Clustering criterion for inertial particles in two-dimensional time-periodic and three-dimensional steady flows

Themistoklis Sapsis[1] and George Haller[2]
[1]Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA
[2]Department of Mechanical Engineering, McGill University, Montreal QC H3A 2K6, Canada

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We derive an analytic condition that predicts the exact location of inertial particle clustering in three-dimensional steady or two-dimensional time-periodic flows. The particles turn out to cluster on attracting inertial Lagrangian coherent structures that are smooth deformations of invariant tori. We illustrate our results on three-dimensional steady flows, including the Hill's spherical vortex and the Arnold–Beltrami–Childress flow, as well as on a two-dimensional time and space periodic flow that models a meandering jet in a channel. © *2010 American Institute of Physics*.
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The motion of finite-size or inertial particles in fluids is an important phenomenon encountered in a wide series of phenomena in nature and technology. As it has been observed both experimentally and numerically the dynamics of finite-size particles can differ markedly from infinitesimal particle dynamics. An example of such behavior is clustering, i.e., preferential concentration, observed in various contexts (plankton patchiness, planetesimal formation, pollutants transportation in the atmosphere, etc.). In this work we use analytical techniques to derive a necessary criterion that predicts smooth clustering surfaces, i.e., inertial Lagrangian coherent structure (ILCS), where particles will concentrate due to their finite size. This condition applies to two-dimensional time-periodic flows and three-dimensional (3D) steady flows that contain a closed two-dimensional stream surface.

I. INTRODUCTION

Small particles in fluid flows are commonly encountered in nature (e.g., contaminant dispersion in the atmosphere) as well as in technological applications (e.g., chemical systems involving particulate reactant mixing). A well-documented phenomenon displayed by inertial particles is clustering, i.e., concentration into narrow bands.

Several studies have analyzed inertial particle dynamics in either analytically defined or numerically generated fluid flows (cf. Refs. 1–11). These studies are based on the Maxey–Riley equations,[1] the equation of motion for small spherical particles in an unsteady nonuniform flow velocity field.

The first systematic attempt to predict particle clustering appears to be by Rubin *et al.*,[8] who study the settling of aerosol particles in a two-dimensional cellular flow field. Applying the results of singular perturbation theory, they show the existence of a globally attracting slow manifold to which inertial particle velocities converge. Reduction to the slow manifold coupled with a subharmonic Melnikov calculation reveals that particles will be attracted to (and hence cluster around) an attracting periodic path as they settle downward through a cellular flow field. Sedimentation patterns for Stokes particles in a weakly time-periodic flow have been studied by Angilella[12] using similar methods.

Burns *et al.*[10] investigate the motion of small, dilute spherical particles in the far wake of a bluff body flow model. Using the approach of Rubin *et al.*,[8] they show numerically the existence of a periodic attractor, i.e., the location of clustering in the wake. A more recent numerical study by Vilela *et al.*[13] visualizes the attractor around which heavy particles cluster in a time-periodic flow.

Haller and Sapsis[11] analyzed the dynamics of small inertial particles in a general 3D, unsteady fluid flow. They have derived a reduced-order inertial equation that governs the asymptotic motion of particles on a slow manifold. This leads to a rigorous criterion for clustering locations in two-dimensional steady flows.[11] Specifically, the clustering locations are zeros of a weighted average of Okubo–Weiss Q parameter (i.e., one-half of the squared difference of the vorticity and the rate of strain) taken along closed streamlines of the flow.

The objective of the present paper is to derive a general criterion for predicting inertial particle clustering in 3D steady velocity fields of the form

$$\mathbf{u}=(u(\mathbf{x}),v(\mathbf{x}),w(\mathbf{x})),\quad \mathbf{x}=(x,y,z)\in\mathbb{R}^3$$

and in two-dimensional time-periodic velocity fields of the form

$$\mathbf{u}=(u(\mathbf{x}),v(\mathbf{x}),\omega),\quad \mathbf{x}=(x,y,\phi)\in\mathbb{R}^2\times S^1. \tag{1}$$

The latter velocity field is also represented as 3D, including the third velocity component $\dot{\phi}=\omega$ in the 3D extended phase space of the spatial variables (x,y) and the phase variable ϕ on the standard unit circle S^1.

The main assumption we make is that the underlying fluid velocity field contains at least one closed two-dimensional stream surface. This certainly holds if $\mathbf{u}$ describes a 3D steady Euler flow in which the Beltrami condition does not hold, i.e., vorticity and velocity are never parallel. In this case, the flow is integrable and the flow domain is foliated by continuous families of stream surface diffeomorphic cylinders or tori.[14] Isolated closed stream surfaces will also exist in 3D nonintegrable flows; a well-known example is the nonintegrable Arnold–Beltrami–Childress (ABC) flow which has KAM (Kolmogorov–Arnold–Moser) tori.[14] Finally, KAM tori typically exist in two-dimensional, incompressible flows; their signature is a closed invariant curve for the associated Poincaré map.

Under the above assumption, we use the results of Haller and Sapsis[11] to reduce the full Maxey–Riley dynamics of small inertial particles to a 3D slow manifold. Given the existence of a closed stream surface S_0, we derive a necessary condition that guarantees the existence of a nearby particle attractor on the slow manifold. The criterion requires the integral of the normal component of the material derivative

$$\frac{D\mathbf{u}}{Dt} = \mathbf{u}_t + (\nabla\mathbf{u})\mathbf{u}$$

over S_0 to vanish for a nearby attractor S_ε to exist for particles of mass ε. The vanishing of this integral on S_0, therefore, predicts clustering on a nearby surface S_ε which is diffeomorphic to S_0.

For the special case when the fluid particle motion is dense in S_0, we use ergodic theory to reformulate our clustering criterion. The result is a simplified clustering criterion that only requires the evaluation of a line integral along a single fluid trajectory in S_0. This formulation is particularly helpful for numerically or experimentally generated velocity fields, where exact expressions for closed stream surfaces are not readily available, but individual fluid trajectories are simple to generate.

We illustrate our clustering criteria for inertial particles in Hill's spherical vortex flow, the ABC flow, and a flow model of a meandering jet in a channel with time-dependent perturbation.

To put our results in a broader perspective, we note that the clustering locations S_ε we identify in this paper are attracting ILCSs, as defined in Sapsis and Haller.[15] These attracting surfaces exist in the phase space of the inertial particle motion and depend on the size of the inertial particle. Sapsis and Haller[15] show how these structures can be located numerically using finite-time Lyapunov exponents. The present paper shows how ILCS can be located semianalytically in a 3D steady or two-dimensional time-periodic flow that admits closed stream surfaces.

II. FORMULATION

A. Equation of motion for inertial particles

Consider a particle p of density ρ_p immersed in a *steady* 3D fluid with velocity field

$$\mathbf{u}(\mathbf{x}) = (u(x,y,z), v(x,y,z), w(x,y,z)), \tag{2}$$

where the particle position $\mathbf{x}=(x,y,z)$ is taken from a bounded spatial domain $\mathcal{D}$. Let U be the characteristic velocity of the flow, ν the kinematic viscosity of the fluid, and $\mathrm{Re}=UL/\nu$ the Reynolds number. For a spherical particle in the flow having radius $a \ll L$, we denote with $\mathbf{x}(t)$ its position and with $\mathbf{v}(t)=\dot{\mathbf{x}}(t)$ its Lagrangian velocity.

We restrict our analysis to the dilute regime, where the particle concentration is sufficiently small for the interaction among particles and the effect of the particle motion on the fluid flow can be neglected. Under these conditions, the particle motion is dominated by the force exerted by the undisturbed flow, the Stokes drag, the added mass term resulting from part of the fluid moving with the particle, and the buoyancy force. The particle then satisfies the Maxey–Riley equation of motion (cf., e.g., Refs. 1, 16, and 17)

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{v}, \\ \epsilon\dot{\mathbf{v}} &= \mathbf{u}(\mathbf{x}) - \mathbf{v} + \epsilon\frac{3R}{2}\frac{D\mathbf{u}(\mathbf{x})}{Dt} + \epsilon\left(1 - \frac{3R}{2}\right)\mathbf{g}, \end{aligned} \tag{3}$$

where

$$\epsilon = \frac{1}{\mu} \ll 1, \quad \mu = \frac{R}{\mathrm{St}}, \quad R = \frac{2\rho_f}{\rho_f + 2\rho_p},$$

St is the Stokes number

$$\mathrm{St} = \frac{2}{9}\left(\frac{a}{L}\right)^2 \mathrm{Re},$$

and $\mathbf{g}$ is the constant vector of gravity.

