Almost-invariant sets and invariant manifolds – Connecting probabilistic and geometric descriptions of coherent structures in flows

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A B S T R A C T

We study the transport and mixing properties of flows in a variety of settings, connecting the classical geometrical approach via invariant manifolds with a probabilistic approach via transfer operators. For non-divergent fluid-like flows, we demonstrate that eigenvectors of numerical transfer operators efficiently decompose the domain into invariant regions. For dissipative chaotic flows such a decomposition into invariant regions does not exist; instead, the transfer operator approach detects almost-invariant sets. We demonstrate numerically that the boundaries of these almost-invariant regions are predominantly comprised of segments of co-dimension 1 invariant manifolds. For a mixing periodically driven fluid-like flow we show that while sets bounded by stable and unstable manifolds are almost-invariant, the transfer operator approach can identify almost-invariant sets with smaller mass leakage. Thus the transport mechanism of lobe dynamics need not correspond to minimal transport.

The transfer operator approach is purely probabilistic; it directly determines those regions that minimally mix with their surroundings. The almost-invariant regions are identified via eigenvectors of a transfer operator and are ranked by the corresponding eigenvalues in the order of the sets’ invariance or “leakiness”. While we demonstrate that the almost-invariant sets are often bounded by segments of invariant manifolds, without such a ranking it is not at all clear which intersections of invariant manifolds form the major barriers to mixing. Furthermore, in some cases invariant manifolds do not bound sets of minimal leakage.

Our transfer operator constructions are very simple and fast to implement; they require a sample of short trajectories, followed by eigenvector calculations of a sparse matrix.

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1. Introduction

Transport and mixing processes play an important role in many natural phenomena and their mathematical analysis has received considerable interest in the last two decades. Areas of application include astrodynamics, molecular dynamics, fluid dynamics, and ocean dynamics; see e.g. \cite{1–4} for discussions of transport phenomena. Analytical and numerical treatments of transport typically assume that the motion of a passive particle is completely determined by an underlying autonomous or nonautonomous velocity field. A variety of different concepts from dynamical systems theory may then be used to detect barriers to particle transport, to explain the transport mechanisms at work, and to quantify transport in terms of transition rates or probabilities. Two different families of approaches have been developed in the past for the analysis of transport and mixing processes in dynamical systems: (i) geometric methods which make use of invariant manifolds and related concepts and (ii) probabilistic techniques which attempt to approximate so-called almost-invariant sets. One of the main aims of this work is to demonstrate numerically in a number of case studies that there is a strong connection between the two approaches and that the combination of the two types of analyses leads to a richer understanding of the global dynamics.

The notion that geometrical structures such as invariant manifolds play a key role in dynamical transport and mixing for fluid-like flows has been around for almost two decades. In autonomous settings, invariant cylinders and tori form impenetrable dynamical barriers. This follows directly from the uniqueness of trajectories of the underlying ordinary differential equation (ODE). Slow mixing and transport in periodically driven maps and flows can sometimes be explained by lobe dynamics of invariant manifolds \cite{5,6,3}. In non-periodic time-dependent settings, finite-time hyperbolic material lines \cite{7} and surfaces \cite{8} have been proposed as barriers to mixing. Both the theoretical and the numerical analysis of these Lagrangian coherent structures in mixing fluids in many different application areas has been the focus of considerable interest over the last decade and a half, see e.g. \cite{7–13}, and the references therein.

Unions of segments of invariant manifolds may form either complete or partial boundaries of regions that are completely or
partially dynamically isolated. These dynamically isolated regions are either invariant sets or almost-invariant sets. One of the main aims of this work is to demonstrate numerically that the regions that are maximally almost-invariant often have boundaries comprised of segments of invariant manifolds.

Almost-invariant sets arose in the context of smooth maps and flows on subsets of $\mathbb{R}^d$ [14,15] about a decade ago. The main theoretical and computational tool is the Perron–Frobenius (or transfer) operator, and almost-invariant sets were estimated heuristically from eigenfunctions of the Perron–Frobenius operator. Further theoretical and computational extensions have since been constructed [16–18]. A parallel series of work specific to time-symmetric Markov processes and applied to identifying molecular conformations was developed in [19] and surveyed in [19,20]. The constructions of [20] are transfer operator based and the transfer operator is derived directly from ensemble simulation of the dynamics. Related ideas have also been developed for finite-state Markov chains [21,22], where the starting point is a Markov chain model of some physical system that is similar in spirit to a transfer operator.

Connections between eigenmodes of evolution operators and slow mixing in fluid flow have recently begun to appear. Liu and Haller [23] observe via simulation a transient "strange eigenmode" as predicted by classical Floquet theory. Pikovsky and Popovych [24,25] numerically integrated an advection–diffusion equation to simulate the evolution of a passive scalar, observing that it is the subdominant eigenmode of the corresponding transfer operator that describes the most persistent deviation from the unique steady state. The particular form of flow used in [24,25] admitted a convenient Fourier series representation that allowed calculation of leading eigenmodes. The numerical methods we describe in the present paper can be used to estimate eigenmodes for flows that are continuous in space and time and require only the calculation of many short trajectories.

Prior work related to connections between geometric and statistical objects include [26,27], where ergodic averages of observables have been used to identify invariant sets in autonomous and periodically driven fluid-like flows in two and three dimensions. Connections with finite-time invariant manifolds have been studied numerically in the aperiodically driven setting [28]. The approaches [26–28] have the disadvantages of (i) requiring possibly lengthy integration times and (ii) the ambiguity of selecting an observable to ergodically average. In contrast, our transfer operator approach employs relatively short integration times and directly constructs slow eigenmodes that carry information about invariant and almost-invariant sets. The first connection between almost-invariant sets and invariant manifolds appeared in [29], where graph algorithms were applied to analyse transport in astrodynamics. The present paper significantly extends the results of [29] by treating a wide variety of systems and framing the probabilistic approach in terms of eigenfunctions of transfer operators rather than graph partitioning. The spectral approach is more natural, especially under variation of initial flow times and flow durations and delivers significant benefits in terms of the transfer operator describing the global dynamics.

