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Citation for published version (APA):

DOI:
10.1063/1.4819901

Document status and date:
Published: 01/01/2013

Document Version:
Publisher's PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:
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Citation: Phys. Fluids 25, 093602 (2013); doi: 10.1063/1.4819901
View online: http://dx.doi.org/10.1063/1.4819901
View Table of Contents: http://pof.aip.org/resource/1/PHFLE6/v25/i9
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Three-dimensional Lagrangian transport phenomena in unsteady laminar flows driven by a rotating sphere

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(Received 14 February 2013; accepted 16 August 2013; published online 11 September 2013)

Magnetic actuation of microscopic beads is a promising technique for enhancement and manipulation of scalar transport in micro-fluidic systems. This implies laminar and essentially three-dimensional (3D) unsteady flow conditions. The present study addresses fundamental transport phenomena in such configurations in terms of 3D coherent structures formed by the Lagrangian fluid trajectories in a 3D time-periodic flow driven by a rotating sphere. The flow field is represented by an exact Stokes solution superimposed by a nonlinear closed-form perturbation. This facilitates systematic “activation” and exploration of two fundamental states: (i) invariant spheroidal surfaces accommodating essentially 2D Hamiltonian dynamics; (ii) formation of intricate 3D coherent structures (spheroidal shells interconnected by tubes) and onset to 3D dynamics upon weak perturbation of the former state. Key to the latter state is emergence of isolated periodic points and the particular foliation and interaction of the associated manifolds, which relates intimately to coherent structures of the unperturbed state. The occurrence of such fundamental states and corresponding dynamics is (qualitative) similar to findings on a realistic 3D lid-driven flow subject to weak fluid inertia. This implies, first, a universal response scenario to weak perturbations and, second, an adequate representation of physical effects by the in essence artificial perturbation. The study thus offers important new insights into a class of flow configurations with great practical potential.

I. INTRODUCTION

Scope of the present study is manipulation and enhancement of transport of scalar quantities (chemical species, pathogens, nutrients, and proteins) in micro-fluidic systems via magnetically actuated beads. This is a promising technique for application in emerging diagnostic and biosensing technologies.1–5 Fundamental to micro-fluidic transport, notwithstanding the diversity in systems, is that it happens under laminar flow conditions.6–8 Moreover, given that bead actuation typically involves sequences of rotations and translations in multiple directions, transport in the current class of systems is essentially three-dimensional (3D) and unsteady. However, insight into 3D laminar transport, despite considerable advancement since the mid-1980s, remains limited to date.9 Progress in micro-fluidics technologies may strongly benefit from better understanding of its underlying mechanisms, though. This motivates our study, which aims at deepening insight into 3D laminar transport in the particular context of 3D micro-flows driven by actuated beads.

Transport is investigated in terms of tracers that are passively advected by the flow. This enables topological analyses based on 3D coherent structures formed by Lagrangian fluid trajectories and has found application in a great variety of 3D transport problems.10–20 Such structures geometrically determine the transport properties and insight into their formation, characteristics and response to parametric variations is key to better understanding — and, ultimately, systematic manipulation — of 3D transport. The traditional objective is accomplishment of efficient mixing, which here
becomes synonymous with chaotic advection and absence of certain coherent structures (i.e., transport barriers). However, manipulation of coherent structures in principle admits functionalities beyond mixing (e.g., systematic compartmentalization of flow domains by controlled emergence of transport barriers). Such multi-functionality has particular potential for advanced micro-fluidic applications. Hence, our study, instead of concentrating on mixing alone, concerns flow topology versus 3D transport in general in bead-driven micro-flows.

The configuration investigated here consists of a 3D laminar flow in an unbounded domain set in motion by a rotating solid sphere. Three-dimensionality and unsteadiness (two key elements of realistic bead-driven flows) are introduced by time-periodic reorientations of a steady base flow due to rotation about a fixed axis. Transport is studied via numerical simulation of tracer advection, employing an exact solution to the Stokes limit superimposed by a nonlinear analytical perturbation. The latter emulates nonlinear effects by, e.g., weak fluid inertia and is essential to attain the rich dynamics characteristic of 3D systems. Important to note is that the analytical perturbation, though strictly artificial and in violation of momentum conservation, adequately represents physical phenomena. This is substantiated by fundamental similarities between the (perturbed) analytical flow and a realistic 3D flow subject to weak fluid inertia. (This is elaborated hereafter.) Thus the adopted approach admits efficient and accurate analysis of 3D Lagrangian transport phenomena without compromising physical relevance.

The exposition is organized as follows. The model problem is introduced in Sec. II. Fundamental dynamical states of time-periodic sphere-driven flows are demonstrated in Sec. III. The flow topologies for the essentially 2D and 3D cases are addressed in Secs. IV and V, respectively. Conclusions are given in Sec. VI.

II. MODEL DESCRIPTION

A. Introduction

The present study considers 3D time-periodic flow in an unbounded domain, driven by a rotating solid sphere (radius $R$ and angular velocity $\Omega$) with step-wise reorientation of the rotation axis via some forcing protocol (Figure 1(a)). The flow dynamics is characterized by the Reynolds number $\text{Re} = \Omega R^2/\nu$ and Strouhal number $\text{Sr} = \tau_d/\tau$, with $R$ and $\Omega$ as before, $\nu$ the kinematic viscosity, $\tau$ the time-period of the forcing, and $\tau_d = R^2/\nu$ the diffusion time scale. Typical bead radii in biosensor/microfluidic applications are $R \sim O(5 \mu \text{m})$, angular velocities $\Omega \sim O(2\pi \text{ rad/s})$, time scales $\tau \sim O(\Omega^{-1})$, and water as working fluid$^{2-5}$ yield $\text{Re} \sim O(10^{-4})$ and $\text{Sr} \sim O(10^{-4})$. This admits approximation by $\text{Re} = 0$ (Stokes limit) and $\text{Sr} = 0$ (instantaneous adjustment of the flow to reorientation of the rotation axis of the sphere) and implies that the time-periodic flow

$$u(x, t) = u(x, t + \tau)$$

FIG. 1. Schematic of the base-flow configuration (a) and typical Poincaré sections of the corresponding tracer dynamics (b). Spherical fluid layers $\tilde{r} = \text{constant}$ perform solid-body rotation at layer-dependent rotation axes and angular velocities. Left and right panels in (b) show layer-wise circular tracer orbits at $\tilde{r}_0 = 1.5$ and $\tilde{r}_0 = 2.0$, respectively, for the same forcing protocol. Arrows indicate rotation axes.
is composed of successive reorientations of a steady base flow governed by the incompressible steady Stokes equations
\[ 0 = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u}, \quad \nabla \cdot \mathbf{u} = 0, \tag{2} \]
with \( \rho \) the fluid density and \( p \) the pressure. Base flow and resulting time-periodic flow are treated in more detail in Secs. II B and II C, respectively.

The corresponding Lagrangian motion of passive tracer particles is governed by the kinematic equation
\[ \frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}, t), \quad \mathbf{x}(0) = \mathbf{x}_0 \quad \Rightarrow \quad \mathbf{x}(t) = \Phi_t(\mathbf{x}_0), \tag{3} \]
where \( \mathbf{x}(t) \) and \( \mathbf{x}_0 \) are the current and initial tracer position, respectively. The formal solution \( \Phi_t \) describes the continuous Lagrangian flow of the tracer particle, with \( \mathcal{X}(\mathbf{x}_0, t) = \{ \Phi_t(\mathbf{x}_0) \mid 0 \leq \xi \leq t \} \) its corresponding trajectory connecting \( \mathbf{x}_0 \) and \( \mathbf{x}(t) \). These trajectories identify with fluid trajectories and streamlines for unsteady and steady flows, respectively, in the present case of passive tracers.

For time-periodic flows \( \mathbf{u} \) according to (1) the flow \( \Phi_t \) admits an alternative representation as a map
\[ \mathbf{x}_{n+1} = \Phi_T(\mathbf{x}_n) = \Phi^*_{n+1}(\mathbf{x}_0), \quad \mathbf{x}_n \equiv \mathbf{x}(nT), \quad \Phi_T \equiv \int_0^T \mathbf{u}(\mathbf{x}(\xi), \xi) d\xi, \tag{4} \]
which directly links consecutive tracer positions after each cycle. The set of these tracer positions, i.e., \( \mathcal{X}_n(\mathbf{x}_0) \equiv \{ \mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_n, \mathbf{x}_{n+1} \} \), gives the discrete representation of the underlying fluid trajectory \( \mathcal{X} \) as if illuminated by a stroboscope synchronized with the periodicity of the flow. This "stroboscopic picture" \( \mathcal{X}_n \) defines the so-called Poincaré section of a tracer trajectory and will play a key role in the analysis of tracer dynamics hereafter.

### B. Base flow

Define the base flow \( \mathbf{u} \) as the steady flow governed by (2) due to rotation of the sphere about the \( z \)-axis. This implies boundary conditions \( \mathbf{u}|_{r=R} = \Omega \mathbf{e}_\theta \), with radii \( r = \sqrt{x^2 + y^2} \) and \( \tilde{r} = |\mathbf{x}| \), and yields the analytical solution
\[ \mathbf{u}(\mathbf{x}) = -\tilde{\Omega} \mathbf{e}_x + \tilde{\Omega} x \mathbf{e}_y = \tilde{\Omega} r \mathbf{e}_\theta, \quad \tilde{\Omega}(\tilde{r}) = \frac{\Omega R^3}{\tilde{r}^3}, \tag{5} \]
with \( \mathbf{e}_{x,y,\theta} \) the standard unit vectors of Cartesian and cylindrical coordinate systems. This flow in essence concerns "solid-body rotations" of spherical fluid layers \( \tilde{r} = \text{constant} \) about the \( z \)-axis with angular velocity \( \tilde{\Omega}(\tilde{r}) \).