Note that the larger the inertia parameter μ, the less significant the effect of inertia; in the $\mu \to \infty$ limit, Eq. (3) describes the motion of a passive ideal tracer particle. The density ratio R distinguishes neutrally buoyant particles ($R=2/3$) from aerosols ($0<R<2/3$) and bubbles ($2/3<R<2$). In what follows, we consider only non-neutrally buoyant particles, as neutrally buoyant particles cannot exhibit clustering.[11]

Using an extension of classic geometric singular perturbation ideas, Haller and Sapsis[11] proved that for $\epsilon>0$ small enough, Eq. (3) admits a globally attracting invariant slow manifold of the form

$$M_\epsilon = \left\{(\mathbf{x},\mathbf{v}_s) : \mathbf{v}_s = \mathbf{u}(\mathbf{x}) + \epsilon\left(\frac{3R}{2} - 1\right)\left[\frac{D\mathbf{u}(\mathbf{x})}{Dt} - \mathbf{g}\right] + \mathcal{O}(\epsilon^2)\right\}. \tag{4}$$

(The result is established for general 3D unsteady flows; here we only recall the results for 3D steady flows.)

A reduction in the dynamics to the slow manifold M_ϵ leads to the *inertial equation*

$$\dot{\mathbf{x}} = \mathbf{u}(\mathbf{x}) + \epsilon\left(\frac{3R}{2} - 1\right)\left[\frac{D\mathbf{u}(\mathbf{x})}{Dt} - \mathbf{g}\right] + \mathcal{O}(\epsilon^2). \tag{5}$$

Inertial particle motion will converge exponentially fast to the trajectories of the inertial equation (5), as long as the slow manifold is attractive. This is the case if ϵ is small enough to satisfy

$$\lambda_{\max}\left[-\frac{\nabla \mathbf{v}_s(\mathbf{x})+(\nabla \mathbf{v}_s(\mathbf{x}))^T}{2}\right]<\frac{1}{\epsilon} \tag{6}$$

for all $\mathbf{x}\in\mathcal{D}$ (cf. Refs. 18 and 19). Here $\lambda_{\max}[A]$ denotes the maximal eigenvalue of a tensor A. In the present paper, we assume that Eq. (6) holds over the whole domain $\mathcal{D}$.

The above results also hold for unsteady flows with the appropriate modifications. Specifically, for a two-dimensional velocity field $(u(x,y,\omega t),v(x,y,\omega t))$ that is $2\pi/\omega$-periodic in time, we let

$$\mathbf{x}=(x,y,\phi),\quad \mathbf{u}=(u(\mathbf{x}),v(\mathbf{x}),\omega) \tag{7}$$

and observe that the inertial equation (5) remains valid. As a result, particle trajectories of such two-dimensional flows approach asymptotically the trajectories of Eq. (5), as long as ϵ is small enough for condition (6) to hold on the domain of interest.

III. NECESSARY CONDITION FOR CLUSTERING

For the setting described above, we have the following main result—a necessary condition—for the location of inertial particle clustering. Assume that the 3D vector field $\mathbf{u}$ [defined as Eq. (2) or Eq. (7)] is incompressible, i.e., has zero divergence with respect to its arguments $\mathbf{x}$. Also assume that S_0 is a compact, two-dimensional stream surface for $\mathbf{u}$. Let us denote the outward unit normal of S_0 at point $\mathbf{x}$ by $\mathbf{n}(\mathbf{x})$. Then the following holds:

Theorem: *Assume that the 3D vector field* $\mathbf{u}$ *[defined as Eq. (2) or Eq. (7)] is incompressible, i.e., has zero divergence with respect to its arguments* $\mathbf{x}$. *Also assume that* S_0 *is a compact, two-dimensional stream surface for* $\mathbf{u}$. *Let us denote the outward unit normal of* S_0 *at point* $\mathbf{x}$ *by* $\mathbf{n}(\mathbf{x})$. *Then the following holds.*

(i) A necessary condition for the existence of an inertial particle attractor S_ϵ *that is* $O(\epsilon)$ C^1*-close to* S_0 *is the following:*

$$\int_{S_0}\frac{D\mathbf{u}}{Dt}\cdot\mathbf{n}\,dA=0,$$
$$(3R-2)\int_{S_0}\nabla\left[\frac{D\mathbf{u}}{Dt}\cdot\mathbf{n}\right]\cdot\mathbf{n}\,dA<0. \tag{8}$$

(ii) Assume that S_0 *is a two-dimensional torus filled densely with the trajectories of the system* $\dot{\mathbf{x}}=\mathbf{u}(\mathbf{x})$. *Let* $\boldsymbol{\xi}(t)$ *be one of these dense trajectories on* S_0. *Then condition (8) is equivalent to*

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T|\dot{\boldsymbol{\xi}}(t)|\left\{\frac{D\mathbf{u}}{Dt}\cdot\mathbf{n}\right\}_{\mathbf{x}=\xi(t)}dt=0,$$
$$\lim_{T\to\infty}\frac{3R-2}{T}\int_0^T|\dot{\boldsymbol{\xi}}(t)|\left\{\nabla\left[\frac{D\mathbf{u}}{Dt}\cdot\mathbf{n}\right]\cdot\mathbf{n}\right\}_{\mathbf{x}=\xi(t)}dt<0. \tag{9}$$

Proof: Let S_ϵ be a compact, two-dimensional, differentiable invariant manifold (i.e., a two-dimensional surface diffeomorphic to a sphere or a torus) for the inertial equation (5). Let S_ϵ vary smoothly for $\epsilon\geq 0$, as assumed in (i) above.

By the invariance of S_ϵ, the phase space volume enclosed by S_ϵ does not change in time. By Liouville's theorem (see, e.g., Ref. 20), this conservation of phase space volume can be expressed as

$$\frac{d}{dt}\text{volume}(S_\epsilon)=\int_{\text{int}(S_\epsilon)}\nabla\cdot\left[\mathbf{u}+\epsilon\left(\frac{3R}{2}-1\right)\left[\frac{D\mathbf{u}(\mathbf{x})}{Dt}-\mathbf{g}\right]+\mathcal{O}(\epsilon^2)\right]dV$$
$$=\frac{1}{2}\epsilon(3R-2)\int_{\text{int}(S_\epsilon)}\nabla\cdot\left[\frac{D\mathbf{u}}{Dt}+\mathcal{O}(\epsilon)\right]dV=0, \tag{10}$$

where we used the incompressibility of $\mathbf{u}$ and the notation $\text{int}(S_\epsilon)$ for the interior of S_ϵ.

Dividing by ϵ and taking the $\epsilon\to 0$ limit in Eq. (10), we obtain that

$$\int_{\text{int}(S_0)}\nabla\cdot\frac{D\mathbf{u}}{Dt}dV=0 \tag{11}$$

must hold for the compact stream surface S_0. Then an application of the divergence theorem to Eq. (11) proves the first condition in Eq. (8).

To prove the second condition, note that if S_ϵ is an attractor, then for any two-dimensional surface S_ϵ^+ that is C^1 close enough to S_ϵ and contains S_ϵ in its interior, we have $d[\text{volume}(S_\epsilon^+)]/dt<0$ under the flow of the inertial equation (5). Similarly, for any two-dimensional surface S_ϵ^- that is C^1 close enough to S_ϵ and is contained in the interior of S_ϵ, we have $d[\text{volume}(S_\epsilon^-)]/dt>0$. Therefore, if S_ϵ^δ is a smooth family of small deformations S_ϵ, such that each S_ϵ^δ is a C^1 graph over S_ϵ and

$$S_\epsilon^{-\delta}\subset S_\epsilon^0\equiv S_\epsilon\subset S_\epsilon^\delta$$

holds for any $\delta>0$, then we have

$$\frac{d}{d\delta}\left[\frac{d}{dt}\text{volume}(S_\epsilon^\delta)\right]_{\delta=0}<0, \tag{12}$$

since $d[\text{volume}(S_\epsilon^\delta)]/dt$ moves from positive to negative values when δ is increasing in the neighborhood of 0.