In this work via a number of case studies in two and three dimensions, for autonomous and time-periodic flows, and for fluid-like and dissipative flows, we compare the geometric, manifold based decomposition of the phase space with the decomposition provided by the transfer operator approach. We will show that the two approaches are largely compatible in the sense that the manifolds often form at least partial boundaries of the regions identified by the transfer operator approach. In such situations the methods are complementary: (see also Fig. 1)

- the probabilistic approach determines which regions are the most dynamically isolated and therefore which manifold intersections are the most important in defining the boundaries of such regions,
- recognising that the boundaries of the almost-invariant regions are pieces of invariant manifold allows a more detailed understanding of the dynamics near the boundaries of the sets and how transport occurs in and out of the almost-invariant regions.

An outline of this paper is as follows. In Section 2 we provide background definitions for invariant sets, invariant measures, and ergodic measures, and summarise the four dynamical settings we will investigate. In Section 3 we define almost-invariant sets and the Perron–Frobenius operator. We then describe our numerical method for producing a finite-rank approximation of the operator and detail an algorithm for using eigenvectors of this finite-rank operator to determine almost-invariant sets. In Section 4 we investigate the connection between the probabilistic description of coherent structures via almost-invariant sets and the geometric description using invariant manifolds. Sections 5–8 contain our four major case studies in which we demonstrate the efficiency of the transfer operator approach in determining and extracting the largest, most coherent structures. In each case study we additionally compute major geometrical structures and demonstrate a high degree of correlation between the geometric structures and the almost-invariant sets. We find one exception to this correlation in the second part of our final case study where we show that lobe related transport need not correspond to minimal leakage from a set.

2. Background: Flows, invariant sets, and invariant measures

Let $M \subset \mathbb{R}^d$ be compact and $F : M \times \mathbb{R} \rightarrow \mathbb{R}^d$ be a smooth vector field. Let $m$ denote Lebesgue measure, normalised so that $m(M) = 1$. We consider the ODE

$$\dot{x} = F(x, t).$$

(1)

In the case where $F(x, t) = F(x)$, we will call the ODE autonomous, otherwise we call it nonautonomous or time-dependent. Let $\phi_t : M \times \mathbb{R} \rightarrow M$ be the flow, i.e. $\phi_t(x_0, t_0)$ is a solution to the ODE (1) with initial condition $x(t_0) = x_0$ and satisfies

$$\frac{d\phi_t}{dt}(x_0, t_0)|_{t=0} = F(x_0, t_0), \quad \text{for all } x_0 \in M, t_0 \in \mathbb{R}. \quad (2)$$
If a trajectory is at \( x_0 \in M \) at time \( t_0 \), then \( \tau \) time units later, the trajectory is at \( \phi_\tau(x_0, t_0) \).

**Remark 1.** In this contribution we will mainly deal with autonomous systems. For this reason and to simplify notation we will state all definitions and theoretical results in terms of an autonomous flow map \( \phi(x) = \phi(x, 0) = \phi(x, t) \forall t \in \mathbb{R} \). In the fourth case study of a periodically driven velocity field we will directly apply these concepts to the time-dependent flow map \( \phi(x, t) \).

**Definition 1.** We will call a set \( A \subseteq M \) invariant if \( \phi_{-\tau}(A) = A \) for all \( \tau \in \mathbb{R} \).

**Definition 2.** Endow \( M \) with the Borel \( \sigma \)-algebra and let \( \mu \) be a probability measure on \( M \). We call \( \mu \) an invariant measure for \( \phi \) if \( \mu(\phi_{-\tau}(A)) = \mu(A) \forall \tau \in \mathbb{R}, A \subseteq M \).

**Definition 3.** Let \( \mu \) be an invariant probability measure on \( M \) and \( A \subseteq M \) a measurable set. We call \( \mu \) an ergodic measure for \( \phi \) if \( \mu(\phi_{-\tau}(A)) = \mu(A) \forall \tau \in \mathbb{R}, A \subseteq M \), and either \( \mu(A) = 0 \) or \( \mu(A) = 1 \).

The settings we consider will fall into several different classes. We make a distinction between autonomous and time-periodic flows, those in 2D and those in 3D, and those for which the flow is fluid-like (divergence free) or dissipative (negative divergence). We will denote by \( \Lambda \) the "maximal invariant set". In fluid-like flows, \( \Lambda = M \), the entire compact domain; for dissipative flows, \( A \subseteq M \), for example, \( A_0 := \bigcap_{\tau \ge 0} \phi(\Lambda) \) may be a chaotic attractor.

Briefly, our four settings are:

1. **Autonomous fluid-like 2D flow (steady double-gyre flow):** We consider an autonomous flow with a double-gyre pattern. The model is a time-independent version of the double-gyre flow analysed in [11]. The domain \( M = [0, 2] \times [0, 1] \) is invariant and so \( \Lambda = M \). The flow preserves Lebesgue measure \( m \), which is not ergodic. This example will be used throughout the text to illustrate several fundamental concepts.

2. **Autonomous 3D fluid-like flow (steady ABC flow):** We consider an Arnold–Beltrami–Childress (ABC) flow on a compact domain. Restricting the dynamics to the torus \( M = \mathbb{T}^3 \) the domain is invariant so \( \Lambda = M \). The flow preserves Lebesgue measure \( m \), which is not ergodic. The steady ABC flow is our first case study, which illustrates how the transfer operator approach can be used to detect and approximate invariant sets.

3. **Autonomous 3D dissipative chaotic flows (Lorenz flow and Chua circuit):** These flows are models of convection rolls [31] and of a simple electronic circuit [32], respectively. In both cases the domain \( M \) is a neighbourhood of the origin in \( \mathbb{R}^3 \) and \( \Lambda \subseteq M \) numerically appears to be a chaotic attractor. The flow numerically appears to preserve an ergodic physical invariant measure \( \mu \). The Lorenz flow and the Chua circuit are our second and third case studies.

4. **Nonautonomous 2D fluid-like flow (unsteady double-gyre flow):** This time-periodic flow is introduced in [11] and serves as a simplified model of the double-gyre pattern that can be observed in many realistic flows. The domain \( M = [0, 2] \times [0, 1] \) is invariant and so \( \Lambda = M \). At all times \( \tau \in \mathbb{R} \), the flow preserves Lebesgue measure \( m \), which numerically appears to be not ergodic. The unsteady double-gyre flow is our fourth case study.