Rescaling variables via \( \mathbf{x}' = \mathbf{x}/R, \mathbf{u}' = \mathbf{u}/\Omega R, \) and \( t' = \Omega t \) gives
\[ \mathbf{u}'(\mathbf{x}') = -\omega y' \mathbf{e}_x + \omega x' \mathbf{e}_y = \omega x' \mathbf{e}_\theta, \quad \omega(\tilde{r}') = \frac{1}{\tilde{r}'^3}, \quad \frac{d\mathbf{x}'}{dt'} = \mathbf{u}'(\mathbf{x}'), \tag{6} \]
as non-dimensional counterpart to velocity (5) and corresponding kinematic equation (3). The latter admits analytical integration, resulting in the closed-form expression
\[ r(t) = r_0, \quad \theta(t) - \theta_0 = \omega_0 t, \quad z(t) = z_0, \quad \omega_0(\tilde{r}_0) = \frac{1}{\tilde{r}_0^3}, \tag{7} \]
for the Lagrangian base flow \( \mathbf{x}(t) = \mathbf{F}_z(\mathbf{x}_0) \), where the subscripts 0 refer to the corresponding initial values. (Primes are dropped for brevity.) The corresponding streamlines describe closed circles centred on the \( z \)-axis along which tracers perform a steady rotation over an angle \( \Delta \theta = \omega_0 \tau \) for a given time interval \( t \in [0, \tau] \). Hence, the Lagrangian base flow in fact constitutes a rotation, i.e.,
\[ \mathbf{F}_z(\omega_0 \tau) = \mathbf{R}_z(\omega_0 \tau) \cdot \mathbf{x}, \tag{8} \]
with \( \mathbf{R}_z(\eta) = \cos \eta (\mathbf{e}_x + \mathbf{e}_z) + \sin \eta (\mathbf{e}_y - \mathbf{e}_z) + \mathbf{e}_z \), the standard rotation operator accomplishing counter-clockwise rotation by an angle \( \eta \) about the \( z \)-axis. Note that the non-dimensional
angular velocity of the sphere amounts to \( \omega_0(1) = 1 \), meaning it completes one full revolution for \( \tau = 2\pi \).

C. Composition of time-periodic flows

Time-periodic flows are composed of successive reorientations of the steady base flow \( \mathbf{u} \) via step-wise reorientation of the rotation axis via some forcing protocol. Thus the map (4) for an \( N \)-step protocol takes the form

\[
\Phi_T = F_N F_{N-1} \ldots F_2 F_1, \quad F_i = M_i^{-1} F_i(\beta_i) M_i, \quad \beta_i = \omega_0, \tau_i, \quad (9)
\]

with \( M_i \) the step-wise similarity transformation accomplishing reorientation of the Lagrangian base flow \( F_1 \) and \( \beta_i \) the step-wise rotation angle. The step-wise durations \( \tau_i \) combined add up to the period time: \( \sum_{i=1}^{N} \tau_i = T \). Important to note is that, since \( \tilde{r} = \sqrt{\tilde{r}_x^2 + \tilde{r}_y^2} \), base flow (7) implies \( \tilde{r}(t) = \tilde{r}_0 \) and thus \( \tilde{r}_n = \tilde{r}_0 \), meaning that tracers subject to map (9) are confined to spheroids \( \tilde{r} \) constant. This, in turn, implies \( \beta_i = \tau_i/\tilde{r}_0^3 \).

The present study is restricted to the two-step forcing protocol \( (N = 2) \) consisting of subsequent rotation about the \( \z \)-axis and the \( x \)-axis for equal duration \( \tau = T/2 \), implying equal step-wise rotation angles \( \beta_1 = \beta_2 = \beta(\tilde{r}_0) = \tau/\tilde{r}_0^3 = T/2\tilde{r}_0^3 \). This yields the map

\[
\Phi_T = F_2 F_1, \quad F_1 = F_{\z}(\tau/\tilde{r}_0^3), \quad F_2 = M_2 F_{\z}(\tau/\tilde{r}_0^3) M_2, \quad (10)
\]

with \( M_2 = e_x e_x + e_y e_y + e_z e_z \) the similarity transformation that identifies the axis of rotation with the \( x \)-axis. (Here \( M_1 = I \) and \( M_2^{-1} = M_2^T \), with subscript \( T \) indicating transpose). The step-wise durations are fixed at \( \tau = 5 \) in the analysis below, which corresponds to about 4/5 of a full revolution (Sec. II B). This value is chosen for no particular reason other than demonstrating typical dynamics. In-depth parametric studies are beyond the present scope and subject of ongoing investigations.

Important to note is that time-periodic flows composed of step-wise reorientations of a base flow in principle fall within the scope of the so-called Linked-Twist-Maps (LTMs) proposed in literature.\(^{18,25}\) The LTM formalism relies on composition of the fluid trajectories from piecewise isometries (translations, rotations, and reflections) and has found successful application for Lagrangian transport studies in a range of 3D mixing flows.\(^{17,18,20}\) This may suggest that the LTM is also the appropriate framework for the current flow. However, despite certain connections, its applicability is limited in the present context. A number of similarities and differences with LTMs are highlighted in the discussion below so as to properly position the current study relative to other approaches towards 3D transport studies.

III. FUNDAMENTAL DYNAMICAL STATES OF TIME-PERIODIC FLOWS

A. Standard base flow: Essentially 1D dynamics

Generic time-periodic maps \( \Phi_T \) with composition (9) consist of reoriented base flows \( F_{\z} \) and, by virtue of structure (8), in fact constitute a sequence of rotations under angles \( \beta_i \) about various axes. This effectively yields one overall rotation, implying a map of the form

\[
\Phi_T = R_{\hat{z}}(\hat{\eta}) \cdot \mathbf{x}, \quad R_{\hat{z}}(\hat{\eta}) = \cos \hat{\eta} (e_x e_x + e_y e_y + e_z e_z) + \sin \hat{\eta} (e_x e_y - e_y e_x) + e_z e_z, \quad (11)
\]

with unit vectors \( e_x, e_y, e_z \) spanning a Cartesian reference frame, where \( e_z \) is the axis of rotation and \( \hat{\eta} \) is the net rotation angle.\(^{26,27}\) The latter properties are defined implicitly through \( R_{\hat{z}} \cdot e_z = e_z \) and \( trace(R_{\hat{z}}) = 1 + 2 \cos \hat{\eta} \). Representing the map \( \Phi_T \) in terms of polar coordinates relative to \( e_{\hat{x}, \hat{y}, \hat{z}} \) gives

\[
\hat{\tilde{r}}_n = \tilde{r}_0, \quad \hat{\theta}_n = \hat{\theta}_0 + n \hat{\eta}, \quad \hat{\zeta}_n = \hat{\zeta}_0, \quad (12)
\]

which is the mapping counterpart of flow (7). Thus tracers describe circular orbits within the \( (\tilde{x}, \tilde{y}) \)-plane of the Poincaré section in a similar way as the underlying continuous flow describes closed circular streamlines. Important to note is that, since \( \tilde{r}_n = \tilde{r}_0 \) — and thereby \( \hat{\tilde{r}}_n = \tilde{r}_0 \) — and \( \beta_i = \tau_i/\tilde{r}_0^3 \) (Sec. II C), the effective rotation (11) is a function of \( \tilde{r}_0 \). Thus the circular orbits described by (12)
run parallel within a given sphere of radius \( r_0 \) yet smoothly change orientation \( e_{\hat{r}, \hat{\phi}, \hat{z}} \) and rotation angle \( \hat{\eta} \) with varying \( r_0 \). This generic structure of the Poincaré section is demonstrated in Figure 1(b) for the two-step forcing (10) at \( \tau = 5 \). The tracer motion is obtained by numerical integration of (3) with an explicit third-order Taylor-Galerkin scheme with adaptive step size.28

The map (12), irrespective of its particular composition, invariably possesses two constants of motion, viz., \( r_0 \) and \( \hat{z}_0 \), rendering it a two-action map. Such maps are fully integrable — and thus intrinsically non-chaotic — in that tracer motion is restricted to closed orbits.10, 13 Thus the transformation of motion, viz., \( \dot{x} = \epsilon z f(x, t) g(t), \quad \dot{y} = \epsilon x f(x, t) g(t), \quad \dot{z} = -2\epsilon xy f(x, t) / g(t), \) (13)

that is subject to conditions

\[
\nabla \cdot \mathbf{u}^\prime = 0, \quad \mathbf{u}^\prime|_{r=1} = 0, \quad \text{(14)}
\]

so as to maintain incompressibility (\( \nabla \cdot \mathbf{u} = 0 \)) and the no-slip condition on the sphere surface. Physical causes for \( \mathbf{u}^\prime \) may, e.g., be fluid inertia or pressure-induced fluctuations in the background flow. However, on grounds of simplicity and mathematical accessibility the present study adopts

\[
\mathbf{u}^\prime = \epsilon y z f(x, t) g(t), \quad \dot{x} = \epsilon x z f(x, t) g(t), \quad \dot{z} = -2\epsilon x y f(x, t) / g(t), \quad \text{(15)}
\]

with

\[
f(x, t) = e^{1-(x^2+y^2+z^2)} - 1, \quad g(t) = 1 + k \sin t, \quad \text{(16)}
\]

as closed-form analytical perturbation satisfying conditions (14). This in essence artificial perturbation may at first glance seem of limited physical relevance. However, below it is demonstrated that, provided \( |\mathbf{u}^\prime| \ll |\mathbf{u}_0| \), the effect upon the dynamics is qualitatively equivalent to that of weak fluid inertia. This is consistent with the fact that weak perturbations, provided they preserve physical properties as incompressibility and boundary conditions, typically have a generic impact on the dynamics independent of its particular structure.10, 13, 29 This further supports the current course of action.

Perturbation \( \mathbf{u}^\prime \) has two tuning parameters, viz., \( \epsilon \) and \( k \), which control its amplitude and degree of unsteadiness, respectively. Vanishing \( \epsilon \), evidently, results in the standard base flow and, inherently, maps of the form (11); non-zero \( \epsilon \) breaks the rotational forms (8) and (11) by coupling the velocity components and is a prerequisite for more complex dynamics. However, steady (\( k = 0 \)) and unsteady (\( k > 0 \)) perturbations have fundamentally different impacts upon the dynamics. This is inextricably
linked to the motion in \( \tilde{r} \)-direction, which for the perturbed flow is governed by

\[
\frac{d\tilde{r}}{dt} = \frac{\mathbf{x} \cdot \mathbf{u}}{\tilde{r}} = \frac{2\epsilon xy z f(x, t)[g^2(t) - 1]}{g(t)\tilde{r}}
\]

implying

\[
\frac{d\tilde{r}}{dt} = 0 \quad \text{for} \quad k = 0, \quad \text{and} \quad \frac{d\tilde{r}}{dt} \neq 0 \quad \text{for} \quad k > 0,
\]

for arbitrary \( \epsilon > 0 \) due to \( g = 1 \) for \( k = 0 \). This has fundamental ramifications for the tracer dynamics, which is elaborated below.