Again, applying Liouville's theorem to Eq. (12), we obtain

$$\frac{d}{d\delta}\left[\frac{d}{dt}\text{volume}(S_\epsilon^\delta)\right]_{\delta=0}=\frac{d}{d\delta}\left\{\int_{\text{int}(S_\epsilon^\delta)}\nabla\cdot\left[\mathbf{u}+\epsilon\left(\frac{3R}{2}-1\right)\left[\frac{D\mathbf{u}(\mathbf{x})}{Dt}-\mathbf{g}\right]+\mathcal{O}(\epsilon^2)\right]dV\right\}_{\delta=0}$$
$$=\frac{1}{2}\epsilon(3R-2)\frac{d}{d\delta}\left\{\int_{\text{int}(S_\epsilon^\delta)}\nabla\cdot\left[\frac{D\mathbf{u}}{Dt}+\mathcal{O}(\epsilon)\right]dV\right\}_{\delta=0}<0.$$

Dividing by $\epsilon>0$, taking the limit $\epsilon\to 0$, and applying the divergence theorem yields

$$\frac{1}{2}(3R-2)\frac{d}{d\delta}\left\{\int_{\mathrm{int}(S_0^\delta)}\nabla\cdot\frac{D\mathbf{u}}{Dt}dV\right\}_{\delta=0}$$
$$=\frac{1}{2}(3R-2)\frac{d}{d\delta}\left\{\int_{S_0^\delta}\frac{D\mathbf{u}}{Dt}\cdot\mathbf{n}dA\right\}_{\delta=0}<0. \tag{13}$$

We now select a particular surface family S_0^δ defined as

$$S_0^\delta=\{\mathbf{x}\in\mathcal{D}:\mathbf{x}=\mathbf{x}_0+\delta\mathbf{n}(\mathbf{x}_0),\ \ \mathbf{x}_0\in S_0\},$$

with $\mathbf{n}(\mathbf{x}_0)$ denoting the outward normal of S_0 at the point $\mathbf{x}_0\in S_0$. For this choice of the family S_0^δ, we can rewrite the second line of Eq. (13) as

$$\frac{1}{2}(3R-2)\frac{d}{d\delta}\left\{\int_{S_0^\delta}\frac{D\mathbf{u}}{Dt}\cdot\mathbf{n}dA\right\}_{\delta=0}$$
$$=\frac{1}{2}(3R-2)\frac{d}{d\delta}\left\{\int_{S_0}\frac{D\mathbf{u}(\mathbf{x}_0+\delta\mathbf{n}(\mathbf{x}_0))}{Dt}\cdot\mathbf{n}(\mathbf{x}_0+\delta\mathbf{n}(\mathbf{x}_0))dA\right\}_{\delta=0}$$
$$=\frac{1}{2}(3R-2)\int_{S_0}\frac{d}{d\delta}\left\{\frac{D\mathbf{u}(\mathbf{x}_0+\delta\mathbf{n}(\mathbf{x}_0))}{Dt}\cdot\mathbf{n}(\mathbf{x}_0+\delta\mathbf{n}(\mathbf{x}_0))\right\}_{\delta=0}dA$$
$$=\frac{1}{2}(3R-2)\int_{S_0}\left\{\nabla\left[\frac{D\mathbf{u}(\mathbf{x}_0+\delta\mathbf{n}(\mathbf{x}_0))}{Dt}\cdot\mathbf{n}(\mathbf{x}_0+\delta\mathbf{n}(\mathbf{x}_0))\right]\cdot\mathbf{n}(\mathbf{x}_0)\right\}_{\delta=0}dA$$
$$=\frac{1}{2}(3R-2)\int_{S_0}\nabla\left[\frac{D\mathbf{u}}{Dt}\cdot\mathbf{n}\right]\cdot\mathbf{n}dA.$$

Using this result in Eq. (13) proves the second condition in Eq. (8) and completes the proof of statement (i) of the theorem.

To prove statement (ii), we observe that if S_0 is a two-dimensional torus filled densely by trajectories of the inertial equation, then the flow of the inertial equation is ergodic on S_0 (see, e.g., Ref. 20). Consequently, the spatial averages in Eq. (8) taken over S_0 are equal to temporal averages over the same quantities taken over a single trajectory $\boldsymbol{\xi}(t)$ in S_0, weighted according to the modulus of the velocity $|\dot{\boldsymbol{\xi}}(t)|$ (see, e.g., Ref. 20). More specifically, we have

$$\int_{S_0}\frac{D\mathbf{u}}{Dt}\cdot\mathbf{n}dA=\lim_{T\to\infty}\frac{1}{T}\int_0^T|\dot{\boldsymbol{\xi}}(t)|\left\{\frac{D\mathbf{u}}{Dt}\cdot\mathbf{n}\right\}_{\mathbf{x}=\xi(t)}dt,$$

$$\int_{S_0}\nabla\left[\frac{D\mathbf{u}}{Dt}\cdot\mathbf{n}\right]\cdot\mathbf{n}dA=\lim_{T\to\infty}\frac{1}{T}\int_0^T|\dot{\boldsymbol{\xi}}(t)|\times\left\{\nabla\left[\frac{D\mathbf{u}}{Dt}\cdot\mathbf{n}\right]\cdot\mathbf{n}\right\}_{\mathbf{x}=\xi(t)}dt.$$

Substituting these expressions into statement (i) proves statement (ii) of the theorem.

We observe that gravity does not enter the clustering criterion. Hence, the main mechanism for clustering of non-neutrally buoyant, finite-size particles is due to their inertia which creates a spatially inhomogeneous perturbation to the velocity field that governs their motion [Eq. (5)] and leads to preferential concentration. This is consistent with other studies (see, e.g., Refs. 31 and 21–23) showing that inertial effects are those which induce clustering of finite-size particles.

We note that 3D incompressible flows that are invariant under the action of a volume-preserving symmetry group always admit a first integral B (cf. Ref. 24). If such a first integral exists for the inertial equation (5), then the normal $\mathbf{n}$ featured in the criteria (8) and (9) can be computed as

$$\mathbf{n}=\nabla B/|\nabla B|. \tag{14}$$

We also note that the second condition (inequality) in the criteria (i) and (ii) of the theorem can be relaxed. A close inspection of the proof of the theorem shows that it is enough for the functional

$$\mathcal{I}(S_0)=\int_{S_0}\frac{D\mathbf{u}}{Dt}\cdot\mathbf{n}dA$$

or

$$\mathcal{I}(S_0)=\lim_{T\to\infty}\frac{1}{T}\int_0^T|\dot{\boldsymbol{\xi}}(t)|\left\{\frac{D\mathbf{u}}{Dt}\cdot\mathbf{n}\right\}_{\mathbf{x}=\xi(t)}dt, \tag{15}$$

respectively, to change from positive to negative as one crosses S_0 from its interior toward its exterior. In other words, it is enough for S_0 to be a topologically transverse zero set for $\mathcal{I}(S_0)$—as opposed to a transverse zero set required by the inequalities in Eqs. (8) and (9). This observation makes the evaluation of our criteria simpler: instead of computing the inequalities in Eqs. (8) and (9), we simply compute the functional $\mathcal{I}(S_0)$, locate its compact, two-dimensional zero sets, and verify its sign inside and outside those zero sets.

Example: (Inertial particles in a point vortex). We will now illustrate the above criterion for a simple two-dimensional point vortex with velocity field given by

$$\mathbf{u}(\mathbf{x})=r\Omega(r)\vec{\mathbf{e}}_\theta,\qquad r=\sqrt{x^2+y^2}.$$

In this case, the fluid particle trajectories are circular. The material derivative of the velocity field vector is given by

$$\frac{D\mathbf{u}}{Dt}(\mathbf{x})=-r\Omega^2(r)\vec{\mathbf{e}}_r.$$

Therefore we will have

$$\int_{S_0}\frac{D\mathbf{u}}{Dt}\cdot\mathbf{n}dA=-2\pi r^2\Omega^2(r).$$

This expression vanishes at $r=0$ and becomes negative when $r>0$. According to our clustering criterion, therefore, centers of point vortices are clustering locations for bubbles.