In the case studies we will concentrate our analysis on the Lorenz system and the double-gyre flow, while the ABC flow and the Chua circuit will be discussed only briefly.

### 3. Transfer operators and almost-invariant sets

In this section, we briefly recount some of the background relevant to almost-invariant sets, define the Perron–Frobenius operator, and describe how transfer operator constructions can be used to identify invariant and almost-invariant sets.

**Definition 4.** Let \( \mu \) be preserved by \( \phi \). We will say that a set \( A \subseteq M \) is almost-invariant over the interval \([0, \tau]\) if

\[
\rho_\mu(\tau)(A) := \frac{\mu(A \cap \phi_{-\tau}(A))}{\mu(A)} \approx 1.
\]

**Example 1 (Autonomous Double-Gyre).** Consider the two-dimensional autonomous ODE defined by

\[
\begin{align*}
\dot{x} &= -\pi \sin(\pi y) \\
\dot{y} &= \pi \cos(\pi x) \sin(\pi y)
\end{align*}
\]

on the domain \( M = [0, 2] \times [0, 1] \). This autonomous ODE has been constructed from a snapshot of the nonautonomous double-gyre system [11]. There is no transport between the left-hand square \([0, 1] \times [0, 1]\) and the right-hand square \([1, 2] \times [0, 1]\). Each square is foliated with periodic orbits centred about one of the points \((1/2, 1/2)\) and \((3/2, 1/2)\); see Fig. 2. The flow preserves Lebesgue measure on each square, but the measure is not ergodic.
measure (normalised so that \( m([0, 2] \times [0, 1]) = 1 \)) and Lebesgue measure is not ergodic. For example, the left and right squares \([0, 1] \times [0, 1] \) and \([1, 2] \times [0, 1] \) are each invariant sets of measure 1/2. Note that the densities \( \chi_{[0, 1]}(x) \) and \( \chi_{(1, 2] \times [0, 1]}(x) \) are both fixed under \( P \) for all \( \tau \).

3.1. Numerical estimation of \( \mathcal{P}_\tau \)

In order to analyse specific flows with the Perron–Frobenius operator, we require an explicit numerical estimate for \( \mathcal{P}_\tau \). A Galerkin approximation known as Ulam’s method [36] has been widely used to estimate \( \mathcal{P}_\tau \). One partitions \( M \) into small connected sets \( \{B_1, \ldots, B_n\} \) (usually a fine grid of boxes) and applies the projection \( \pi_n : L^1(M) \rightarrow \text{sp}(X_{B_1}, \ldots, X_{B_n}) \) defined by

\[
\pi_n f = \sum_{i=1}^n \left( \frac{1}{m(B_i)} \int_{B_i} f \, dm \right) \chi_{B_i}
\]

to \( \mathcal{P}_\tau \) to form \( \pi_n \mathcal{P}_\tau \). The action of \( \mathcal{P}_\tau \) on \( \text{sp}(X_{B_1}, \ldots, X_{B_n}) \) is given by the matrix \( \rho_{P_n,\tau,ij} = \frac{m(B_i \cap \phi_{\tau}(B_j))}{m(B_j)} \).

The matrix \( P_{\tau,n} \) is stochastic and therefore has a spectral radius of one and has at least one fixed point \( p_n \) (satisfying \( p_n P_{\tau,n} = p_n \) and \( \sum_{i=1}^n p_{n,i} = 1 \)), which by the Perron–Frobenius Theorem (see e.g. [37]) is nonnegative. If for a given \( \tau \), \( x \mapsto \phi_{\tau}(x) \) preserves an ergodic invariant probability measure \( \mu \) that is absolutely continuous with respect to Lebesgue measure, then \( P_{\tau,n} \) is eventually positive; the eigenvalue 1 is simple, and the corresponding eigenvector \( p_n \) is strictly positive; see Proposition 2.3 [38]. An estimate of the (unique) fixed point \( h_{\tau} \) of \( \mathcal{P}_\tau \) is constructed by setting

\[
h_{\tau} := \sum_{i=1}^n \frac{p_{n,i}}{m(B_i)} \chi_{B_i}.
\]

A corresponding approximate invariant probability measure is defined by

\[
\mu_{n}(A) := \int_A h_{\tau} \, dm.
\]

3 For simplicity of exposition, we will assume throughout that \( m(B_i) = m(B_j) \) for all \( i \neq j \). If this is not the case, the expression on the RHS of (7) should have \( m(B_i) \) in the denominator; the resulting matrix is then not necessarily stochastic. In order to make this matrix stochastic, we can perform a similarity transformation using the diagonal matrix with \( m(B_i) \), \( i = 1, \ldots, n \) on the diagonal.

4 We assume that \( p_n \) provides a good estimate of an invariant measure \( \mu \) via the density \( h_\tau \); see [35] and the references therein for details. As \( \mu \) does not depend on \( \tau \), in practice \( p_n \) has negligible time dependence. We will therefore drop the \( \tau \) dependence for \( p_n \) and its corresponding density \( h_{\tau} \).

5 A matrix \( P \) is eventually positive if there exists a finite positive integer \( k \) such that \( P^k > 0 \).

Convergence of the peripheral spectrum and eigenprojections of the transition matrix (7) to the true transfer operator as the partition is refined has been considered in a variety of autonomous settings [39–41]. To numerically estimate the fractions in (7), within each \( B_i \), \( i = 1, \ldots, n \), we will define a set of \( N \) test points \( x_{1}, \ldots, x_{N} \) and numerically integrate trajectories to obtain \( \phi_{\tau}(x_{k,i}), k = 1, \ldots, N \).

Then

\[
P_{n,\tau,ij} = \frac{\#\{k : x_{k,i} \in B_j, \phi_{\tau}(x_{k,i}) \in B_j\}}{N}.
\]

The flow time \( \tau \) should be chosen long enough so that most test points leave their partition set of origin, otherwise at the resolution given by the partition \( \{B_1, \ldots, B_n\} \), the approximate operator appears similar to the identity operator (i.e. \( P_{n,\tau} \approx \text{Id}_{\mathcal{P}_M} \)). There is no upper limit on \( \tau \), however, if \( \phi \) acts to separate nearby points, clearly the longer \( \tau \) is, the greater \( N \) should be in order to maintain a good representation of the images \( \phi_{\tau}(B_i) \).