The one-to-one correspondence with LTMs is broken upon perturbation. The latter aims at inducing minute continuous variations in the flow field — and, inherently, the resulting fluid trajectories — so as to emulate weak nonlinear departures from the integrable state by, e.g., fluid inertia (Sec. I). This renders a decomposition of the fluid trajectories into isometries impossible (or at the very least highly impractical). Hence, the LTM formalism is ill-suited for analyzing (perturbed) 3D flows of continuous media as that considered here.

1. **Case \( k = 0 \): Essentially 2D dynamics**

Property (18) for the limit \( k = 0 \) puts forward the radius \( \tilde{r} \) as a constant of motion. This admits reduction of the equations of motion (3) to the generic form (A1). Consider to this end transformation of the system into spherical coordinates \((\tilde{r}, \theta, \rho)\) (relating to the Cartesian frame via \( x = \tilde{r} \cos \theta \sin \rho, \ y = \tilde{r} \sin \theta \sin \rho, \ z = \tilde{r} \cos \rho)\). Expression in terms of the generic curvilinear system following Appendix A 1 via \( \xi = (\xi_1, \xi_2, \xi_3) = (\theta, \rho, \tilde{r}), \ h_1 = \tilde{r} \sin \rho, \ h_2 = \tilde{r}, \) and \( h_3 = 1 \) yields

\[
\tilde{r} \sin \rho \frac{d\theta}{dt} = v_{\theta} = -\frac{1}{\tilde{r}} \frac{\partial H}{\partial \rho}, \quad \tilde{r} \frac{dp}{dt} = v_{\rho} = \frac{1}{\tilde{r} \sin \rho} \frac{\partial H}{\partial \theta}, \quad \frac{d\tilde{r}}{dt} = 0,
\]

where

\[
H(\theta, \rho; \tilde{r}, \epsilon) = \frac{\cos \rho}{\tilde{r}} + \frac{\epsilon f^3}{4} \cos 2\theta (\cos 2\rho - 1),
\]

using \( f = f(\tilde{r}) = e^{1-\tilde{r}^2} - 1 \) and \( g = 1 \) for \( k = 0 \). Thus for \( k = 0 \), the equations of motion collapse on the Hamiltonian form (A2), where Hamiltonian \( H \) is parameterized by \( \tilde{r} \) and \( \epsilon \). The absence of explicit time-dependence for \( k = 0 \) means that the intra-surface dynamics of the base flow, irrespective of \( \epsilon \), remains integrable; motion takes place along closed curves given implicitly by the level sets of \( H \). Hence, for \( k = 0 \), the perturbed base flow remains topologically equivalent to its standard counterpart, viz., \( \epsilon = 0 \), in that tracers are confined. However, for non-zero \( \epsilon \) the motion no longer coincides with simple rotations. This is an essential difference with fundamental consequences.

Reorientation during time-periodic forcing following (11) involves step-wise steady coordinate transforms of the form \((\theta, \rho) \rightarrow (\theta + \Delta \theta(t), \rho + \Delta \rho(t))\), which retains the Hamiltonian structure (20) yet introduces time-dependence: \( H(\theta + \Delta \theta(t), \rho + \Delta \rho(t); \tilde{r}, \epsilon) \). This results in non-integrable Hamiltonian dynamics within the spheres due to the breakdown of the purely rotational motion for \( \epsilon > 0 \) and in principle admits intra-surface chaotic dynamics. Figure 2 demonstrates this by way of the Poincaré section of a single tracer (released at the position indicated by the bullet and the accompanying arrow) for the two-step forcing (10) at \( \epsilon = 0.1 \) and \( k = 0 \). Here panels (a) and (b) give the 3D Poincaré section and its corresponding projection in the \( rz \)-plane, respectively. Tracers exhibit chaotic advection yet indeed remain restricted to an invariant sphere, implying essentially 2D Hamiltonian chaos. Hence, non-zero \( \epsilon \) in combination with \( k = 0 \) increases the freedom of motion of tracers by transforming the system from a two-action map (confinement to circular orbits; Sec. II B) to a one-action map (confinement to spheres).10, 13 Moreover, the invariant spheres constitute convex closed surfaces, meaning that the dynamics is dominated by period-1 lines30 (Appendix A 4). This is examined in greater detail in Sec. IV.
FIG. 2. 3D Poincaré section (a) and corresponding projection in the \(rz\)-plane (b) of a single tracer released at the (red) bullet \((\tilde{r}_0 = 2.0)\) with arrow for \(\epsilon = 0.1\) and \(k = 0\).

2. Case \(k > 0\): Towards essentially 3D dynamics

Property (18) implies that the invariant spheres vanish and the above Hamiltonian structure breaks down for \(k > 0\), meaning tracers can in principle move freely throughout the 3D domain. This is demonstrated in Figure 3 by the Poincaré section for a single tracer (released at the position indicated by the bullet and the arrow) for the two-step forcing (10) at \(\epsilon = 0.1\) and \(k = 0.01\). Here the \(rz\)-projection (panel (b)) reveals a significant migration in \(\tilde{r}\)-direction, implying essentially 3D tracer motion. However, instead of being fully unrestricted, tracer dynamics is nonetheless dictated by coherent structures. The Poincaré section namely exposes shell-like layers connected by tubes, the formation of which is intimately related to the breakdown of periodic lines into isolated periodic points for non-zero yet sufficiently small \(k\) (Appendix A5). This is investigated in detail in Figure 3.

FIG. 3. 3D Poincaré section (a) and corresponding \(rz\)-projection (b) of a single tracer released at the same position as in Figure 2 (red bullet in \(\tilde{r}_0 = 2.0\) with arrow) for \(\epsilon = 0.1\) and \(k = 0.01\).
Sec. V. The breakdown of the invariant spheres further increases the freedom of motion of tracers and renders the system a zero-action map for non-zero \( k \) and \( \epsilon \).\(^9,10,13\)

The above dynamics, though strictly induced by an artificial perturbation, bears great resemblance to realistic phenomena observed in the 3D lid-driven cylinder flow studied in Refs. 15, 16, 19, 28, 31, and 32. This pertains in particular to cylinder flows driven by a sequence of translations of a single endwall. This gives rise to a time-periodic flow with the same composition as (9), where base flow \( \mathbf{F}_c \) corresponds with the steady flow set up by steady translation of the driving wall in a fixed direction. In the Stokes limit \( \text{Re} = 0 \), signifying absence of fluid inertia, tracers are restricted to spheroidal invariant surfaces\(^33\) within which they exhibit (chaotic) Hamiltonian dynamics in essentially the same manner as the present flow for \( \epsilon > 0 \) and \( k = 0 \) (Figure 2). Moreover, periodic lines are key to this behavior, which is a further fundamental commonality with the current system (Sec. IV). Noteworthy to mention is that similar behavior has been observed in continuum representations of 3D granular flows.\(^17,18\) Fluid inertia (\( \text{Re} > 0 \)) breaks down the invariant spheroids and, for sufficiently small Re, leads to the formation of shell-like layers connected by tubes akin to the present flow for \( \epsilon > 0 \) and \( k > 0 \) (Figure 3). Thus, given non-zero \( \epsilon \), perturbation parameter \( k \) has an equivalent effect upon the dynamics as fluid inertia: the dynamics of the perturbed system for \( k > 0 \) and \( k > 0 \) are qualitatively similar to the cylinder flow for \( \text{Re} = 0 \) and \( \text{Re} > 0 \), respectively. Non-zero \( \epsilon \) ensures topological equivalence between the base flow of the cylinder flow and the current system. The former namely consists of concentric closed orbits yet with dynamics more complex than a simple rotation; the simple rotational form of the latter breaks down for \( \epsilon > 0 \). These fundamental similarities between the cylinder flow and the present flow imply that the artificial perturbation introduced before (at least qualitatively) represents realistic mechanisms. This justifies the artificial perturbation as a simple yet nonetheless physically meaningful way to break the integrability. The present (perturbed) flow namely is, on grounds of its relatively simple mathematical structure, far more amenable to detailed investigation than, e.g., the cylinder flow or any other realistic system due to the lack of closed-form expressions.

IV. FLOW TOPOLOGY FOR THE ESSENTIALLY 2D CASE \( \epsilon > 0 \) AND \( k = 0 \)

A. Periodic lines

Period-1 lines are key elements in the dynamics of the essentially 2D case \( \epsilon > 0 \) and \( k = 0 \) (Sec. III B). Presence of a time-reversal symmetry \( S \) according to (A8) facilitates systematic isolation of such periodic lines. For the two-step forcing (10) a symmetry \( S \), if existent, emanates from symmetries of its individual forcing steps \( \mathbf{F}_1 \) and \( \mathbf{F}_2 \) and can be derived by a symmetry analysis similar to that of Refs. 15, 16, and 19. (These studies partially lean on the analysis of Ref. 34.) This reveals that relevant step-wise symmetries are

\[
\mathbf{F}_1 = S_y \mathbf{F}_1^{-1} S_y, \quad \mathbf{F}_2 = S_y \mathbf{F}_2^{-1} S_y, \quad (21)
\]

with \( S_y : (x, y, z) \rightarrow (x, -y, z) \) effectuating reflection about the plane \( y = 0 \). Substitution into (10) and using the property that \( S_y \) is involutive \( (S_y^2 = I) \) yields

\[
\Phi_T = \mathbf{F}_2 \mathbf{F}_1 = (S_y \mathbf{F}_2^{-1} S_y)(S_y \mathbf{F}_1^{-1} S_y) = S_y \mathbf{F}_2^{-1} \mathbf{F}_1^{-1} S_y = S_y (\mathbf{F}_1 \mathbf{F}_1^{-1}) S_y = S_y (\mathbf{F}_2 \mathbf{F}_1^{-1}) (\mathbf{F}_2 \mathbf{F}_1^{-1})^{-1} = S \Phi_T^{-1} S,
\]

\[
(22)
\]

with \( S = S_y \mathbf{F}_1 \), satisfying \( S = S^{-1} \) due to (21), the sought-after time-reversal reflectional symmetry of map (10). Note that forcing steps \( \mathbf{F}_{1,2} \) possess further symmetries yet these are immaterial with respect to time-reversibility.

