where $K(X)$ is the bailout function whose properties
determine which trajectories of the embedded map will
be eventually abandoned by the embedding. The particu-
lar choice—naturally imposed by the particle dynam-
ics—of the gradient as the bailout function in a flow
translates in the map setting to

$$K(X) = e^{-\lambda} \cdot \nabla T.$$  

(3)

Bailout embeddings have been used to investigate target-
ing of KAM tori in Hamiltonian systems, as well as to
explore generic properties of the distribution of small
particles immersed in incompressible two-dimensional
fluid flows [5], which are also of a Hamiltonian nature.

Here we consider the bailout embedding of a class of
non-Hamiltonian systems: three-dimensional volume-
preserving maps. In particular, we choose to represent
qualitatively chaotic three-dimensional incompressible
base flows that are periodic in time by ABC maps, a
family

$$T = T_{ABC}:(x_n, y_n, z_n) \rightarrow (x_{n+1}, y_{n+1}, z_{n+1}),$$  

(4)

where

$$x_{n+1} = x_n + A \sin z_n + C \cos y_n \mod 2\pi,$$

$$y_{n+1} = y_n + B \sin x_{n+1} + A \cos z_n \mod 2\pi,$$

$$z_{n+1} = z_n + C \sin y_{n+1} + B \cos x_{n+1} \mod 2\pi,$$

(5)

that displays all the basic features of interest of the
evolution of fluid flows. Depending on the parameter
values, this map possesses two quasi-integrable behav-
iors: the one-action type, in which a KAM-type theorem
exists, and with it invariant surfaces shaped as tubes or
sheets; and the two-action type displaying the phenome-
non of resonance-induced diffusion leading to global
transport throughout phase space [7].

Let us now study the dynamics defined by Eqs. (2)–(5).
We first concentrate on the cases in which the flow is
dominated by one-action behavior. In these we find an
interesting generalization of the behavior already seen in
two dimensions: particles are expelled from the chaotic
regions to finally settle in the regular KAM tubes. As an
example, we take values of $A$, $B$, and $C$ that lead to almost
ergodic behavior of the fluid map: a single fluid trajectory
almost completely covers the phase space. However, from
randomly distributed initial conditions, the particle tra-
jectories inevitably visit some hyperbolic regions where
they detach from the corresponding fluid trajectory. In
this fashion they find their way inside the invariant ellip-
tic structures where they can finally relax back onto a safe
fluid trajectory. In Fig. 1 we show how a homogeneous
distribution of particles in the fluid flow, after a large
number of stabilization iterations, finally settles inside the
tubular KAM structures for different values of the pa-
rameter $\lambda$. When the value of $\lambda$ decreases, more random
trajectories follow this evolution: more particles fall into
the invariant tubes.

In the two-action case, the eigenvalues of the Jacobian
are very small on large portions of the trajectory, so that
separation may occur only sporadically during the short
time intervals in which the fluid parcel crosses the fast-motion resonances [7]. Most of the time, particles, and fluid parcels follow exponentially convergent trajectories, causing the separations to be practically unobservable except for very small values of $\lambda$. Most probably, once the particles converge to the fluid dynamics, they remain attached. However, by adding a small amount of white noise, we can continually force the impurity to fluctuate around the flow trajectory [13]. From the application point of view, this noise may be considered to represent the effect of small scale turbulence, thermal fluctuations, etc., but here we use it only as a dynamical device. With this, the particles arrive in the neighborhood of the resonances with a non-negligible velocity mismatch with the fluid that is considerably amplified during the transit across the resonance. The measure of this mismatch is then a good detector of the proximity of the resonance.