3.2. Using eigenvectors to find almost-invariant sets

Let \( C_n := \{A \subseteq M : A = \bigcup_{i=1}^n B_i, I \subset \{1, \ldots, n\}\} \). We will search for sets in \( C_n \) that maximise \( \rho_{\mu,\tau} \). In practice, we use the following discretised version of \( \rho \):

\[
\rho_{n,\tau}(A) := \frac{\sum_{i,j} p_{n,i} p_{n,\tau,ij}}{\sum_{i,j} p_{n,i}}.
\]

We now describe a heuristic method for identifying sets in \( C_n \) for which \( P_{n,\tau} \) is close to maximal.

Note that the stochastic matrix \( P_{n,\tau} \) may be viewed as a transition matrix of an \( n \)-state Markov chain. We define a time-reversal version of \( P_{n,\tau} \) by

\[
R_{n,\tau} := (P_{n,\tau} + \hat{P}_{n,\tau})/2,
\]

where \( \hat{P}_{n,\tau} \) is the stochastic matrix governing the time reversal of the finite-state Markov chain with transition matrix \( P_{n,\tau} \), namely

\[
\hat{P}_{n,\tau,ij} = p_{n,j} p_{n,\tau,ji}/p_{n,i}.
\]

A simple calculation [17] reveals that (11) is unchanged if \( R_{n,\tau} \) is substituted for \( P_{n,\tau} \). Thus, for the purposes of calculating \( \rho_{n,\tau} \), we henceforth use \( R_{n,\tau} \). The following proposition shows that the existence of a set \( A \) with \( \rho_{\mu,\tau}(A) \approx 1 \) forces the existence of an eigenvalue of \( R_{n,\tau} \) close to 1 and vice versa.

**Proposition 1.** Let \( \lambda_2 \) denote the second largest eigenvalue of \( R_{n,\tau} \) and \( A = \bigcup_{i=1}^n B_i, I \subset \{1, \ldots, n\} \).

\[
1 - \sqrt{2(1-\lambda_2)} \leq \max_{i,j} \rho_{n,k}(A) \leq \frac{1+\lambda_2}{2}.
\]

**Proposition 1** is a simple reformulation of Theorem 4.3 [42] in our notation. The proof of the upper bound for \( \rho_{n,\tau} \) motivates the following heuristic approach we will use for finding almost-invariant sets. Let \( v_{\delta_{R,\tau}} \) be the right eigenvector of \( R_{n,\tau} \) corresponding to the second largest eigenvalue \( \lambda_2 \) and define the sets

\[
A^+ := \bigcup_{i,j} B_i, \quad A^- := \bigcup_{i,j} B_i.
\]

The pair \( A^+, A^- \) partition \( M \) into two sets between which we expect little communication of trajectories. This heuristic was originally proposed by Dellnitz and Junge [15,14].

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6 Dellnitz and Junge [14] used the left eigenvector \( v_{\delta_{R,\tau}} \) of \( P_{n,\tau} \) corresponding to the second largest eigenvalue \( \lambda_2 \) of \( P_{n,\tau} \) and based their heuristic on a perturbation argument; see [14] for details.
Froyland and Dellnitz [16] extended this heuristic by (i) defining

\[ A^+_c := \bigcup_{i \in \mathbb{N}, i \leq c} B_i, \quad A^-_c := \bigcup_{i \in \mathbb{N}, i > c} B_i, \tag{16} \]

(ii) selecting \( c \) so as to maximise \( \rho_n(A^+_c) \) and \( \rho_n(A^-_c) \), and (iii) by combining the information contained in several eigenvectors that correspond to eigenvalues close to 1. The maximisation over \( c \) was based upon elements of the proof of the lower bound of Proposition 1, from which the presence of a large second eigenvalue of \( R_{n,\tau} \) forces the existence of an almost-invariant set. This dynamical separation procedure is similar in spirit to spectral methods used to decompose graphs, such as described in e.g. [43]. The use of \( R_{n,\tau} \) in place of \( P_{n,\tau} \) was developed in [17]; in the present work this is the approach we take. In summary:

**Algorithm 1.**

1. Partition the state space \( M \) into a collection of connected sets \( \{B_1, \ldots, B_n\} \) of small diameter.
2. Construct the Ulam matrix \( P_{n,\tau} \) (7) according to (10).
3. Compute the unique fixed left eigenvector \( p_0 \) of \( P_{n,\tau} \) and construct the matrix \( \hat{P}_{n,\tau} \) according to (13).
4. Compute \( R_{n,\tau} \) using (12) and compute the second largest eigenvalue \( \lambda_2 \) and corresponding right eigenvector \( \nu_{\lambda_2} \).
5. Form \( A^+_c, A^-_c \) using (16), selecting \( c \) so as to maximise \( \min(\rho_n(A^+_c), \rho_n(A^-_c)) \).

The choice of maximising \( \min(\rho_n(A^+_c), \rho_n(A^-_c)) \) is motivated by the following results.

**Proposition 2.** Let \( \{A^+, A^-\} \) partition \( M \). Then \( \rho_{\mu,\tau}(A^+) < \rho_{\mu,\tau}(A^-) \) if \( \mu(A^+) < \mu(A^-) \).

**Proof.** Note that

\[ 1 = \frac{\mu(A^+ \cap \phi_{-\tau}(A^+)) + \mu(A^+ \cap \phi_{-\tau}(A^-))}{\mu(A^+)} = \frac{\rho_{\mu,\tau}(A^+)}{\mu(A^+)}, \tag{17} \]

and

\[ 1 = \frac{\mu(A^- \cap \phi_{-\tau}(A^-)) + \mu(A^- \cap \phi_{-\tau}(A^+))}{\mu(A^-)} = \frac{\rho_{\mu,\tau}(A^-)}{\mu(A^-)}. \tag{18} \]

Further, note that

\[ \rho_{\mu,\tau}(A^+ \cap \phi_{-\tau}(A^+)) + \rho_{\mu,\tau}(A^+ \cap \phi_{-\tau}(A^-)) = \mu(A^+), \tag{19} \]

and

\[ \rho_{\mu,\tau}(A^- \cap \phi_{-\tau}(A^-)) + \rho_{\mu,\tau}(A^- \cap \phi_{-\tau}(A^+)) = \mu(A^-). \tag{20} \]