Time-reversal symmetry (22) has the fundamental implication that a period-1 line \( \mathcal{P}^{(1)} \) must sit within the corresponding symmetry plane \( I_S = S I_S \). This line is defined by the intersection of \( I_S \) with its forward mapping \( \Phi_T (I_S) \) according to relation (A9). Here \( I_S \) in fact constitutes a convoluted surface instead of a true plane and can be isolated as follows. Property (21) implies \( S I_S = S_y \mathbf{F}_1 I_S = \mathbf{F}_1^{-1} S_y I_S = I_S \), in turn leading to \( \mathbf{F}_1^{-1/2} S_y I_S = \mathbf{F}_1^{1/2} I_S \), with \( \mathbf{F}_1^{1/2} \) indicating mapping over half of
the first step. Since (21) also holds for \( \mathbf{F}_{1}^{1/2} \), i.e., \( \mathbf{F}_{1}^{1/2} = S_{y} \mathbf{F}_{1}^{-1/2} S_{y} \), implying \( \mathbf{F}_{1}^{-1/2} S_{y} = S_{y} \mathbf{F}_{1}^{1/2} \), this readily yields \( S_{y} \mathbf{F} = \mathbf{F} \), with \( \mathbf{F}_{} = \mathbf{F}_{1}^{1/2} I_{S} \), meaning that \( \mathbf{F} \) is the symmetry plane of \( S_{y} \) and thus coincides with the plane \( y = 0 \). Hence, \( I_{S} \) is defined by

\[
I_{S} = \mathbf{F}_{1}^{1/2} I_{y}.
\]

which follows from backward mapping of \( I_{y} \) over half the first step.

The type of periodic points is determined by the deformation tensor \( \mathbf{F} \) following (A3). The map (4) in terms of the spherical coordinates \( \xi = (\xi_1, \xi_2, \xi_3) = (\theta, \rho, \tilde{r}) \) introduced in Sec. III B takes the form

\[
\mathbf{x}_{n+1} = \Phi_{T} (\mathbf{x}_{n}) = \tilde{r} \mathbf{e}_{\tilde{r}} (\tilde{\xi}_{n}), \quad \tilde{\xi}_{n+1} = \Phi_{\xi} (\xi_{n}), \quad \tilde{\xi} = (\theta, \rho),
\]

with \( \mathbf{e}_{\tilde{r}}(\tilde{\xi}) = \sin \rho \cos \theta \mathbf{e}_{x} + \sin \rho \sin \theta \mathbf{e}_{y} + \cos \rho \mathbf{e}_{z} \) and \( \Phi_{\xi} = (\Phi_{\xi_{1}}, \Phi_{\xi_{2}}) \) the map on invariant spheres. The corresponding deformation tensor reads

\[
\mathbf{F} = \mathbf{e}_{\cdot} \mathbf{e}_{\cdot} + \tilde{\mathbf{F}}, \quad \tilde{\mathbf{F}} = \frac{\partial \Phi_{\rho}}{\partial \theta} \mathbf{e}_{\theta} \mathbf{e}_{\rho} + \sin \rho \frac{\partial \Phi_{\theta}}{\partial \rho} \mathbf{e}_{\rho} \mathbf{e}_{\theta} + \frac{1}{\sin \rho} \frac{\partial \Phi_{\rho}}{\partial \theta} \mathbf{e}_{\theta} \mathbf{e}_{\rho} + \frac{\partial \Phi_{\rho}}{\partial \rho} \mathbf{e}_{\rho},
\]

with \( \tilde{\mathbf{F}} \) the deformation tensor within a given invariant sphere (using \( \partial \mathbf{e}_{\cdot}/\partial \theta = \sin \rho \mathbf{e}_{\theta}, \partial \mathbf{e}_{\cdot}/\partial \rho = \mathbf{e}_{\rho} \) and constant \( \tilde{r} \)). (Note that \( \tilde{\mathbf{F}} \) concerns the action of \( \mathbf{F} \) in \( \xi_{1,2} \)-directions and for generic curvilinear coordinates \( \xi \) differs from the Jacobian \( \tilde{\mathbf{J}} = \partial \Phi/\partial \hat{\xi} \).) This implies

\[
J = \tilde{J} + 1, \quad \tilde{J} = \text{trace}(\tilde{\mathbf{F}}),
\]

with \( J \) according to (A4), meaning that the classification of periodic points on periodic lines following Appendix A.2 may alternatively be expressed in terms of \( J \): elliptic (\( J < 2 \)) and hyperbolic (\( J > 2 \)). This connection with \( \tilde{J} \) enables specification of the generic link between the formation of periodic lines and the type of constituent periodic points according to Appendix A.5. Here criterion (A7) namely becomes

\[
\Sigma^{0} \neq 0, \quad \Sigma^{0} = |\mathbf{F}| - 1 - \tilde{J} = 2 - \tilde{J},
\]

using property \( |\mathbf{F}| = |\tilde{\mathbf{F}}| = 1 \), and through the above implies that periodic points merge into periodic lines whenever they are elliptic (\( J < 2 \iff \Sigma^{0} > 0 \)) or hyperbolic (\( J > 2 \iff \Sigma^{0} < 0 \)).\(^{35}\) Existence criterion (27) is violated at parabolic points (\( \tilde{J} = 2 \iff \Sigma^{0} = 0 \)), meaning that strictly only single-type periodic lines form. However, parabolic points, if occurring, typically emerge as isolated degenerate points and, by virtue of continuity, positions of periodic points on adjacent invariant surfaces will change smoothly. Thus parabolic points, if indeed isolated, effectively are “contact points” of neighboring elliptic and hyperbolic lines, causing the latter to effectively constitute one periodic line comprising of segments of different type.\(^{36}\) This is consistent with observations in the before-mentioned cylinder flow studied in Refs. 15, 16, 19, 28, 31, 32 and happens also in the present flow.

Each invariant surface accommodates at least one period-1 point due to the fact that the flow always possesses at least one period-1 line intersecting these surfaces (Appendix A.4). However, further generic statements on the intra-surface arrangement of periodic points cannot be made \textit{a priori}. Stagnation points of steady flow fields are configured according to the Poincare-Hopf theorem;\(^{37}\) an equivalent for their time-periodic counterparts in maps, on the other hand, is absent. Generalization of the former to maps is possible only in case of fully integrable intra-surface dynamics. The impact of chaotic conditions on the topological make-up within invariant spheres is highly non-trivial.

Figure 4(a) gives the period-1 lines within the range \(-4 \leq x, y, z \leq 4\), as defined by (A9) and using the symmetry plane \( I_{S} \) according to (23), for \( \epsilon = 0.05 \) and \( k = 0 \). This results in three separate lines with \( \Sigma^{0} > 0 \) throughout their extent, implying fully elliptic types. Slightly augmenting the perturbation maintains the three separate period-1 lines but causes \( \Sigma^{0} \) to vanish at isolated positions, signifying segmentation into elliptic (\( \Sigma^{0} > 0 \)) and hyperbolic (\( \Sigma^{0} < 0 \)) sections by parabolic points (\( \Sigma^{0} = 0 \)) following the above scenario. This is demonstrated in Figure 4(b) for \( \epsilon = 0.1 \), where dark and bright parts of period-1 lines indicate elliptic and hyperbolic segments, respectively. The
period-1 lines in the center and to the right each on one end connect with the sphere; the line on the left, on the other hand, is completely detached from the sphere.

Note that, since the period-1 lines by definition coincide with the intersection of two surfaces, they must occur in one of only four kinds: (i) fully closed; (ii) both ends attached to the sphere; (iii) one end attached to sphere and one end extending to infinity; and (iv) both ends extending to infinity. Two lines in Figure 4(b) belong to category (iii); the remaining line may be either category (i) or (iv). A larger portion of the flow domain must be investigated to conclusively establish this. However, this is beyond the scope of the present study.

B. Intra-surface dynamics

The period-1 lines dominate the dynamics within the invariant spheres in that their intersections with the latter constitute period-1 points \((\theta^0, \rho^0)\) of the intra-surface Hamiltonian systems (19). Such period-1 points are key to Hamiltonian dynamics.\(^{21, 22}\) This is investigated in more detail below for \(\epsilon = 0.1\) and \(k = 0\); here the segmentation of period-1 lines namely implies both elliptic and hyperbolic points and thus gives rise to the typical — and in dynamical sense most interesting — situation of coexisting chaotic and non-chaotic regions, either within invariant spheres or on neighboring spheres.