IV. APPLICATIONS

In this section, we illustrate the criteria proved in the theorem for three different flows. We first consider Hill's spherical vortex problem which is an example of a 3D, steady, rotational solution of Euler's equation. Additionally, it admits a volume-preserving continuous symmetry group, hence the normal to stream surfaces can be computed from an appropriate first integral B, as shown in Eq. (14).

In the other two applications we consider, the normal vector $\mathbf{n}(\mathbf{x})$ is not known analytically, and hence has to be determined numerically. Specifically, in the second example we show how our criterion predicts the clustering location in a nonintegrable ABC flow. As a third application, we apply to predict clustering locations in a two-dimensional, temporally and spatially periodic model of a perturbed meandering jet in a channel.

A. Hill's spherical vortex

We consider the integrable case of a Hill's spherical vortex amended with a line vortex at the z-axis. The corresponding velocity field is given by (cf. Ref. 25)

$$\mathbf{u}(\mathbf{x}) = \begin{pmatrix} xz - 2cy/(x^2+y^2) \\ yz + 2cx/(x^2+y^2) \\ 1 - 2(x^2+y^2) - z^2 \end{pmatrix}. \quad (16)$$

We note that for $c \neq 0$ the velocity field is singular along the z-axis. Moreover, this flow generates (compact) toroidal stream surfaces inside the spherical stream surface $\{\mathbf{x} \in \mathbb{R}^3 : |\mathbf{x}| \leq 1\}$. We, therefore, restrict our analysis to the two-dimensional tori in the $|\mathbf{x}| \leq 1$ region.

As described by Haller and Mezić,[24] the velocity field (16) admits the first integral

$$B(x,y,z) = \tfrac{1}{2}(x^2+y^2) - \tfrac{1}{2}(x^2+y^2)^2 - \tfrac{1}{2}(x^2+y^2)z^2.$$

By Eq. (14), we therefore obtain that the unit normal to any two-dimensional stream surface of Eq. (16) can be written as

$$\mathbf{n}(\mathbf{x}) = \alpha \begin{pmatrix} x - 2x(x^2+y^2) - xz^2 \\ y - 2y(x^2+y^2) - yz^2 \\ -z(x^2+y^2) \end{pmatrix}, \quad (17)$$

where $\alpha > 0$ is an appropriate normalization factor to ensure that $|\mathbf{n}(\mathbf{x})| = 1$.

We use the expression (17) to evaluate the clustering criterion derived from Sec. III. Note that in the region $|\mathbf{x}| \leq 1$, a randomly selected initial condition will fall on a quasiperiodic invariant torus with probability one (resonant tori with nondense trajectories form a set of measure zero).

Therefore, we can calculate the formulation (ii) of our clustering criterion numerically for a grid of initial conditions within the unit sphere. This is because all initial conditions on the grid will be dense within their stream surfaces with probability one. For the integration of the flow field from a grid of initial conditions, we use a multistep algorithm, the variable-order Adams–Bashforth–Moulton PECE (predict-evaluate–correct-evaluate) solver (cf. Ref. 26), with integration tolerance of 10^{-6}.

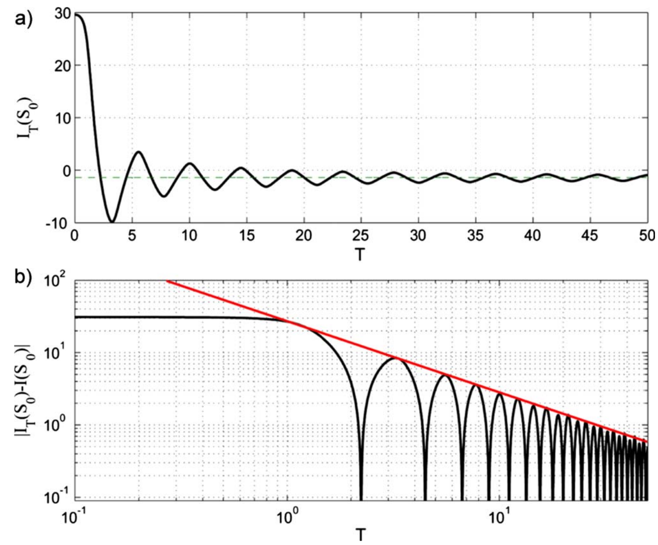

FIG. 1. (Color online) (a) Time series of the nonlinear functional $I_T(S_0,\mathbf{x}_0)$ for $c=0$ and initial condition $\mathbf{x}_0=(0.7216,0,0)^T$. (b) Rate of convergence of $I_T(S_0,\mathbf{x}_0)$.

We choose a set of initial conditions, each one lying on a different torus, and compute the corresponding trajectory for an integration time length $T=50$. Next, we calculate the corresponding value of

$$\mathcal{I}_T(S_0,\mathbf{x}_0) = \frac{1}{T}\int_0^T |\dot{\boldsymbol{\xi}}(t)| \left\{ \frac{D\mathbf{u}}{Dt} \cdot \mathbf{n} \right\}_{\mathbf{x}=\boldsymbol{\xi}(t)} dt \quad (18)$$

for each torus S_0 with $\boldsymbol{\xi}(0)=\mathbf{x}_0$. Note that $\mathcal{I}_T(S_0,\mathbf{x}_0)$ will be a good approximation of $\mathcal{I}(S_0)$ [see Eq. (15)] for large enough T. To avoid complications arising from the sign of the factor $(3R-2)$, we will use the quantities

$$I_T(S_0,\mathbf{x}_0) = \mathcal{I}_T(S_0,\mathbf{x}_0)/(3R-2),$$

$$I(S_0) = \mathcal{I}(S_0)/(3R-2)$$

to present our results.

In Fig. 1(a) we show the value of $I_T(S_0,\mathbf{x}_0)$ as a function of the integration time T for a typical case [$c=0$ and $\mathbf{x}_0=(0.7216,0,0)^T$]. In Fig. 1(b) the absolute error $|I_T(S_0,\mathbf{x}_0) - I(S_0)|$ is shown in a logarithmic scale. We observe that the convergence rate is of order $O(T^{-1})$, as predicted by the central limit theorem.

We will present our computations using a Poincaré map generated by the section $x=0$, superimposed by a color map that will represent the value of $I_T(S_0,\mathbf{x}_0)$ on every stream surface. Thus, closed curves on the Poincaré map will correspond to intersections of two-dimensional toroidal stream surfaces with the $x=0$ plane. If such a closed curve is the zero set $I_T(S_0,\mathbf{x}_0)$, and $I_T(S_0,\mathbf{x}_0)$ changes its sign from positive to negative as we cross the closed curve, then we will have a clustering location $O(\epsilon)$ C^1-close to S_0, as predicted by the theorem.

In Figs. 2(a), 2(c), and 3(a) we show the corresponding plots for three cases of the vortex strength, namely, $c=0$, 1, and 0.15.

We also present $I_T(S_0,\mathbf{x}_0)$ as a function of the first integral $B(\mathbf{x}_0)$. Note that $B(\mathbf{x})$ attains its minimum value $B(\mathbf{x})=0$