Equalities (19) and (20) together yield

\[ \rho_{\mu,\tau}(A^+ \cap \phi_{-\tau}(A^+)) + \rho_{\mu,\tau}(A^- \cap \phi_{-\tau}(A^+)) = \mu(A^+ \cap \phi_{-\tau}(A^+)), \tag{21} \]

Making the substitution from (21) in Eq. (18) we obtain

\[ \rho_{\mu,\tau}(A^+) + \frac{\mu(A^+ \cap \phi_{-\tau}(A^-))}{\mu(A^+)} = \rho_{\mu,\tau}(A^-) + \frac{\mu(A^- \cap \phi_{-\tau}(A^-))}{\mu(A^-)}, \]

from which the result follows. \( \square \)

**Corollary 1.** For any \( c \in \mathbb{R} \),

\[ \min(\rho_{\mu,\tau}(A^+_c), \rho_{\mu,\tau}(A^-_c)) = \begin{cases} \rho_{\mu,\tau}(A^+_c), & \text{if } \mu(A^+_c) \leq 1/2; \\ \rho_{\mu,\tau}(A^-_c), & \text{if } \mu(A^-_c) < 1/2. \end{cases} \]

**Proof.** Immediate from Proposition 2. \( \square \)

Thus in Step 5 of Algorithm 1 by selecting a value of \( c \) to maximise \( \min(\rho_{\mu,\tau}(A^+_c), \rho_{\mu,\tau}(A^-_c)) \), Corollary 1 guarantees that whichever set \( A^+_c \) or \( A^-_c \) has the lower \( \rho \) value also has \( \mu \)-mass less than 1/2 and thus the bound of Proposition 1 applies.

**Remark 2.** In the following, to simplify notation, the index \( \tau \) will be dropped whenever the flow duration is clear, i.e. \( P_n \) denotes \( P_{n,\tau} \).

**Remark 3.** The eigenvectors of \( R_n \) will rank invariant and almost-invariant sets according to how "leaky" they are. That is, if one orders the eigenvalues of \( R_n \) as \( \lambda_1 > \lambda_2 > \lambda_3 > \ldots \), then the sets identified by an eigenvector \( v^m \) of \( \lambda_m \) are less leaky than those identified by an eigenvector \( v^m \) with \( m > k \); see [44] for a formal statement. In fact, the eigenvectors \( v^m \), \( k = 1, \ldots, n \) are pairwise orthogonal under the \( p_0 \)-weighted inner product \( \langle v, x \rangle_{p_0} := \sum_{i=1}^n v_i x_i p_{0,i} \) (see e.g. [42, Chapter 6.2.1]). Thus each eigenvector provides information on different almost-invariant sets. In the present paper we focus on the eigenvector \( v^1 \) and relate the associated almost-invariant sets to invariant manifolds. We refer the reader to [16,44,17,45] for discussion on further subdominant eigenvectors.

**Example 2.** Continuing with Example 1, we partition \( M = [0, 2] \times [0, 1] \) into \( n = 16384 \) boxes and estimate \( P_n \) from (5) and (10) with \( \tau = 0.2 \). Each box is sampled uniformly with 400 points and the 16384 \( \times \) 16384 matrix \( P_n \) is constructed. We form \( \hat{P}_n \) and \( R_n \) via (12) and (13), and compute the outer spectrum of \( R_n \). The spectrum of the matrix \( R_n \), including a zoom of a neighbourhood of 1, is shown in Fig. 3.

We note that the eigenvalue 1 has multiplicity 2. There are two eigenvectors spanning the corresponding eigenspace. One of these eigenvectors is the invariant density \( h \equiv 1/2 \), and the other is the zero mean function \( h_2(x) := \frac{1/2, 0 \leq x \leq 1/2 \quad 1/2 \leq x \leq 1} {1/2}. \) Identifying each half of the domain as an invariant set.

In this example, since the "second" eigenvalue \( \lambda_2 \) equals 1, the bounds \( \lambda_2 \) force the existence of a subset \( A \subset [0, 2] \times [0, 1] \) with \( \rho_n(A) = 1 \). There are two such sets, namely \( [0, 1] \times [0, 1] \) and \( [1, 2] \times [0, 1] \) each of which is a union of partition elements from \( \{B_1, \ldots, B_{16384}\} \).

**Remark 4.** In Example 2, the partition sets were aligned to the boundaries of the two invariant sets \([0, 1] \times [0, 1] \) and \([1, 2] \times [0, 1] \) and these invariant sets could be constructed as unions of partition elements. In general, however, this may not be the case and the spatial discretisation will destroy invariant sets unless the partition boundaries are adapted to the boundaries of the invariant sets. Thus, a matrix \( P_{n,\tau} \) may be ergodic (viewed as a Markov chain) even when \( \phi_{\tau}(\cdot) \) is not transitive. Any true positive measure invariant sets of \( \phi_{\tau}(\cdot) \) should be detected as almost-invariant sets via (16) with corresponding eigenvalues extremely close to 1. Furthermore, we expect these eigenvalues to converge to 1 as \( n \to \infty \).

This is in contrast to true almost-invariant sets, for which the corresponding eigenvalues bound the "probability of leakage" from sets (via (14)). In this case we expect the eigenvalues to converge to numbers strictly less than 1.
4. Invariant manifolds and almost-invariant sets

The transfer operator approach is a probabilistic view of dynamics. The classical geometric approach to analysing flows is through the study of equilibria, periodic orbits, and invariant manifolds. One of our main aims is to demonstrate that the transfer operator approach is often compatible with this classical approach and that by combining the two approaches, one obtains an even sharper analysis of a system. In this section, we briefly review how invariant manifolds determine invariant sets in fluid-like flows and discuss how these geometric objects can play a role in defining almost-invariant sets in chaotic dissipative systems.