Figure 5(a) displays a 3D Poincaré section in which the intra-surface tracer dynamics is governed by both elliptic and hyperbolic points. Here tracers are released at strategic locations on a sphere of radius \(\tilde{r}_0 \approx 2.4\) intersected by both elliptic and hyperbolic segments of the period-1 lines, and the forcing protocol was repeated sufficiently long for features to become visible. The coexistence of chaotic and non-chaotic regions is evident from the presence of distinct elliptic islands (surrounded by the characteristic island chains) embedded in a chaotic sea. Darker gray dots (blue online) and lighter gray dots (red online) correspond to mappings of tracers released in the chaotic and non-chaotic regions, respectively. Each island corresponds to an elliptic point of the intra-surface Hamiltonian system. Two of these points are due to the intersection of the elliptic segment of the period-1 line with the invariant surface. Other elliptic points and their corresponding islands are associated with periodic lines of higher order. This has been verified by identifying the locations of higher-order elliptic points within the spherical surface (not shown in Figure 5). The intra-surface dynamics is characteristic of perturbed Hamiltonian systems, where the island behavior is described by the well-known Poincaré-Birkhoff and KAM theorems.\(^{22}\)

The Hamiltonian dynamics within invariant spheres intersected only by hyperbolic segments of period-1 lines is entirely governed by the corresponding hyperbolic points. This is demonstrated by the Poincaré section in Figure 5(b) for a sphere of radius \(\tilde{r} = 4.0\). Evidently, no period-1 islands are present and the dynamics exhibited 2D Hamiltonian chaos throughout the entire sphere. The
chaotic tracer transport is “driven” by the transversely intersecting stable-unstable manifold pairs of the hyperbolic points. Lighter/darker curves (green/red online) indicate one stable/unstable manifold pair. These intra-surface manifolds, in turn, identify with intersections between said sphere and transversely intersecting 2D manifolds $W_{1D}^u$ and $W_{1D}^s$ of hyperbolic segments of the period-1 lines (Appendix A 3). (The 1D intra-surface manifolds are computed with the method described in Ref. 38.) Case $\epsilon > 0$ and $k = 0$ thus nicely demonstrates the essentially 2D nature of chaotic advection associated with periodic lines. This is primarily due to the periodic lines; similar (Hamiltonian-like) dynamics occurs without strict confinement to invariant surfaces.\(^{16}\)

V. FLOW TOPOLOGY FOR THE ESSENTIALLY 3D CASE $\epsilon > 0$ AND $k > 0$

A. Isolated periodic points

The presence of periodic lines for the essentially 2D case $k = 0$ investigated in Sec. IV has fundamental ramifications for the topology of the truly 3D case $k > 0$. Periodic lines for $k = 0$, by virtue of existence criterion (A11), namely imply isolated periodic points for sufficiently small yet non-zero $k$ in their direct proximity (Appendix A 5). Moreover, the type of isolated periodic points is inextricably linked to the properties of the underlying periodic lines. Generically, $D > 0$ and $D < 0$ results in a node-type and focus-type periodic point, respectively, with $D$ the discriminant following (A4) (Appendix A 2). The latter depends on the deformation tensor $\mathbf{F}$. The case $k = 0$, given by (25), becomes

$$
\mathbf{F}^* = \frac{\partial \Phi^*_\rho}{\partial \rho} \mathbf{e}_\rho + \frac{\partial \Phi^*_\theta}{\partial \theta} \mathbf{e}_\theta + \frac{\partial \Phi^*_\phi}{\partial \phi} \mathbf{e}_\phi + \frac{1}{\rho} \frac{\partial \Phi^*_\rho}{\partial \theta} \mathbf{e}_\theta + \frac{1}{\rho} \frac{\partial \Phi^*_\phi}{\partial \rho} \mathbf{e}_\phi + \bar{\mathbf{F}}^* = \mathbf{F} + O(k),
$$

(28)

for small yet non-zero $k$ on similar grounds as those underlying the approximate existence criterion (A11). Here the star again, consistent with Appendix A 4, indicates a minute departure from the essentially 2D limit ($k = 0$). Hence, $J^* = J + O(k)$, meaning that to good approximation $J^* = J$, which, via (26) and (27), yields $J^* = 3 - \Xi^0$. Furthermore, it can be shown that $\text{trace}(\mathbf{F}^{*2}) = \text{trace}(\mathbf{F}^2) + O(k)$ meaning that the unit eigenvalue associated with the period-line case $k = 0$ is
FIG. 6. Isolated period-1 points for perturbations with amplitude \( \epsilon = 0.1 \) and two degrees of unsteadiness: (a) \( k = 10^{-6} \) and (b) \( k = 0.01 \). Circles and crosses indicate foci and nodes, respectively; dark and bright curves represent elliptic and hyperbolic segments of the period-1 lines in case of only steady perturbation \( (k = 0) \) (Figure 4(b)).

Isolated period-p points are located by a root-finding algorithm applied to \( \Phi^p(x) = x \) (Appendix B). Figure 6(a) demonstrates the emergence of isolated periodic points within the range \(-4 \leq x, y, z \leq 4\) for \( \epsilon = 0.1 \) and \( k = 10^{-6} \). Circles/crosses indicate focus/node-type period-1 points; dark/bright lines represent elliptic/hyperbolic segments of the period-1 lines of the unperturbed counterpart \( k = 0 \) shown in Figure 4(b). This exposes consistency with two fundamental theoretical predictions. First, isolated periodic points emerge in the direct vicinity of periodic lines. Second, their type correlates with that of the adjacent segments of the periodic line: elliptic (dark) \( \rightarrow \) focus (circle); hyperbolic (bright) \( \rightarrow \) node (cross). Note the occurrence of two foci in Figure 6(a) at a relatively large distance from the period-1 lines. This by no means implies a contradiction of theory. The latter predicts isolated points near periodic lines yet does not rule out emergence of points elsewhere. Moreover, Figure 6(a) shows period-1 lines only within the symmetry plane \( IS \); further periodic lines may exist that possibly correlate with said foci.

Intensifying the degree of unsteadiness \( k \) breaks the link between periodic points and periodic lines. This is demonstrated in Figure 6(b) for \( \epsilon = 0.1 \) and \( k = 0.01 \). Periodic points typically emerge far away from former periodic lines. Moreover, even if located in close proximity, the correlation between types is lost. Note, e.g., the node near the center of the elliptic segment of the leftmost period-1 line, which clearly violates theory. This implies that the influence of the periodic lines on the isolated periodic points reaches only up to perturbations of \( k \sim O(0.01) \). Thus for larger \( k \), isolated periodic points may, due to the non-convexity of the 3D flow domain, completely cease to exist (Appendix A5).

### B. Manifold dynamics: Focus versus node

Manifolds associated with hyperbolic (segments of) periodic lines and isolated periodic points play a crucial role in the 3D tracer dynamics, since they dictate the flow by (i) forming transport
barriers or (ii) accomplishing chaotic advection through transverse interactions (Appendix A3). Here we demonstrate typical manifold dynamics of isolated periodic points for a focus-type and a node-type period-1 point for the essentially 3D case $\epsilon > 0$ and $k = 0.01$. Computational methods for demarcating the manifold pairs $(W_1^{\mu u}, W_2^{\mu u})$ of a given periodic point are following Ref. 38. Note that, for reasons of computational efficiency, 2D manifolds $W_2$ are approximated by curves $\tilde{W}_2$ emanating from the vector $\mathbf{n}' = \mathbf{n}_2 + \mathbf{n}_3$, with $\mathbf{n}_{2,3}$ the eigenvectors of the deformation tensor associated with $W_2$. Relation (18) implies that for $k > 0$ tracers are no longer restricted to invariant spheres and therefore may migrate in $\tilde{r}$-direction. This facilitates the emergence of isolated periodic points from periodic lines discussed above. Moreover, this allows the associated manifolds to (in principle) proliferate freely in the 3D domain. This is demonstrated in Figure 7 by the perspective view of the $W_1$ manifold of a period-1 focus (panel a) and the corresponding projection in the $rz$-plane (panel b), where the circle with arrow indicates the focus. This exposes remarkable behavior. The manifold basically comprises three segments: two segments that each extend within separate spheroidal shells; one segment connecting the latter. Thus the manifold exhibits largely quasi-2D dynamics by, reminiscent of the invariant spheres for $k = 0$, remaining within spheroidal shells yet locally displays essentially 3D dynamics by linking different shells. This is consistent with findings in Ref. 29.

Within each spheroidal shell, the manifold exhibits stretching and folding similar to that observed for the manifolds of the hyperbolic segments of the period-1 lines for the limit $k = 0$ (Figure 5). Each shell gradually expands when time progresses, but for sufficiently small $k$ this expansion is extremely small, so that the present topology is preserved over thousands of periods. The accompanying $\tilde{W}_2$ manifold (not shown) remains entirely within one spheroidal shell that largely coincides with the inner shell of $W_1$. (This strongly suggests homoclinic transverse intersections $W_2^{\mu u} \cap W_1^{\mu u}$.) Here multiple shells and connecting segments are absent, implying quasi-2D dynamics for the whole manifold. These results are characteristic of all focus-type period-1 points considered, which has important consequences for the 3D tracer dynamics (see below).

As a second example, we consider the manifold dynamics associated with a period-1 node. Figure 8 shows the perspective view of the manifold pair $(\tilde{W}_2, W_1^{\mu u})$ of a period-1 node (panel a) and its projection in the $rz$-plane (panel b). The period-1 node is indicated by the cross and the arrow, whereas the $\tilde{W}_2$ and $W_1^{\mu u}$ manifolds are represented by the lighter gray curve (green online) and darker gray curve (red online), respectively. It is evident that the manifold pair remains confined to a spheroidal shell within which the dynamics is chaotic and essentially quasi-2D. (This implies
homoclinic transverse intersections \( W_{2D}^2 \cap W_{1D}^2 \). Similar to foci, the shell gradually expands when time progresses, but for sufficiently small \( k \) also here the state is preserved for prolonged time spans. However, a fundamental difference with foci exists in that the entire manifold pair remains within one spheroidal shell. Links between concentric shells, as via the 1D manifolds of foci, do not occur for the node.

Reconciling the behavior of the focus and node reveals a mutual influence. The spheroidal shell occupied by the manifold pair of the node approximately coincides with the outer shell of the focus. The 2D manifold of the node is stable (\( W_{2D}^2 \)) and thus acts as transport barrier to any manifold of the same stability (Appendix A 3). Hence, \( W_{2D}^2 \) of the node prevents further outward radial extension of \( W_{1D}^1 \) of the focus. Conversely, the unfolding of \( W_{1D}^1 \) within a spheroidal shell defines a transport barrier for inward radial growth of \( W_{2D}^2 \). This mutual blocking of radial extension is demonstrated in Figure 8(b), which shows \( W_{1D}^1 \) of the focus (black line; blue online) together with \( W_{2D}^2 \) (lighter gray curve; green online) and \( W_{1D}^1 \) (darker gray curve; red online) of the node. The inset highlights the strong mutual influence of manifolds \( W_{1D}^1 \) and \( W_{2D}^2 \). Close inspection of the corresponding 3D view (not shown) reveals that they closely align yet indeed never join or intersect. The causality in the interaction, i.e., whether \( W_{2D}^2 \) (node) prohibits proliferation of \( W_{1D}^1 \) (focus) or vice versa, is not evident, however. Manifold \( W_{2D}^2 \) constitutes a strict transport barrier in the sense of defining a continuous surface and in that respect likely dominates the observed behavior. The dense winding of \( W_{1D}^1 \) within shells, on the other hand, yields surface-like entities that may play equally dominating roles.