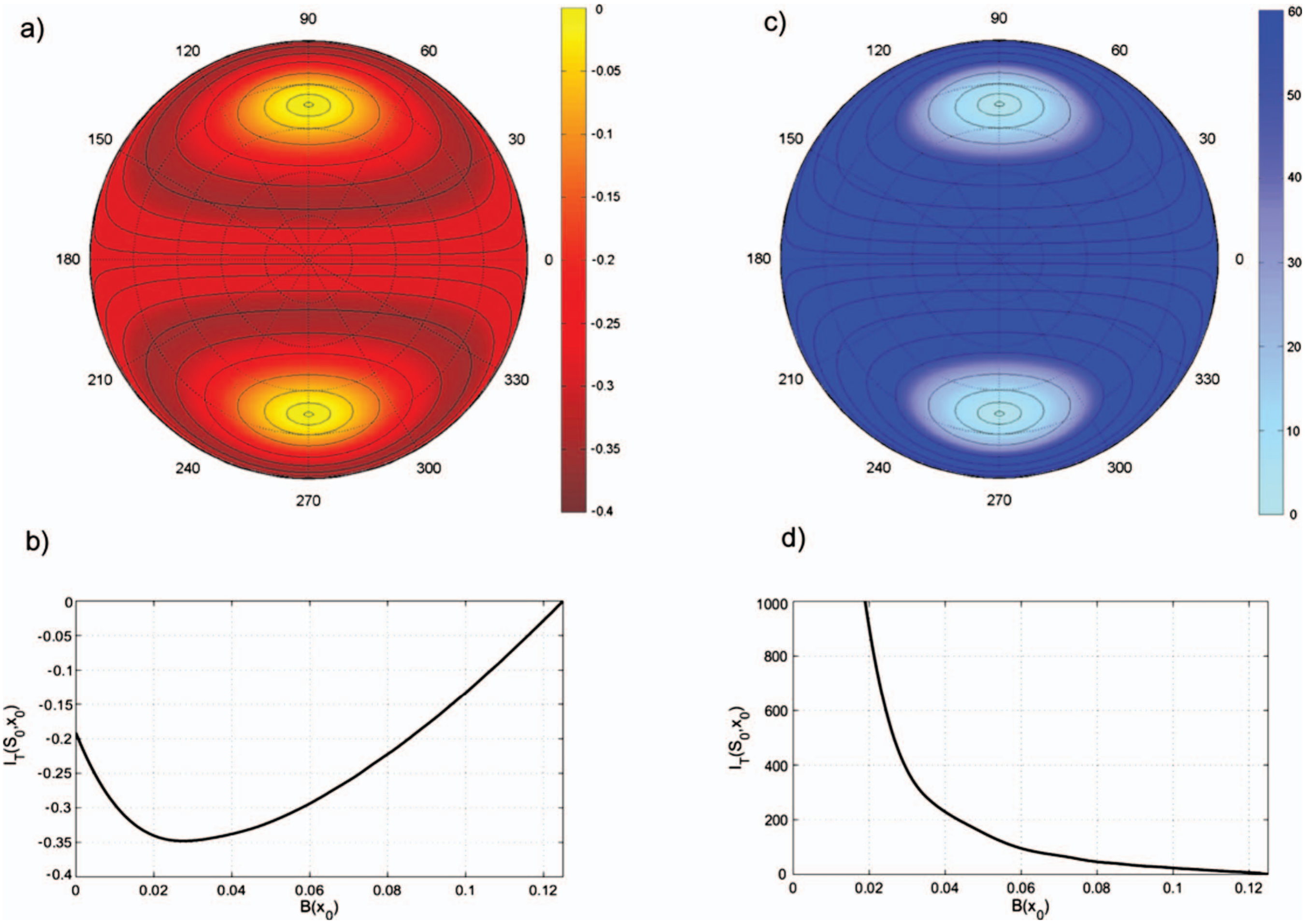

FIG. 2. (Color) (a) Poincaré section at $x=0$ of the Hill's spherical vortex for $c=0$. The color map represents the values of the functional $I_T(S_0,\mathbf{x}_0)$. (b) The nonlinear functional $I_T(S_0,\mathbf{x}_0)$ as a function of $B(\mathbf{x}_0)$ for $c=0$. (c) Poincaré section at $x=0$ and I_T-color map for $c=1$. (d) $I_T(S_0,\mathbf{x}_0)$ as a function of $B(\mathbf{x}_0)$ for $c=1$.

at the separatrix $\{|\mathbf{x}|=1\}\cup\{x^2+y^2=0,\ |z|<1\}$ and its maximum value $B(\mathbf{x})=\frac{1}{8}$ at the degenerate stream surface $\mathbf{x}_c(t)=(1/\sqrt{2}\sin t, 1/\sqrt{2}\cos t, 0)$.

We observe that in cases $c=0$ and $c=1$, there will be no two-dimensional clustering surface as $I_T(S_0,\mathbf{x}_0)\neq 0$ holds for all closed curves in the Poincaré map. However, for all three cases there is a pair of points on the Poincaré map at $\mathbf{p}_c=\pm(0,1/\sqrt{2})$ for which $I_T=0$. These points correspond to the closed streamline $\mathbf{x}_c(t)$ which always persist as a one-dimensional attractor for inertial particles. Moreover, as it can be deduced from the color around $\mathbf{p}_c$ that this closed streamline will attract bubbles $(2/3<R<2)$ when $c=0$ and $c=0.15$, it will, however, attract aerosols $(0<R<2/3)$ when $c=1$.

For $c=0.15$ [Figs. 3(a) and 3(b)], we observe a closed invariant curve of the Poincaré map on which I_T vanishes. As a result, the theorem gives a necessary condition for the existence of a two-dimensional surface where inertial particles will cluster. Indeed, the color distribution close to the closed curve in the Poincaré map suggests that the persistent stream surface will attract aerosols $(0<R<2/3)$.

We verify the above prediction by solving numerically the inertial equation (5) and constructing the Poincaré map for aerosols for which $\epsilon(3R/2-1)=-0.01$ [red dots—Fig. 3(c)].

B. ABC flow

The stream surfaces of nonintegrable steady flows will typically exhibit complex geometry, which will not allow us to express analytically the stream surfaces. A typical example is the ABC flow, a simple steady-state solution of Euler's equations.

Dombre *et al.*[27] observed that for most parameter values, the ABC flow admits a set of closed helical streamlines which are surrounded by a finite region of KAM tori. In McLaughlin[21] the effect of inertia on particle motion in the ABC flow was studied using Poincaré maps and it was shown that for this case chaotic behavior is suppressed. Here we will apply the main theorem to seek clustering surfaces for inertial particles near the toroidal stream surfaces of the fluid flow.

For the ABC flow the velocity field is given by

$$\mathbf{u}(\mathbf{x})=\begin{pmatrix} A\sin z + C\cos y \\ B\sin x + A\cos z \\ C\sin y + B\cos x \end{pmatrix}. \tag{19}$$

As stream surfaces are not available analytically for this flow, we will compute the normal $\mathbf{n}$ appearing in our clustering criteria by exploiting the ergodic property of the flow