4.1. Invariant manifolds and Lagrangian coherent structures

Consider the autonomous ordinary differential equation \( \dot{x} = F(x), x \in M \subseteq \mathbb{R}^n, t \in \mathbb{R} \), and its flow \( \phi \). Let \( \bar{x} \in M \) be a hyperbolic fixed point. Smooth local stable and unstable manifolds of \( x \) which are tangent to the stable and unstable eigenspaces of \( DF(\bar{x}) \) exist according to the Stable Manifold Theorem (see e.g. [46], Thm. 1.3.2). In the local stable manifold \( W^s_{loc}(\bar{x}) \) contraction is exponential with rates given by the real parts of the stable eigenvalues of \( DF(\bar{x}) \), likewise for the unstable manifold \( W^u_{loc}(\bar{x}) \) if the system is considered under time reversal. The global stable and unstable manifolds are defined as

\[
W^s(\bar{x}) = \left\{ y \in M \mid \lim_{t \to -\infty} \phi_t(y) = \bar{x} \right\}
\]

\[
W^u(\bar{x}) = \left\{ y \in M \mid \lim_{t \to +\infty} \phi_t(y) = \bar{x} \right\}
\]

respectively.

In general, invariant manifolds cannot be obtained analytically. However, (22) and (23) suggest a numerical scheme for the approximation of these objects: starting from the local manifolds (which can be approximated in terms of eigenspaces) one obtains the global stable and unstable manifolds by looking at the preimages and images of these local objects, respectively. A variety of numerical algorithms are based on this idea (see [47] for a survey) and we will in particular use the set-oriented continuation scheme introduced in [48], see also [49,50] for details.

We note that stable and unstable manifolds of hyperbolic fixed points or periodic orbits often can also be characterised from a variational point of view. The exponential contraction/expansion near the fixed point and Palis’ Lambda-Lemma (see e.g. [46], Thm. 5.2.10) suggest that pairs of points straddling a stable manifold will typically separate exponentially fast, likewise for the unstable manifold when the system is considered under time-reversal (see e.g. [51] for a detailed treatment). In nonlinear7 systems such exponential behaviour distinguishes these initial conditions from other arbitrary pairs of points. Hence, candidate manifolds can be detected by searching for such distinguished initial conditions. However, if the vector field \( F(x, t) \) is time-varying, time-asymptotic structures such as stable and unstable manifolds may not exist. Nevertheless, so-called Lagrangian coherent structures (LCS) have been defined [7,8,11], using the variational view described above. A quantity that measures the exponential divergence of infinitesimal perturbations is the finite-time Lyapunov exponent:

Definition 6 (Finite-Time Lyapunov Exponent). Let \( \bar{x} = F(x, t) \) be a nonautonomous ODE with flow \( \phi_t \). Fix initial time \( t_0 \) and flow time \( \tau \) and denote by \( D\phi_\tau(x_0, t_0) \) its spatial derivative at \( x_0 \). Define

\[
\mathcal{E}_\tau(x_0, t_0) = \frac{1}{2\tau} \log(\lambda_{\max}(D\phi_\tau(x_0, t_0)^T D\phi_\tau(x_0, t_0))),
\]

where \( \lambda_{\max}(D) \) is the largest eigenvalue of a matrix \( D \). The argument of \( \lambda_{\max} \) in (24) is symmetric and \( \mathcal{E}_\tau(x_0, t_0) \) represents the largest relative length growth of any vector under the action of \( D\phi_\tau(x_0, t_0) \). \( \mathcal{E}_\tau(x_0, t_0) \) is called the largest finite-time Lyapunov exponent associated with the trajectory \( \phi_s(x_0, t_0), s \in [0, \tau] \). For the time-reversed system we define

\[
\tilde{\mathcal{E}}_\tau(x_0, t_0) := \mathcal{E}_{\tau-s}(x_0, t_0)
\]

\[
= \frac{1}{2\tau} \log(\lambda_{\max}(D\phi_{-\tau-s}(x_0, t_0)^T D\phi_{-\tau-s}(x_0, t_0))).
\]

So-called “ridges” in the scalar fields \( \mathcal{E}_\tau(x_0, t_0) \) or \( \tilde{\mathcal{E}}_\tau(x_0, t_0) \) indicate the location of repelling and attracting LCS [7,8,11,12]. In the autonomous setup considered in Sections 5–7 LCS can be viewed as an approximation of the classical invariant manifolds (see e.g. [11,12]). The same applies for the Poincaré return map of the periodically driven flow in Section 8.

In Sections 5, 7 and 8 we estimate stable and unstable manifolds by applying a set-oriented methodology [51] to Definition 6. A box-valued approximation of the finite-time Lyapunov exponent field is computed; for each box in the covering \( \{B_i, \ldots, B_n\} \) we define the expansion rate of a box \( B_i, i = 1, \ldots, n \), as

\[
\delta_i(B_i, t) := \max_{x \in B_i} \mathcal{E}_\tau(x, t),
\]

and

\[
\tilde{\delta}_i(B_i, t) := \max_{x \in B_i} \tilde{\mathcal{E}}_\tau(x, t),
\]

respectively.

Each box carries local upper bounds for the two FTLE fields. If the box shrinks to a point \( x \) then via the continuity of the FTLE fields the quantities \( \mathcal{E}_\tau(x, t) \) and \( \tilde{\mathcal{E}}_\tau(x, t) \) are recovered. In practice, the expansion rates (26) and (27) are approximated using a collection of uniformly distributed initial conditions in each box and taking the maximum in (26) and (27) with respect to these points. The individual \( \mathcal{E}_\tau(x, t) \) and \( \tilde{\mathcal{E}}_\tau(x, t) \) are either computed by solving the variational equation as in Eqs. (24) and (25), or alternatively via computing the growth rate of the relative distance of pairs of particle trajectories. The latter approach has the advantage that it is derivative free and is therefore particularly suitable when the Jacobian is difficult to obtain; for instance when the RHS of the ODE is only given in terms of discrete data. Accuracy of the approximation is ensured by sufficiently small initial perturbations and sufficiently fine sampling. More details on the set-oriented expansion rate approach and convergence statements can be found in [51].

4.2. Autonomous flows in two dimensions

Invariant manifolds of autonomous flows on compact surfaces form impenetrable barriers for trajectories. If unions of segments of invariant manifolds form a closed curve, then the region enclosed by this curve is an invariant set. In this way, the invariant manifolds form a skeleton of the dynamics, dividing the domain into uncommunicating regions. In the autonomous double-gyre of Example 1, taking a geometric approach, we note that there is a heteroclinic connection of the unstable manifold of the fixed point \( (1, 1) \) and the stable manifold of the fixed point \( (1, 0) \). This invariant manifold separates the two halves of the domain \( M \) into the invariant sets \([0, 1] \times [0, 1] \) and \([1, 2] \times [0, 1] \). Taking a transfer operator approach, the two invariant sets \([0, 1] \times [0, 1] \) and \([1, 2] \times [0, 1] \) can be detected by the second eigenvector of \( \mathcal{K} \). Thus the
maximally almost-invariant sets can be easily identified via the
eigenfunction of the transfer operator corresponding to the second
largest eigenvalue. We remark that the separating heteroclinic
orbit would also be clearly detected by both fields $\mathcal{E}_1$ and $\mathcal{E}_2$.