The above properties and scenarios are characteristic of all (period-1) foci and nodes identified in the present system. Manifold pairs of nodes as well as 2D manifolds of foci remain entirely within one spheroidal shell and induce quasi-2D motion. The 1D manifolds of foci, in contrast, generically divide over two spheroidal shells that are connected by a single segment and thus promote radial tracer transport. Moreover, strong mutual influence between periodic points occurs in that (in particular 2D) manifolds act as transport barriers to other manifolds of the same stability. Such interactions have a significant impact on the formation and structure of the flow topology.
C. Coherent structures

Isolated periodic points and associated manifolds as those investigated above result in essentially 3D coherent structures in the Poincaré sections of tracers. Formation of such structures is demonstrated in Figure 3(b) by the Poincaré section for a single tracer with $\epsilon = 0.1$ at $k = 0.01$, which exposed spheroidal shells and interconnecting tubes. Careful analysis revealed that the tracer initially remains confined to a spheroidal shell and at some point starts to migrate radially outward along three tube-like structures while jumping from one tube to the other in a period-3 fashion. This behavior is intimately related to the presence of isolated periodic points (here of period-3) and the corresponding manifold dynamics. This is examined in more detail below.

Figure 9(a) shows the positions of isolated period-3 points, defined by $x = \Phi^3_T(x)$, in the $rz$-plane (dotted semi-circles indicate spheres $\tilde{r}$ = constant) for $\epsilon = 0.1$ and $k = 0.01$ within the domain $-6 \leq z \leq 6$ and $0 \leq r \leq 7$. $-4 \leq x, y, z \leq 4$. Foci and nodes are again indicated by circles and crosses, respectively. Each isolated period-3 point $x$ is a member of a triplet of period-3 points of the same type: $\{x, \Phi^1_T(x), \Phi^2_T(x)\}$. Here each triplet is virtually located at a given sphere with radius $\tilde{r}$ (dotted semi-circles in Figure 9(a) serve as reference spheres). Note the strict spatial segregation of types: triplets between the solid sphere ($\tilde{r} = 1$) and sphere $\tilde{r} = 2$ are invariably of the focus-type; triplets outside $\tilde{r} = 2$ are all of the node-type. The reason for this is unknown.

The intimate link between coherent structures and (manifolds of) isolated periodic points is demonstrated in Figure 9(b) by an overlay of the Poincaré section (Figure 3(b)) and the period-3 triplets. Each tube, consistent with the period-3 behavior of the corresponding tracer motion, is accompanied by one focus-type period-3 point of the same triplet. Moreover, each tube is centered on one of the associated 1D manifolds $W_{1D}^u$ (solid lines). This exposes a direct link between the formation of coherent structures and the existence of focus-type periodic points. The segments of $W_{1D}^u$ transverse to the spheroidal shells cause the formation of tubes that facilitate exchange of
FIG. 10. 3D view of the projected Poincaré section shown in Figure 9(b) combined with the manifold pairs \( (W_u^{1D}, \tilde{W}_u^{2D}) \) of the upper triplet of period-3 nodes in the outer shell at \( \tilde{r}_0 \approx 2.6 \) (a) and the manifold pairs \( (W_s^{1D}, \tilde{W}_s^{2D}) \) of the triplet of period-3 nodes in between inner and outer shell at \( \tilde{r}_0 \approx 2 \) (b). Stable and unstable manifolds are indicated by the lighter gray curve (green online) and darker gray curve (red online), respectively; the (red) bullet with arrow indicates the initial tracer position.

Material between inner and outer shells. Here the outer shell, similar to the period-1 focus in Figure 7, coincides with the 1D manifolds. (They do not occupy the entire shell, because only a small part is computed.) However, the inner shell, in contrast with its period-1 counterpart, accommodates only the 2D manifolds \( W_s^{2D} \) of the triplet (not shown). The 1D manifolds further extend radially inward and form heteroclinic orbits with a neighboring period-3 triplet closer to the solid sphere. This implies the formation of inward tubes on the inner shell (not shown), which is substantiated by the observation that, depending on the initial position relative to \( W_s^{2D} \), tracers migrate either radially inward or outward through tubes centered on \( W_u^{1D} \).

The deflection of the outwardly extending 1D manifolds \( W_u^{1D} \) in the outer shell is, akin to the period-1 focus in Figure 7, likely to be caused by the formation of transport barriers through smooth mergers \( S = W_s^{2D} \cup W_u^{2D} \) or by manifolds of the same type (Appendix A 3). Examination of the two triplets of period-3 nodes in the outer shell \( (\tilde{r} \approx 2.6) \) reveals in both cases \( (W_s^{2D}, W_u^{1D}) \) manifold pairs. Figure 10(a) gives \( \tilde{W}_s^{2D} \) (lighter gray curve; green online) and \( W_u^{1D} \) (darker gray curve; red online) together with the Poincaré section of the tracer. The particular stability properties rule out mergers \( S = W_s^{2D} \cup W_u^{2D} \) as transport barriers to further radial proliferation of \( W_u^{1D} \). This leaves two mechanisms: (i) formation of a surface-like transport barrier by dense windings of \( W_u^{1D} \) of the period-3 nodes (comparable to the behavior observed in Sec. V B); and (ii) heteroclinic interaction of \( W_u^{1D} \) (period-3 foci) with \( W_s^{2D} \) (period-3 nodes). Establishing whether one mechanism or an interplay of both is active here is highly non-trivial and is therefore not further investigated.

Further analysis of the present case exposes first evidence that 2D manifolds form transport barriers to manifolds of the same type only under the explicit condition that these entities are fully impenetrable. Consider to this end the triplet of period-3 nodes that sits in the region in between inner and outer shell \( (\tilde{r} \approx 2) \) near the tubes (Figure 9(b)). The corresponding manifold pairs \( (W_s^{1D}, \tilde{W}_s^{2D}) \) are foliated within one shell, as shown in Figure 10(b), meaning that the 2D manifolds \( W_u^{2D} \) of the nodes in principle should act as transport barrier to the 1D manifolds \( W_u^{1D} \) of the period-3 foci. However, the latter evidently cross the shell at \( \tilde{r} \approx 2 \), as demonstrated by the tubes in Figure 10(b), implying absence of a “true” transport barrier. The underlying mechanisms are unclear and several scenarios are conceivable. A plausible explanation is that gaps occur between the adjacent 2D manifolds \( W_u^{2D} \) of the period-3 points on grounds of the fact that they, on the one hand, are extremely convoluted yet, on the other hand, can never intersect or merge with one another. This
scenario, if indeed at play, implies that the observed penetrability is a consequence of higher-order periodicity. The individual 2D manifolds of the period-3 triplet still act as transport barriers yet each seal-off only part of the shell. An alternative explanation is that individual 2D manifolds, irrespective of stability or periodicity, generically may admit “holes” that allow tracers — and thus manifolds of identical stability — to penetrate. Conclusive establishment of the actual causes requires deeper analysis.

VI. CONCLUSIONS

The present study concerns transport of passive tracers in the 3D time-periodic flow near the surface of a rotating solid sphere. Time-periodicity is introduced via alternation between two rotation axes. The flow possesses two constants of motion in its Stokes limit, rendering the corresponding map a two-action map, implying essentially non-chaotic tracer motion along closed orbits. Breaking the integrability by “opening up” these orbits is imperative to obtain more complex dynamics, and, ultimately, chaos. To this end we superimpose a nonlinear perturbation that preserves incompressibility and the no-slip condition on the sphere surface. The perturbation is controlled by two tuning parameters, viz., $\epsilon$ and $k$, which regulate its strength and degree of unsteadiness, respectively.

Non-zero $\epsilon$ with $k = 0$ increases the freedom of motion by transforming the system from a two-action map to a one-action map in which tracers remain confined to spheroidal invariant surfaces $\tilde{r} = \text{constant}$. Tracer motion is governed by essentially 2D Hamiltonian mechanics within these spheres. Moreover, intra-surface dynamics is dominated by periodic points that invariably form due to the convexity of the spheres in accord with Brouwer’s fixed-point theorem. These periodic points, in turn, merge into periodic lines in the 3D flow domain. Conversely, intra-surface periodic points are in fact intersections of the invariant spheres with periodic lines. Their type determines the (local) intra-surface dynamics: periodic points associated with elliptic and hyperbolic (segments of) periodic lines result in islands and chaotic regions, respectively. This yields intra-surface Poincaré sections with a composition typical of 2D Hamiltonian systems.

For non-zero $\epsilon$ and $k > 0$, the invariant spheres and corresponding Hamiltonian structure are destroyed. This further increases the freedom of motion by admitting significant tracer migration in $\tilde{r}$-direction. However, instead of being fully unrestricted, tracer dynamics for non-zero yet sufficiently small $k$ is dictated by intricate coherent structures. The invariant spheres develop into shell-like spheroidal layers that exchange material via connecting tubes. The formation of these structures is intimately linked to the disintegration of periodic lines into isolated periodic points for non-zero $k$. Node-type and focus-type periodic points form near hyperbolic and elliptic (segments of) periodic lines, respectively, and the associated manifolds determine the dynamics. The 1D/2D manifolds of nodes and the 2D manifolds of foci foliate primarily in spheroidal direction. The 1D manifolds of foci exhibit segmentation into two disconnected parts, each extending within separate spheroidal shells, connected by a radially oriented segment. The latter segment underlies formation of the before-mentioned tubes; the other (segments of) manifolds cause the emergence of the spheroidal shells.

Remarkable is that the 3D flow domain is unbounded and non-convex, meaning that Brouwer’s fixed-point theorem strictly does not apply and periodic points may be completely absent. However, the existence of convex invariant surfaces (for $\epsilon > 0$ and $k = 0$) fundamentally changes this situation by implying at least one period-1 point within each of these subdomains and, inherently, at least one period-1 line in the 3D domain. The existence of a period-1 line, in turn, implies isolated periodic points in case of weak perturbation by a “small” $k > 0$. Only for “stronger” perturbations may periodic structures completely vanish, consistent with the properties of a generic non-convex domain.