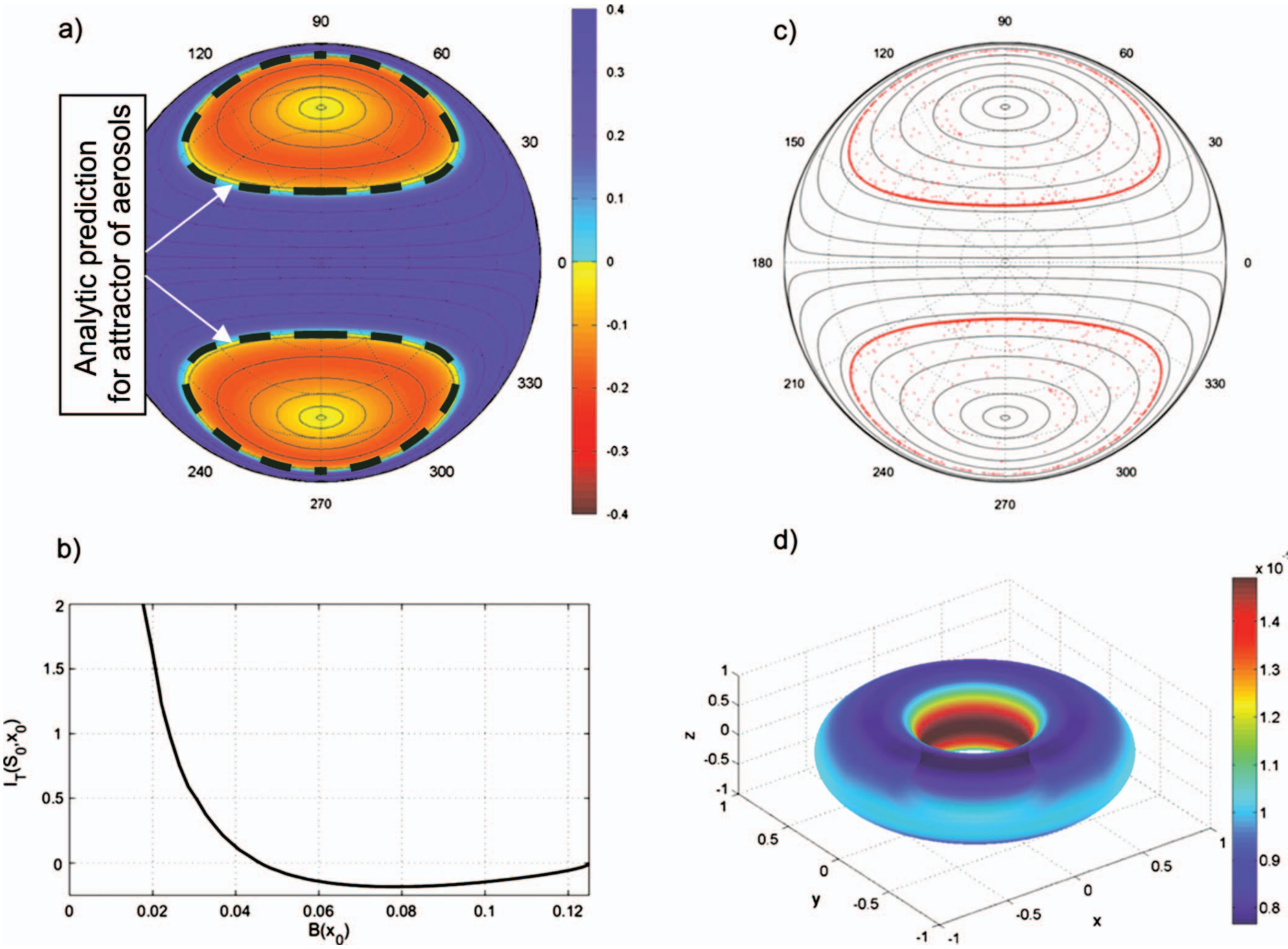

FIG. 3. (Color) (a) Poincaré section at $x=0$ of the Hill's spherical vortex for $c=0.15$. The color map represents the values of the functional $I_T(S_0,\mathbf{x}_0)$. (b) $I_T(S_0,\mathbf{x}_0)$ as a function of $B(\mathbf{x}_0)$ for $c=0.15$. (c) Poincaré map of an inertial particle trajectory computed using the inertial equation (5). (d) Persistent stream surface for inertial particles.

on an invariant surface S_0. Specifically, we express the normal vector $\mathbf{n}$ as

$$\mathbf{n}_T(\boldsymbol{\xi}(t,\mathbf{x}_0)) = \alpha\mathbf{u}(\boldsymbol{\xi}(t,\mathbf{x}_0)) \times [\boldsymbol{\xi}(t,\mathbf{x}_0) - \boldsymbol{\xi}(s,\mathbf{x}_0)], \qquad (20)$$

where $\alpha>0$ is a normalization constant such that $|\mathbf{n}(\mathbf{x})|=1$ and $s\in[0,T]$ is defined as

$$s = \delta_t^{-1}\Big[\inf_{|\tau-t|>\theta}\|\boldsymbol{\xi}(t,\mathbf{x}_0) - \boldsymbol{\xi}(\tau,\mathbf{x}_0)\|\Big]$$

with $\delta_t(s)\equiv\|\boldsymbol{\xi}(t,\mathbf{x}_0)-\boldsymbol{\xi}(s,\mathbf{x}_0)\|$, and θ is the characteristic time for a particle to run over a typical diameter d_{S_0} of S_0 (Fig. 4). In this case, the ergodic property of the flow and the central limit theorem guarantee that $\|\mathbf{n}_T(\mathbf{x})-\mathbf{n}(\mathbf{x})\|\to 0$ as $T\to\infty$, with rate of convergence of order $O(T^{-1})$.

We consider the case $A^2=1$, $B^2=\frac{2}{3}$, $C^2=\frac{1}{3}$ studied by Dombre *et al.*[27] For this choice of parameters, the phase space is divided into ordered and chaotic regions, hence the flow is not integrable. We first compute the Poincaré section defined by the plane $z=\pi$, then calculate the integral I_T (with $T=50$) over the ordered regions where some closed stream surfaces exist. Based on our earlier discussion, we calculate I_T from Eq. (18) for all initial conditions we consider; the result, however, will only be relevant for our clustering criterion if the initial condition falls on a KAM torus.

In Fig. 5(a), we present the Poincaré map for the flow, superimposed with a color map for the value of I_T on every closed stream surface. Note that there is a pair of closed stream surfaces that satisfy the necessary condition for the existence of a nearby inertial clustering surface.

Additionally, there are two points in the Poincaré map at which $I_T=0$. These points correspond to a pair of closed streamlines that give rise to nearby one-dimensional clustering locations (line attractors) for inertial particles. From the distribution of the values I_T we conclude that the two-

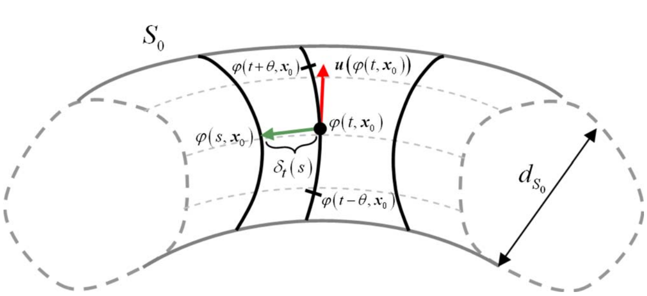

FIG. 4. (Color online) Numerical calculation of the normal vector $\mathbf{n}(\mathbf{x})$.