To conclude we point out that the other major geometric
structures, namely the family of invariant sets enclosed by
foliations of periodicorbits shown in Fig. 2 are also detected by
combining eigenfunctions corresponding to the second and third
largest eigenvalues of the transfer operator.

4.3. Autonomous fluid-like flows in three dimensions

The situation in three dimensions is more complicated.
Studies of fluid-like flows on compact domains such as the
Arnold–Beltrami–Childress (ABC) flow, defined by (29), have
shown that there can exist invariant tori that divide the phase
space into invariant sets. For example, [52] prove that for
small positive $C$ in (29) the ABC flow possesses invariant tori.
However, the numerical identification of these invariant tori and
associated invariant sets can be difficult. Haller [8] has employed
hyperbolicity times and finite-time Lyapunov exponents to obtain
numerical estimates of the 2D stable and unstable manifolds of
hyperbolic periodic orbits that appear to bound invariant regions
identified by Dombre et al. [53]. In our first case study, in Section 5,
we demonstrate that these invariant regions are identified via
our transfer operator approach and are easily extracted from the
eigenvectors of the associated matrix $R_n$.

4.4. Autonomous dissipative flows in three dimensions

For chaotic dissipative flows, such as the Chua [32] and
Lorenz [31] flows (see Sections 6 and 7 for definitions), Lebesgue
almost all trajectories starting in a neighbourhood of the attractors
appear numerically to exhibit a unique ergodic invariant measure.
In fact, Tucker [54] has shown that the Lorenz system has a unique
SBR measure $\mu$ and by ergodicity of $\mu$ there are no invariant sets
with $\mu$-measure strictly between 0 and 1. Nevertheless almost-

invariant sets may exist for such flows and we can ask where these
sets lie in phase space and what relationship they have to invariant
manifolds. We demonstrate in two case studies, in Sections 6 and
7, that there is a very close connection between almost-invariant
sets and primary intersections of stable and unstable manifolds of
equilibrium points and low-period unstable periodic orbits of
the flow. Studies of almost-invariant sets for the Chua and Lorenz
systems have been undertaken in [15,16] respectively, however
the linking of these probabilistic findings with the geometry of
invariant manifolds is completely new.

4.5. Periodically driven fluid-like flows in two dimensions

In periodically driven fluid-like flows such as the double-gyre
flow [11] (see Section 8) stable and unstable manifolds of hyper-

bolic periodic orbits typically intersect transversally giving rise
to horseshoe dynamics. Nonetheless closed curves composed of
segments of stable and unstable manifolds form partial barriers
to transport where the heteroclinic tangle provides the transport
mechanism across the boundary. This concept is known as lobe
dynamics (see e.g. [5,6,3]) and has been successfully applied in a
variety of settings. In addition to chaotic motion induced by
the horseshoe dynamics, in the double-gyre system we can observe re-
gions of regular motion such as invariant tori. The transfer opera-
tor approach picks up regions formed by families of invariant tori
as the most almost-invariant sets. The transfer operator approach
also identifies almost-invariant sets with non-invariant boundaries
close to the manifolds responsible for the heteroclinic tangle.

4.6. Connecting the probabilistic and geometric approaches

The connection between the probabilistic and geometric
approaches is most clear when there is a positive volume region $A$
bounded by unions of invariant manifolds (e.g. the steady double-
gyre and the steady ABC flow). Impenetrability of the manifolds
means that $A$ is invariant and so $\chi_A/m(A)$ is an eigenfunction
of $\mathcal{P}_A$. The connection between the probabilistic and geometric
approaches is less clear when no such invariant set exists.

Let us first discuss the setting of Sections 6 and 7 which study
the Lorenz and Chua systems respectively. The attracting set of
the Lorenz system is known to be transitive [54], and there is
numerical evidence that the attracting set of the Chua system is
also transitive. The dynamics occurs on the unstable manifolds that
comprise the chaotic attractor. By transitivity, it is impossible to
enclose an open invariant set in the attractor by segments of stable
manifold. Nevertheless, there is still the possibility that almost-
invariant sets exist and the geometrical nature of the boundaries
of globally maximal almost-invariant sets may be non-trivial.

Definition 7. Consider a positive $d$-dimensional volume con-
ected set $A \subset M \subset \mathbb{R}^d$. We call the regular part of the boundary
of $A$ that portion of $\partial A$ that may be represented as a finite union
of segments of co-dimension 1 invariant manifolds, with each seg-
ment having positive $(d-1)$-dimensional volume. The remainder
of $\partial A$ we will call an exit boundary.

In Sections 6 and 7 we demonstrate that the boundaries of
globally maximal almost-invariant sets as determined by
the transfer operator formalism are mostly comprised of stable
manifolds. The remaining part of the boundary is not aligned with
a stable manifold and it is only through this piece of the boundary,
which we term an “exit boundary”, that transport is possible.
We conjecture that this is a universal way in which almost-
invariant sets are formed: by bounding them with segments of stable
manifold and leaving a small exit boundary through which
trajectories may leave the almost-invariant set.

We now argue heuristically that if one continuously deforms
the boundary of an almost-invariant set $A$ away from a stable
manifold, the invariance ratio will decrease. We thus argue that
local maxima of $\rho_{\mu,\tau}(A)$ are obtained by matching a segment of the
boundary of $A$ with a stable manifold.

We begin by noting that
\[
\rho_{\mu,\tau}(A) = \frac{\mu(A \cap \phi^{-\tau}_A(A))}{\mu(A)} = \frac{\mu(\phi^{\tau}_A \cap A)}{\mu(A)},
\] (28)

as $\phi_{\tau}$ is invertible and preserves $\mu$. We consider the locally 2D
setting where our set $A$ is contained in a locally 2D attractor $A$;
similar arguments apply in a 3D setting. Suppose that there exists
a stable manifold $W^s(x_0)$ of a hyperbolic fixed point $x_0$ and denote
by $C$ the intersection of some segment $W$ of this manifold with
$A$. Suppose also that there exists an almost-invariant set $A$ in the
vicinity of $C$, but not intersecting $C$; see Fig. 4(a).