The 2D manifolds within spheroidal shells have a strong impact on the dynamics in two ways. First, they define transport barriers akin to the invariant spheroids of $k = 0$ by restricting tracers to quasi-2D motion in substantial parts of the domain. Fundamental differences are that shells (i) do not form a dense family of transport barriers and (ii) admit tracer exchange due to local radial transport along 1D manifolds of foci. Second, our observations strongly suggest that 2D stable/unstable manifolds cause the deflection of radially oriented segments of 1D stable/unstable manifolds of
foci into spheroidal shells. 2D manifolds namely cannot be crossed by manifolds of identical stability. This manifold interplay thus very likely is a key mechanism behind the intricate coherent structures composed of shells and interconnecting tubes. The periodicity of the underlying periodic points seems essential here. Manifolds of period-1 points indeed yield such structures. However, spheroidal shells occupied by 2D manifolds of higher-order periodic points admit crossing by tubes (and thus 1D manifolds of foci). A plausible explanation is that these 2D manifolds, which always occur in clusters, never fully seal-off a spheroidal shell and effectively leave “holes” by which tracers can pass.

The dynamics induced by the rotating sphere bears great resemblance to that of the 3D cylinder flow driven by one endwall studied in literature.\cite{lit1, lit2, lit3, lit4} Cases \(k = 0\) and \(k > 0\) are (given \(\epsilon > 0\)) equivalent to the time-periodic cylinder flow for \(\text{Re} = 0\) and \(\text{Re} > 0\), respectively. The non-inertial limit (\(\text{Re} = 0\)) exhibits 2D Hamiltonian dynamics within invariant spheroids governed by periodic lines; fluid inertia (\(\text{Re} > 0\)) results in intricate coherent structures that comprise spheroidal shells interconnected by tubes. These striking similarities have important implications. First, the observed dynamics are kinematic phenomena triggered by a generic non-integrable perturbation of a solenoidal flow field; momentum conservation is only of secondary importance. (The present flow in fact violates the latter.) Second, the behavior of the cylinder flow, though tied to \(\text{Re}\), is not exclusive to fluid inertia. Presence or absence of the latter — or, more general, momentum conservation — facilitates certain phenomena yet is not the mechanism per se. Third, the findings in the present study, notwithstanding the artificial perturbation, are (qualitatively) representative of the transport induced by actuated beads. Here parameter \(k\) acts as a qualitative counterpart to \(\text{Re}\). It must be stressed that this equivalence pertains specifically to weak perturbations.

Current efforts concentrate on experimental validation of the observed dynamics. To this end a laboratory set-up has been realized for detailed measurement of 3D flow field and Lagrangian fluid trajectories using 3D Particle Tracking Velocimetry (3D-PTV). Past experimental investigations demonstrated the great potential of this technique for 3D Lagrangian transport studies and isolation of 3D coherent structures in laminar flows and turbulence studies.\cite{lit5, lit6, lit7, lit8} Furthermore, transport studies using heat as a tracer are underway. Here, heat-transfer rates from the (heated) sphere to the surrounding fluid (inferred from electrical power supply and temperature measurements by thermocouples) are determined as a function of the actuation. This offers insight into the global transport enhancement by the flow.

ACKNOWLEDGMENTS

We greatly acknowledge financial support by the Dutch Technology Foundation STW under Grant No. 10458.

APPENDIX A: GENERAL PROPERTIES OF 3D FLOW TOPOLOGIES

The following gives an overview of generic topological properties relevant in the present context. The results in Appendix A 1 follow from general vector calculus; Appendices A 2–A 5 are recapitulations from literature with minor additions and modifications.

1. Hamiltonian dynamics within invariant surfaces

The equations of motion (3) under certain conditions may admit reduction to

\[
\begin{align*}
    h_1 \frac{d\xi_1}{dt} &= u_1, \\
    h_2 \frac{d\xi_2}{dt} &= u_2, \\
    \frac{d\xi_3}{dt} &= 0,
\end{align*}
\]

(A1)

with \(x = x(\xi_1, \xi_2, \xi_3)\) and \(\xi = (\xi_1, \xi_2, \xi_3)\) an orthogonal curvilinear coordinate system (scale factors \(h_i = |\partial_x / \partial \xi_i|\)) such that motion in \(\xi_3\)-direction ceases. This may in general, e.g., be the result of a constant of motion or a continuous symmetry in the flow field \(u\).\cite{lit9, lit10} This implies 2D invariant surfaces, coinciding with the level sets of \(\xi_3\), within which effectively 2D flow occurs: \(u = u_1 e_1 + u_2 e_2\). For incompressible flows, the intra-surface equations of motion define a Hamiltonian system.
investigated in Ref. 11.

Periodic points and lines

Periodic points of order \( p \) (or “period-\( p \) points”) of a time-periodic map are material points that will return to their initial positions after \( p \) periods: \( x = \Phi^p(x) \). The local behavior at such period-\( p \) points is determined by

\[
\frac{d \xi_1}{dt} = \frac{-1}{h} \frac{\partial H}{\partial \xi_2}, \quad \frac{d \xi_2}{dt} = \frac{1}{h} \frac{\partial H}{\partial \xi_1},
\]

(A2)

with \( h \equiv h_1 h_2 h_3 \). This follows from expression of the gradient and divergence operators in terms of coordinate system \( \xi \) in conjunction with \( v_3 = 0 \). Reduction of system (3) to the form (A1) thus has fundamental ramifications. First, it restricts the flow to effectively 2D motion within invariant surfaces. Second, it results in essentially Hamiltonian dynamics within these surfaces. Important to note is that the above only holds for a continuous family of invariant surfaces so that the natural reference frame \( \xi \) exists everywhere. Violation of the latter may result in non-Hamiltonian intra-surface dynamics. An example is the isolated invariant sphere bounding the 3D steady flow investigated in Ref. 11.

### 2. Periodic points and lines

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\[
d x_{n+p} = F dx_n, \quad F = \nabla \Phi^p|_x = \sum_{i=1}^{3} \lambda_i n_i n_i, \quad (A3)
\]

with \( dx \) the local frame of reference and \( F \) the deformation tensor (expressed in terms of its eigenvector basis \( (n_1, n_2, n_3) \) with corresponding eigenvalue spectrum \( (\lambda_1, \lambda_2, \lambda_3) \)) representing the locally linearized mapping \( \Phi^p \). The discriminant \( D \), defined as

\[
D = \left[ \frac{(J - \lambda_1)}{2} \right]^2 - 1/\lambda_1, \quad J \equiv trace(F), \quad (A4)
\]

determines the local dynamics and thus the type of periodic point: focus (\( D < 0 \)) or node (\( D > 0 \)). Here \( \lambda_1 \) is the “distinct eigenvalue” in the sense of being (i) the only real eigenvalue or (ii) the sole real eigenvalue below or above unity: \( |\lambda_1| < 1 \) and \( |\lambda_2, 3| > 1 \) or \( |\lambda_1| > 1 \) and \( |\lambda_2, 3| < 1 \). Two basic kinds of periodic points exist, viz., focus (\( D < 0 \)) and node (\( D > 0 \)), each accompanied by a 1D-2D manifold pair, denoted \( (W_1 D, W_2 D) \) hereafter, that delineates the principal transport directions forward (“unstable”) and backward (“stable”) in time. Pairs invariably comprise a stable-unstable combination: \( (W_1 D, W_2 D) \) or \( (W_1 D, W_2 D) \).

A special case exists in periodic lines formed by a continuous string of periodic points. Periodic lines are in essence the 3D counterparts of periodic points in 2D systems in that they induce effectively 2D tracer dynamics in the local plane perpendicular to their tangent. This tangent coincides with one of the eigenvectors of \( F \), say \( n_1 \), that has a corresponding eigenvalue \( \lambda_1 = 1 \), signifying absence of motion in \( \eta_1 \)-direction. This happens in case

\[
J^2 - 2J - trace(F^2) = 0 \quad \Rightarrow \quad J = 1 \pm \sqrt{1 + trace(F^2)}, \quad (A5)
\]

which follows from the characteristic polynomial of \( F \). Eigenvectors \( n_{2,3} \) span the before-mentioned perpendicular plane. Points on periodic lines are, given \( \lambda_1 = 1 \) and discriminant \( D \) according to (A4), fully characterized by the single matrix invariant \( J \). Two kinds exist: elliptic \( (J < 3) \) and hyperbolic \( (J > 3) \) lines. Elliptic lines are centres of families of concentric tubes; hyperbolic lines are, reminiscent of isolated periodic points, the parent entities of 2D-2D manifold pairs \( (W_1 D, W_2 D) \). Periodic lines admit segmentation into elliptic and hyperbolic parts. The invariant \( J \) typically varies smoothly along periodic line and may thus cause division into elliptic \( (J < 3) \) and hyperbolic \( (J > 3) \) segments.
3. Manifold dynamics and interactions

The manifolds of isolated periodic points and hyperbolic segments of periodic lines are essential to the dynamics. Manifold pairs \((W^s_{2D}, W^u_{2D})\) associated with either the same or two different periodic lines or with two different isolated periodic points may merge into one smooth surface \((S = W^s_{2D} \cup W^u_{2D})\) or may intersect transversely \((\mathcal{I} = W^s_{2D} \cap W^u_{2D})\). Merger leads to the formation of transport barriers; intersection results in exponential stretching of material and, inherently, chaotic advection.\(^{16}\) Isolated periodic points furthermore admit mergers \(S = W^s_{1D} \cup W^u_{1D}\) (homo/heteroclinic orbit) and \(S = W^s_{1D} \cup W^u_{1D}\) (heteroclinic orbit) as well as homo/heteroclinic transverse intersections \(\mathcal{I} = W^s_{1D} \cap W^u_{1D}\). (The transversality theorem renders intersections \(W^s_{1D} \cap W^u_{1D}\) unlikely.\(^{42}\)) Here transverse interaction again promotes chaos. Merger, on the other hand, does not signify transport barriers; it merely reflects (local) absence of chaos. Chaos due to periodic lines (locally) is essentially 2D.\(^{15}\) Absence of periodic lines thus is a necessary prerequisite for 3D chaos.