Consider the following stochastic iterative system:

$$X_{n+2} - T(X_{n+1}) = e^{-A} \nabla T \cdot (X_{n+1} - T(X_n)) + \xi_n,$$

where the noise term $\xi_n$ satisfies $\langle \xi_n \rangle = 0$, and $\langle \xi_n \xi_m \rangle = \epsilon (1 - e^{-2A}) \delta_{mn} I$. We can recast Eq. (6) into

$$X_{n+1} = T(x_n) + \delta_n, \quad \delta_{n+1} = e^{-A} \nabla T \cdot \delta_n + \xi_n,$$

if we define the velocity separation between the fluid and the particle as $\delta_n = x_{n+1} - T(x_n)$. We illustrate the behavior referred above by studying the most ergodic two-action case, in which all the fluid trajectories intersect the resonant lines. In Fig. 2(a) we show how $\delta_n$ grows strongly at some points, which correspond to the crossings of the resonant lines. In Fig. 2(b) we plot an $xy$ slice of the three-dimensional cube, choosing those points where the value of $\delta_n$ is greater than a minimum value $\delta_0$. As shown, we recover the resonant structure previously noted [7,8].

This is the most primitive way to obtain useful information from the noisy particle dynamics. A shrewder analysis [13] shows how the variance of the separation $\delta_n$ between particles and fluid trajectories and the variance of the noise $\xi_n$ are related by a function that depends only on the particular point of the phase space that we look at, in a sort of temperature amplitude for the fluctuations of $\delta$.

$$T(x) = \frac{\langle \delta^2 \rangle}{\langle \xi^2 \rangle} = \sum_{j=0}^{\infty} \left( e^{-jA} \cdot \int_{T^{-k}(x)} \nabla T \right)^2.$$  

This amplitude takes different values at different points of the flow. At those points that the particle dynamics tries to avoid, its value increases, so the particle prefers to escape the hot regions and to fall into the cold ones.

In Fig. 3 we illustrate this phenomenon. First we analyze a one-action situation showing the temperature amplitude, as well as the impurity dynamics; Figs. 3(a) and 3(b), respectively. Again we use slices of the three-dimensional cube to show the situation more clearly. Figure 3(a) shows the temperature in a scaled color code. Figure 3(b) shows a histogram of visits that a single particle pays to each bin of the space. The agreement between the higher-temperature regions and the less-visited ones is evident. Next we plot the same pictures but in the two-action case studied before; Figs. 3(c) and 3(d). Finally, we apply this analysis to a generic chaotic case where we do not have any information about the phase space structure. We show in Fig. 3(e) how the invariant manifolds are very twisted, and in Fig. 3(f) how the particles, even so, try to find the coldest regions of the flow.

In order to confirm that the above-described behavior is not an artifact of our mapping-based approach, we have performed analogous simulations using a continuous-time model as a base flow. We have considered neutrally
buoyant particles immersed in a modified version of the ABC flow,

\begin{align*}
\dot{x} &= (1 + \sin 2\pi t) \cdot (A \sin z + C \cos y), \\
\dot{y} &= (1 + \sin 2\pi(t + 1/3)) \cdot (B \sin x + A \cos z), \\
\dot{z} &= (1 + \sin 2\pi(t + 2/3)) \cdot (C \sin y + B \cos x),
\end{align*}

in which each component of the velocity vector field is sinusoidally modulated with a relative phase shift of $2\pi/3$, and where $x$, $y$, and $z$ are to be considered modulo $2\pi$. While a detailed analysis of the dynamical aspects of this flow is beyond the scope of this Letter, we advance that it shows structures similar to those of the ABC maps, i.e., a complex array of KAM sheets and tubes surrounded by chaotic volumes. Neutrally buoyant particles evolved according to the true (simplified) Maxey-Riley equations, Eq. (1), based on this flow, show exactly the same tendency to accumulate inside KAM tubes as in the map case.

This application of bailout embedding is the first to be reported for a non-Hamiltonian dynamical system. Our approach can be pursued with two different goals in mind: on one hand, it contributes to the understanding of the physical behavior of impurities, and on the other, it provides a mathematical device to learn about the dynamical structures of the base flow in situations where these are very difficult to elucidate directly. Both bodies of information are important to improve our presently scant knowledge of the transport properties of three-dimensional fluid flows.

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FIG. 3 (color online). The temperature amplitude—lighter is hotter—for the one-action, two-action, and most chaotic cases [(a), (c), and (e), respectively], together with the corresponding slices of the impurity dynamics (histogram) in the phase space [(b), (d), and (f)]. All images are the $[0, 2\pi] \times [0, 2\pi]$ region in the $xy$ axis, for a slice in the $z$ direction corresponding to the values $z \in [0, 0.49].$

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