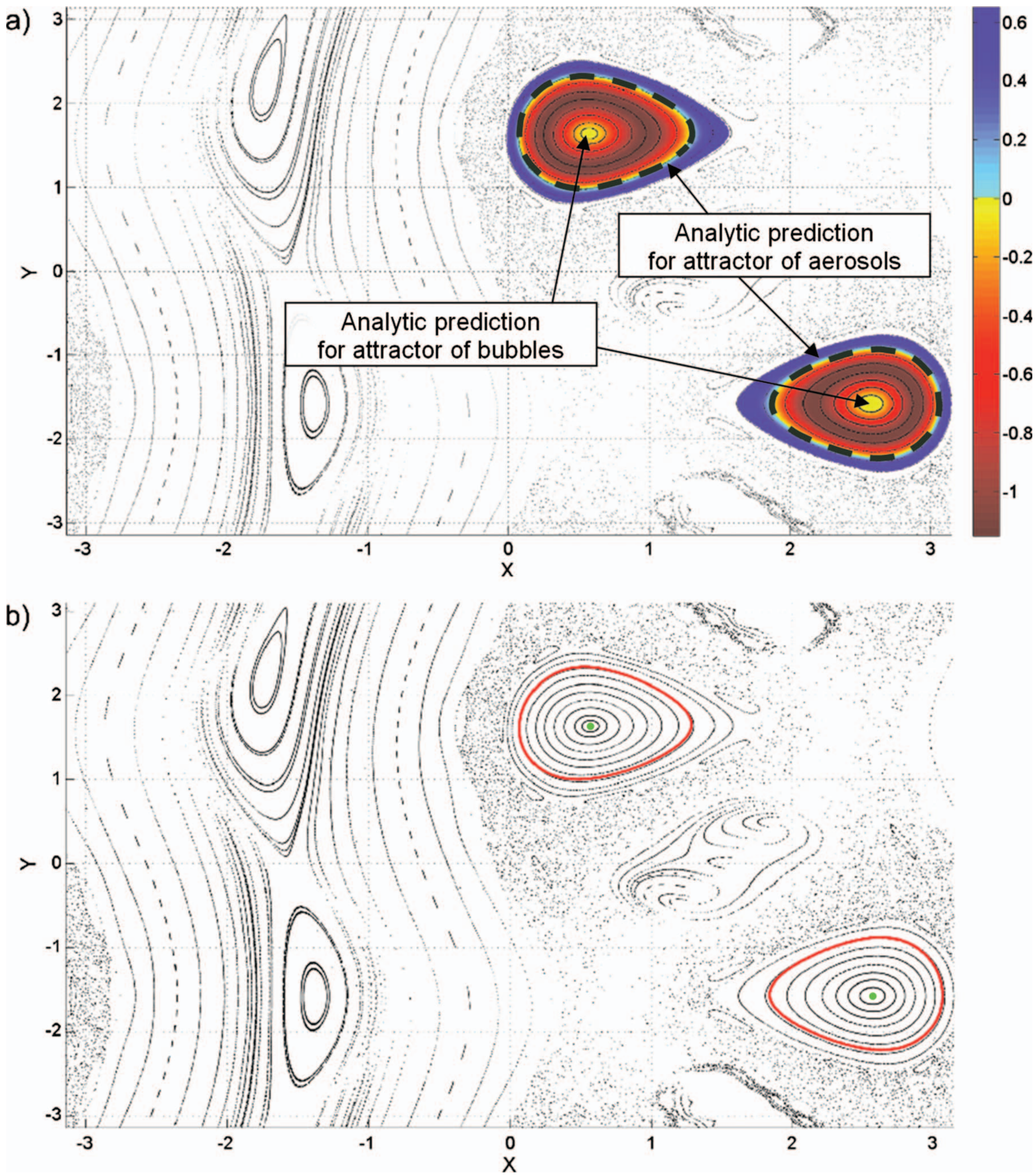

FIG. 5. (Color) (a) Poincaré map of the ABC flow. At any given point, the color refers to the computed value of I_T on the trajectory starting from that point. (b) The stream surface that attracts inertial particles obtained by the direct numerical solution of the inertial equation for $\epsilon(3R/2-1)=-0.01$.

dimensional clustering surface will attract aerosols $(0<R<2/3)$ while the one-dimensional clustering surface will attract bubbles $(2/3<R<2)$.

We verify the results by the direct numerical solution of the inertial equation (5); we present the Poincaré map for aerosols and bubbles with $|\epsilon(3R/2-1)|=0.01$ as red and green dots, respectively [Fig. 5(b)]. Finally, in Fig. 6 we present the persistent clustering surfaces colored according to the modulus of the velocity $|\mathbf{v}_s(\mathbf{x})|$ (red regions indicate intense velocity).

C. Traveling wave in a channel

In our final example, we study the dynamics of inertial particles in a periodically perturbed, traveling wave in a channel. For this problem the stream function that describes the flow in a reference frame (x,y) moving with the primary wave is given by

$$\psi(x,y,t) = -cy + A \sin kx \sin y + \sigma y \sin \omega t,$$
$$(x,y) \in S^1 \times [0,\pi],$$

where $A>0$ is the amplitude, k is the x-wave number, c determines the speed of propagation of the sinusoidal wave form, and σ, ω are the amplitude and frequency, respectively, of the time-periodic perturbation (cf. Refs. 28 and 29).

If $\sigma=0$ and c is chosen appropriately, the above stream function is an exact solution of the barotropic vorticity

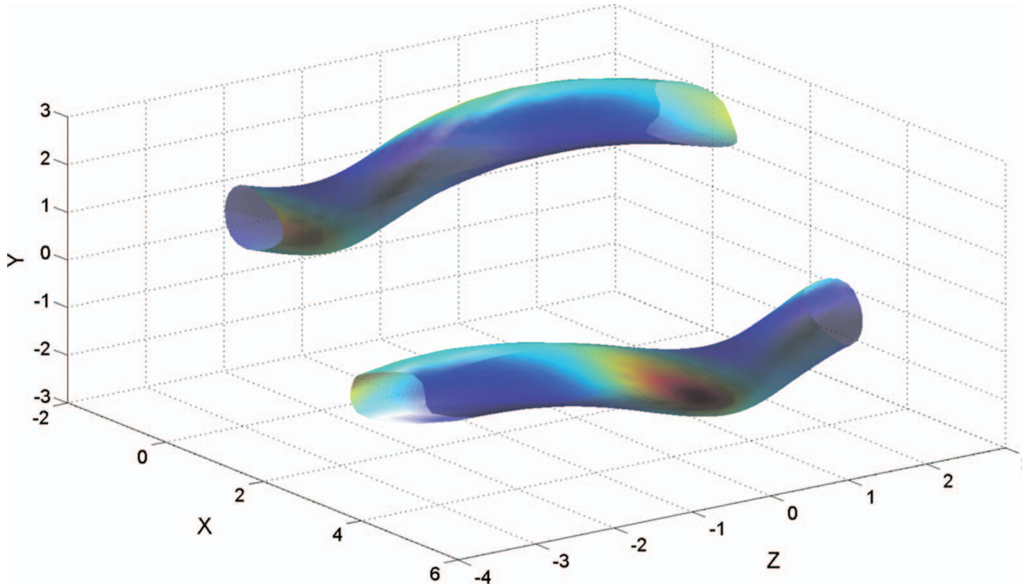

FIG. 6. (Color) Clustering surface for inertial particles colored according to the modulus of the velocity $|\mathbf{v}_s(\mathbf{x})|$.

equation[30] in a channel with rigid boundaries at $y=0$ and $y=\pi$. The equations for the fluid trajectories in the comoving (x,y) frame are

$$\dot{x} = u(x,y,\omega t) = c - A \sin kx \cos y - \sigma \sin \omega t,$$

$$\dot{y} = v(x,y,\omega t) = Ak \cos kx \sin y.$$

The relevant notation for our clustering theory to bear on this flow is given in Eq. (7). For $\sigma=0$, the flow is integrable. In what follows, however, we will consider the case of nonzero σ where integrability is lost. Specifically, we choose the parameters $A=1$, $k=1$, $c=0.5$, $\sigma=0.02$, and $\omega=1$. For this choice, the flow has both chaotic and ordered regions shown in the Poincaré map (Fig. 7). As in the case of the ABC flow, the unit normal vector $\mathbf{n}(\mathbf{x})$ on the invariant surfaces of the extended velocity field $\mathbf{u}=(u(\mathbf{x}),v(\mathbf{x}),\omega)$ cannot be expressed analytically; we will again compute the normal numerically using expression (20).

In Fig. 7(a) we present the calculation of the nonlinear functional $I_T(S_0,\mathbf{x}_0)$ for the ordered regions of the Poincaré map. For the closed circulation regions we observe that $I_T(S_0,\mathbf{x}_0)$ vanishes only at the centers. Moreover, the sign of $I_T(S_0,\mathbf{x}_0)$ indicates that aerosols will always be repelled by the circulation regions, while bubbles will cluster at the centers.

For the jet region, we observe that there is an invariant manifold, a two-dimensional torus, on which the functional $I_T(S_0,\mathbf{x}_0)$ vanishes. The signs of $I_T(S_0,\mathbf{x}_0)$ around this manifold indicate that a nearby clustering surface exists for aerosols.

In Fig. 7(b) we present the Poincaré map for the flow along with the Poincaré map of the inertial equation for two cases of inertial particles: aerosols (red dots) and bubbles (green dots). We observe that the actual clustering locations compare favorably with the predicted ones for both the aerosols and the bubbles. Note that a similar attractor has also been observed by Maxey and Corrsin,[31] where the case of heavy particles in a randomly oriented cell flow was considered in the presence of gravity.

V. CONCLUSIONS

We have derived a criterion that predicts the location of clustering for two-dimensional time-periodic flows and 3D steady flows. Our criterion assumes that the clustering location is a compact surface that deforms smoothly with the particle inertia, which is considered small in this work.

Our theorem provides a necessary condition for existence on a smooth clustering surface, i.e., an ILCS. The necessary condition involves the computation of the projection of the material derivative of the fluid flow on the unit normal of a stream surface. If the average of this quantity (take over a compact stream surface) changes from positive to negative as one crosses a stream surface S_0 toward its exterior, then a nearby clustering surface exists for small enough inertial particles. The clustering surface will be a small deformation of S_0.

For toroidal stream surfaces that are filled densely with fluid trajectories, our criterion can be reformulated using a temporal average instead of a stream surface average. This formulation is particularly useful for nonintegrable fluid flows where analytical expressions for stream surfaces are not available.

We have applied our results to the Hill's spherical vortex amended with a line vortex at the z-axis. We have obtained that for certain parameters, a toroidal surface exists which attracts aerosols, while bubbles are attracted by the single closed streamline that is contained in the flow.