Transverse intersections \(\mathcal{I} = W^s \cap W^u\) are asymptotic limits of the parent entities of the manifolds (i.e., periodic lines or isolated periodic points) and thus must be topologically consistent with the latter. Hence, intersections \(W^s_{2D} \cap W^u_{2D}\) between periodic lines define an infinite set of disconnected curves. However, if at least one of the parent entities is an isolated periodic point, intersections \(W^s_{2D} \cap W^u_{1D}\) define a heteroclinic orbit connecting both parent entities. Intersections \(W^s_{2D} \cap W^u_{1D}\) yield infinite sets of isolated points.

Manifolds of the same stability cannot intersect. This has the fundamental implication that 2D manifolds act as transport barriers to any manifold of identical stability.

4. Existence of periodic lines

A case of particular interest in the present context are systems of the form \((A1)\) with closed invariant surfaces parameterized by \(\xi_3\) that are convex.\(^{43}\) Brouwer’s fixed-point theorem then states that each such invariant surface must accommodate at least one period-1 point \(\hat{\xi}^0\).\(^{16}\) These period-1 points \(\hat{\xi}^0\) are defined implicitly by

\[
G(\hat{\xi}^0) \equiv \Phi_\xi(\hat{\xi}^0) - \hat{\xi}^0 = 0, \quad \hat{\xi}_{n+1} = \Phi_\xi(\hat{\xi}_n),
\]

with \(\Phi_\xi\) the map associated with \((A1)\) in terms of \(\xi\). (The specific relation between \(\Phi_\xi\) and \(\Phi_T\) depends on the transformation \(\mathcal{F}: x \rightarrow \xi\) and, depending on the shape of the invariant surfaces, may be far from trivial.) Period-1 points \(\hat{\xi}^0\) merge into period-1 lines \(\mathcal{P}^{(1)} = (\hat{\xi}^0, \hat{\xi}^0, \hat{\xi}^0)\), with \(\hat{\xi}_3\) as tangent coordinate, whenever

\[
\dot{\xi} = \left[ \frac{\partial G_1}{\partial (\xi_1, \xi_2)} \right]_{\hat{\xi}^0} \neq 0,
\]

which follows from the implicit-function theorem.\(^{29}\) This condition is generically met, save isolated points at which \(\Xi^0 = 0\), meaning that flows with convex invariant surfaces normally exhibit at least one period-1 line \(\mathcal{P}^{(1)}\). Existence criterion \((A7)\) via definition \((A6)\) involves the intra-surface components of the Jacobian \(J = \partial \Phi_\xi / \partial \xi\) that, in turn, relates to the deformation tensor \(F\) in \((A3)\) through coordinate transformation \(\mathcal{F}\). This links the formation of periodic lines and the type of constituent periodic points.\(^{29}\) However, this link may vary for generic curvilinear reference frames \(\xi\) and, instead of providing a universal formulation, is therefore elaborated only specifically for the current system in Sec. IV.

For systems possessing a time-reversal reflectional symmetry \(S\), with \(I_S = SI_S\) the associated symmetry plane,\(^{44}\) according to

\[
\Phi_T = S\Phi_T^{-1}S,
\]

this period-1 line occurs within \(I_S\).\(^{16}\) (Note that \(S\) furthermore implies symmetric pairs of periodic lines outside \(I_S\). However, contrary to \(\mathcal{P}^{(1)}\), these lines should not necessarily exist and are therefore not considered here.) The period-1 line \(\mathcal{P}^{(1)}\) is defined by the intersection of the symmetry plane
with its mapping, i.e.,
\[ \mathcal{P}^{(1)} \equiv I_S \cap \Phi_T(I_S), \]
which facilitates systematic isolation. For time-periodic flows (9), symmetries \( S \) following (A8), if existent, originate from symmetries of the base flow \( F_c \) and its reorientations.15,16,19

5. Emergence of isolated periodic points from perturbed periodic lines

Weak perturbation of the invariant surfaces causes breakdown of the period-1 line \( \mathcal{P}^{(1)} \) into isolated periodic points \( \xi^* \), defined by
\[ G^*(\xi^*) = \Phi^*_T(\xi^*) - \xi^* = 0, \]
where the star indicates the perturbed state with respect to (A1). Isolated points \( \xi^* \) exist if \( G^* \equiv |\partial G^*/\partial \xi|_0 \neq 0 \), which for \( \Phi^*_T = \Phi_T + \epsilon h \) and \( \epsilon \ll 1 \) admits approximation by
\[ \Xi^* = \Xi^0 \frac{\partial G^*_3}{\partial \xi^3} \neq 0 \Rightarrow \Xi^0 \neq 0 \text{ and } \frac{\partial G^*_3}{\partial \xi^3} \neq 0, \]
based on Ref. 29. This links the emergence of isolated periodic points in the perturbed system directly to the existence of periodic lines. Typical 3D perturbations always yield \( \partial G^*_3/\partial \xi^3 = \epsilon \partial h_3/\partial \xi^3 \neq 0 \) and thus periodic lines \( (\Xi^0 \neq 0) \) for \( \epsilon = 0 \) imply isolated periodic points \( (\Xi^0 \neq 0) \) for \( \epsilon > 0 \) in their direct proximity.29 (Note that assumption \( \partial h_3/\partial \xi^3 \neq 0 \) ensures \( G^*_3 = 0 \) — and thereby condition (A10) — is satisfied indeed only in isolated positions.) Moreover, the type of periodic points correlates with the properties of the underlying periodic lines. This is addressed more specifically in Sec. V.

Remarkable in the present context is that the 3D flow domain as a whole is open and non-convex, meaning that Brouwer’s fixed-point theorem in general does not apply and isolated period-1 points normally may yet by no means must exist. However, the existence of convex invariant surfaces fundamentally changes this situation by causing Brouwer’s fixed-point theorem to imply at least one period-1 point within each of these subdomains and, inherently, at least one period-1 line in the 3D domain. The existence of a period-1 line, in turn, implies isolated periodic points in case of a “weakly” perturbed system. Only for “stronger” departures from the invariant-surface state may periodic structures completely vanish, consistent with the properties of a generic non-convex domain.

APPENDIX B: ISOLATION OF PERIODIC POINTS

Period-\( p \) points \( x \) are located by a root-finding algorithm applied to displacement \( dX(x) \equiv x - \Phi^p_T(x) \). This involves the following steps:

1. Subdivision of the area of interest into small boxes, each defined as \( B_i \equiv \{ b_1, \ldots, b_8 \} \), with \( b_i \) (1 ≤ \( i \) ≤ 8) its 8 vertices.
2. Computation of the vertex displacements \( dX_i \equiv dX(b_i) \) for each box.
3. Identification of boxes \( B \) within which the three components of \( dX(x) \) simultaneously have a root. This employs a 3D version of the bi-section method: a given box \( B \) contains a curve \( C \) at which a function \( F(x) \) vanishes (i.e., \( F(x) = 0 \) \( \forall x \in C \)) if \( F(b_i) > 0 \) for at least one and at most 7 vertices \( b_i \). Isolated periodic points \( x_p \) coincide with the intersection of the “root curves” \( C_{x,y,z} \) of the three components of \( dX(x) \): \( x_p = C_x \cap C_y \cap C_z \). Important to note is that existence of \( C_{x,y,z} \) does not imply an intersection \( x_p \). Hence, the bi-section method identifies boxes that may contain isolated periodic points \( x_p \). Actual isolation of \( x_p \) follows from the refinement procedure elaborated below.
4. Refinement of the root finding within each box by a modified version of the 3D Newton-Rhapson method. The original method iterates towards a root of \( dX \) via
\[ x_{k+1} = x_k + dx_k, \quad dx_k = G_k^{-1}dX(x_k), \quad G_k = -\nabla dX|_{x_k} = F|_{x_k} - I, \]
with $x_{k+1}$ the estimated root location, $F$ the deformation tensor following (A3), and $I$ the unit tensor. Initial condition for the iteration is the box center $x_0 = \sum_{i=1}^8 b_i/8$ and convergence is attained in case $e_k + 1 < e_k$, with $e_k = |dX(x_k)|$, implying progression towards the sought-after root ($\lim_{k \to \infty} e_k = 0$). However, convergence is highly sensitive to the initial guess in this approach. This constraint has been relaxed by slightly modifying the method such that the sequence of positions $R = \{x_0, x_1, \ldots, x_{k+1}, \ldots\}$ delineates the path towards the root. To this end the step-wise displacement is rescaled as $dX' = \gamma dX/|dX|$, with $\gamma$ the length of a line segment of $R$, which must be set far smaller than the side length of the box $d$. Numerical experiments put forth $\gamma/d \approx 0.1$ as a good value. Iteration is continued if $e_k$ exhibits monotonic decay ($e_k + 1 < e_k$) and terminated for $k_\ast$ such that $e_{k_\ast} < e_{\min}$, with $e_{\min}$ a preset accuracy threshold ($e_{\min} = 10^{-9}$ in the present study). The iteration is restarted with smaller $\gamma$ in case $e_k + 1 > e_k$ and aborted if multiple restarts fail to produce convergence. Boxes are considered devoid of isolated periodic points in such cases.

30 The term “periodic line” is strictly inappropriate and “periodic curve” should be used instead. However, in the literature on 3D chaotic advection this is a common term for indicating such coherent structures.


33 Spheroid means that these surfaces are not exactly spheres yet are topologically equivalent to spheres (see Ref. 16).


35 Note that the definition of parameter $\Xi^0$ is different from parameter $\Xi$ in Ref. 29.

36 This analysis is based on that of Ref. 29. The latter concerns systems in Cartesian coordinates and results identify with that of the present spherical system. However, it has not been examined to what extent this generalizes to arbitrary curved invariant surfaces and associated curvilinear reference frames $\xi$.

37 M. Henle, A Combinatorial Introduction to Topology (Freeman, San Francisco, 1979).


42 J. Guckenheimer and P. Holmes, Nonlinear Oscillations, Dynamical Systems and Bifurcations of Vector Fields (Springer, New York, 1983).

43 A space is convex if for any pair of points within the space, any point on the line joining them is also within the space. This may also be a curved surface.