We have also considered the ABC flow with parameters away from integrability. For this case, we described a numerical method for the calculation of the unitary normal vec-

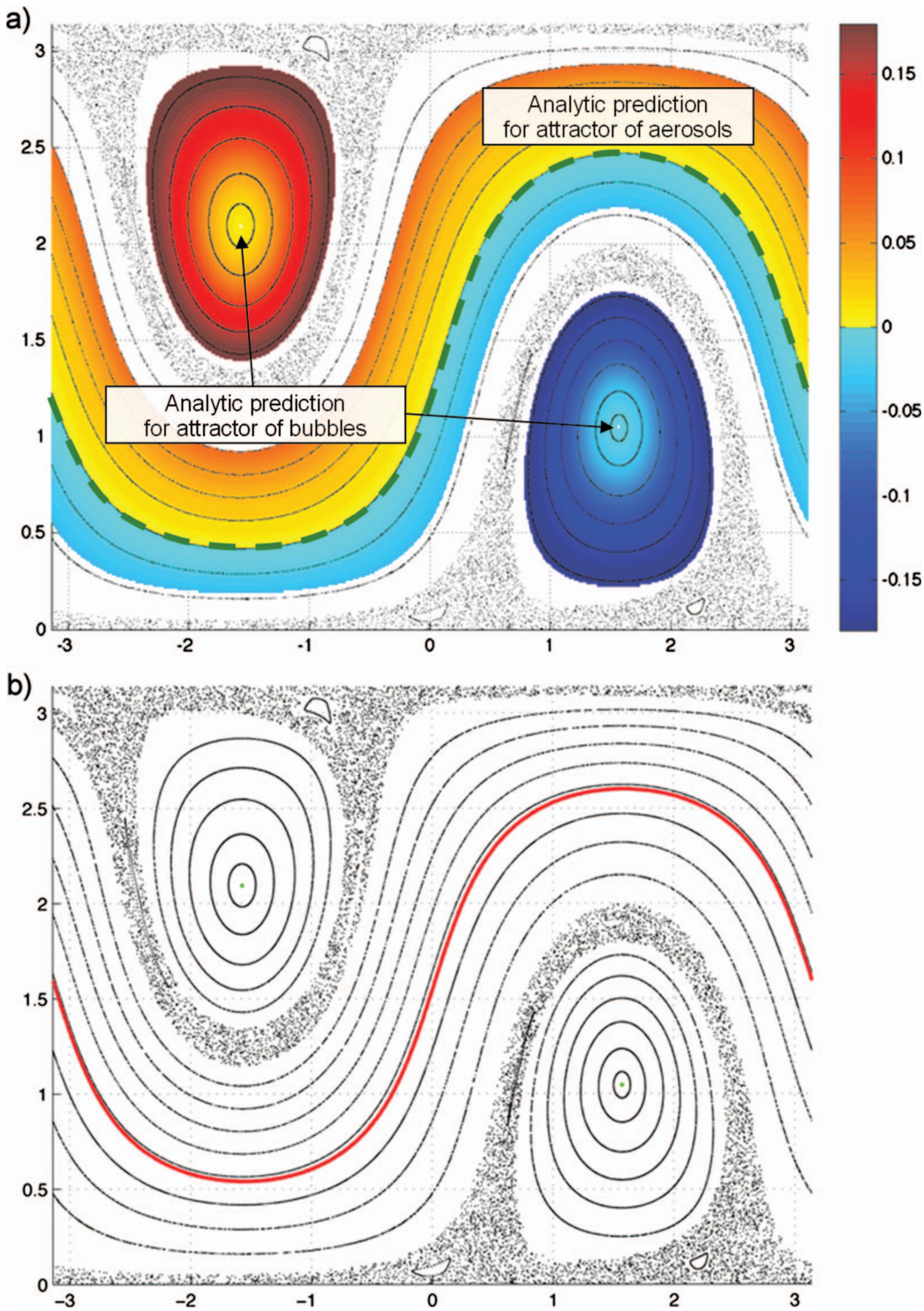

FIG. 7. (Color) (a) Poincaré map for the traveling wave in a channel with parameters $A=1$, $k=1$, $c=0.5$, $\sigma=0.02$, and $\omega=1$; the color refers to the value of I_T on closed stream surfaces. (b) Poincaré maps illustrating the invariant manifolds that attract inertial particles obtained from the numerical solution of the inertial equation for $|\epsilon(3R/2-1)|=0.01$ and for both aerosols (red dots) and bubbles (green dots).

tor using a single nonresonant trajectory. Our criterion in this case predicts the existence of a pair of clustering surfaces for aerosols and a pair of clustering lines for bubbles.

Finally, we have applied the criterion to a two-dimensional time-periodic model of a meandering jet in a channel. In this example, as well as in the other, too, we confirmed the predicted clustering manifolds by direct numerical simulations of the inertial particle equations of motion.

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[1]M. Maxey and J. Riley, Phys. Fluids **26**, 883 (1983).
[2]L. Tang, F. Wen, Y. Yang, C. Crowe, J. Chung, and T. Troutt, Phys. Fluids A **4**, 2244 (1992).
[3]K.-K. Tio, A. Liñán, J. Lasheras, and A. Gañán-Calvo, J. Fluid Mech. **254**, 671 (1993).
[4]B. Marcu, E. Meiburg, and P. Newton, Phys. Fluids **7**, 400 (1995).
[5]J. Martin and E. Meiburg, Phys. Fluids **6**, 1116 (1994).
[6]B. Marcu and E. Meiburg, Phys. Fluids **8**, 715 (1996).
[7]A. A. Vasiliev and A. I. Neishtadt, Chaos **4**, 673 (1994).
[8]J. Rubin, C. K. R. T. Jones, and M. Maxey, J. Nonlinear Sci. **5**, 337 (1995).
[9]C. Crowe, T. Troutt, and J. Chung, Annu. Rev. Fluid Mech. **28**, 11 (1996).
[10]T. Burns, R. Davis, and E. Moore, J. Fluid Mech. **384**, 1 (1999).
[11]G. Haller and T. Sapsis, Physica D **237**, 573 (2008).
[12]J. R. Angilella, Phys. Fluids **19**, 073302 (2007).
[13]R. Vilela, T. Tél, A. P. S. de Moura, and C. Grebogi, Phys. Rev. E **75**, 065203(R) (2007).
[14]V. I. Arnold and B. Keshin, *Topological Methods in Hydrodynamics* (Springer, New York, 1998).
[15]T. Sapsis and G. Haller, J. Atmos. Sci. **66**, 2481 (2009).
[16]I. J. Benczik, Z. Toroczkai, and T. Tél, Phys. Rev. Lett. **89**, 164501 (2002).
[17]A. Babiano, J. H. E. Cartwright, O. Piro, and A. Provenzale, Phys. Rev. Lett. **84**, 5764 (2000).
[18]T. Sapsis and G. Haller, Phys. Fluids **20**, 017102 (2008).
[19]G. Haller and T. Sapsis, "Normally stable and unstable subsets of invariant manifolds," SIAM J. Appl. Dyn. Syst. (to be published).
[20]Y. A. G. Sinai, *Introduction to Ergodic Theory* (Princeton University Press, Princeton, 1976).
[21]J. B. McLaughlin, Phys. Fluids **31**, 2544 (1988).
[22]R. Vilela and A. Motter, Phys. Rev. Lett. **99**, 264101 (2007).
[23]J. R. Angilella, Phys. Rev. E **78**, 066310 (2008).
[24]G. Haller and I. Mezić, Nonlinearity **11**, 319 (1998).
[25]M. J. M. Hill, Philos. Trans. R. Soc. London, Ser. A **185**, 213 (1894).
[26]L. F. Shampine and M. K. Gordon, *Computer Solution of Ordinary Differential Equations: The Initial Value Problem* (Freeman, San Francisco, 1975).
[27]T. Dombre, U. Frisch, J. M. Greene, M. Hinon, A. Mehr, and A. M. Soward, J. Fluid Mech. **167**, 353 (1986).
[28]E. Knobloch and J. Weiss, Phys. Rev. A **36**, 1522 (1987).
[29]R. Samelson and S. Wiggins, *Lagrangian Transport in Geophysical Jets and Waves* (Springer, New York, 2006).
[30]R. Pierrehumbert, Geophys. Astrophys. Fluid Dyn. **58**, 285 (1991).
[31]M. Maxey and S. Corrsin, J. Atmos. Sci. **43**, 1112 (1986).