Consider the local effect on points in $A$ near $C$. By hyperbolicity,
in backward time, points in $A$ near $C$ will be attracted out of $A$
toward $C$; see Fig. 4(a). If $A$ were to enlarge to cross $C$, those points
in $A$ on the right of $C$ would be repelled from $C$ and would leave $A$;
see Fig. 4(b). However, by locally matching precisely the boundary
of $A$ with $C$ both of these effects can be eliminated, reducing the
loss of points from $A$ locally near $C$ in both backward and forward
time, and increasing the value of $\rho_{\mu,\tau}(A)$. Thus, heuristically, we
argue that if one continuously deforms the boundary of an almost-
invariant set $A$ away from a stable manifold, $\rho_{\mu,\tau}(A)$ will decrease
and $\rho_{\mu,\tau}(A)$ will have a local maximum when the boundary of $A$
precisely matches the segment $C$.

Finding the globally maximal almost-invariant sets is highly
non-trivial, and practically impossible using only estimates of

\[
\text{G. Froyland, K. Padberg, Physica D 238 (2009) 1507–1523}
\]
invariant manifolds. It is far from clear which stable manifold segments one should piece together to form a globally maximal almost-invariant set. In Sections 6 and 7 we find that these boundaries are formed from stable manifolds of fixed points or low period orbits. We also find that these stable manifolds are associated with the strongest “ridges” in an FTLE field. One may be tempted to conjecture that globally maximal almost-invariant sets have boundaries formed from stable manifolds associated with the strongest “ridges” in an FTLE field. However, while local deviation of boundaries from such stable manifolds would lead to rapid flux across the new boundary, as argued in Fig. 4, the global structure of the manifolds and the size and position of the exit boundary also play a role.

In Section 8 we show that the global maximum of $\rho_{\mu,\tau}$ does not correspond to a set bounded by stable or unstable manifolds. In this case, we have a boundary with a rather large “exit boundary”, but an exit boundary that is well placed with respect to the dynamics so that mass transfer through the exit boundary is very small.

5. Case Study I — Autonomous fluid-like 3D flow (ABC flow)

To illustrate our methodology we begin with the following 3D system of ordinary differential equations:

$$\begin{align*}
\dot{x} &= A \sin z + C \cos y \\
\dot{y} &= B \sin x + A \cos z \\
\dot{z} &= C \sin y + B \cos x.
\end{align*}$$

(29)

This class of flows is known as ABC (Arnold–Beltrami–Childress) flows and the system (29) is notable for being an exact steady solution of Euler’s equation, exhibiting a nontrivial streamline geometry. We refer the reader to Haller [8] for a numerical analysis, and to Dombre et al. [53] for an analytical investigation. As in [53] we consider the ABC flow on the torus $T^3$, i.e. $0 \leq x, y, z < 2\pi$ in (29). The domain is invariant and preserves Lebesgue measure. For our choice of parameters $A = \sqrt{3}, B = \sqrt{2}, C = 1$ (cf. [8]) the flow is non-integrable and the system exhibits non-trivial invariant sets which are enclosed by 2D invariant manifolds.

The results for the application of the set-oriented expansion rate approach [51] as described in Section 4.1 are shown in Fig. 5(a). Here we used flow time $\tau = 5$ and coloured the boxes $B_i$ from a very fine box discretisation according to $\max[\delta_i(B_i), \delta_i^{-1}(B_i)]$. High values in the scalar field highlight stable and unstable invariant manifolds of hyperbolic periodic orbits and confirm Haller’s results [8]. Moreover the picture gives an indication of the dynamically distinct regions in the ABC flow.

For the numerical approximation of the transfer operator we partition $M = [0, 2\pi]^3$ into $n = 262144$ boxes and estimate $\rho_i$ from (10) with $\tau = 0.2$. Each box is sampled uniformly with 1000 points and the $262144 \times 262144$ sparse matrix $P_\tau$ is constructed. We form $\tilde{P}_\tau$ and $R_\tau$ via (13) and (12), and compute the outer spectrum of $R_\tau$. The largest six eigenvalues $\lambda_1 = 1, \lambda_2 = 0.9986, \lambda_3 = 0.9979, \lambda_4 = 0.9978, \lambda_5 = 0.9971,$ and $\lambda_6 = 0.9968$ are very close to 1. The eigenvector for the eigenvalue $\lambda_1 = 1$ gives the uniform invariant density, while the eigenvectors $v_i, i \geq 2,$ characterise almost-invariant sets, see Fig. 5(b). In fact these sets are truly invariant, the leakage is only due to the numerical discretisation described above; see Remark 4. For a finer discretisation the leading eigenvalues will converge to one and, consequently, the corresponding eigenvectors will relate to invariant sets. We note that the numerical results are very robust in that sense that the leading eigenvectors with respect to a coarser partition of $M$ highlight the same regions.

In order to extract approximations of some of the large invariant sets enclosed by invariant manifolds, we apply the heuristic approach described in Algorithm 1 to the eigenvector $v_i$.

The resulting partition into three sets is shown in Fig. 6(a). In Fig. 6(a) we also overlay the invariant manifolds obtained via taking regions with high values in the combined forward and backward time FTLE field as described above. These structures align exactly with the set boundaries that result from the thresholding approach. This confirms that truly invariant sets of the flow have been approximated.

Fig. 4. (a) Almost-invariant set $A$ in a locally 2D attractor $\Lambda$ with boundary near $C = W_2 \cup A$ where $W_2 \subset W^s(x_0)$ is a locally 1D segment of a stable manifold $W^s(x_0)$ of a hyperbolic fixed point $x_0$. In reverse time, points in $A$ near $C$ are attracted out of $A$ toward $C$. (b) Almost-invariant set $A$ crossing $C = W_2 \cup A$. In forward time, those points in $A$ on the right of $C$ are repelled out of $A$. Both of these effects are minimised when the boundary of $A$ matches $C$.

Fig. 5. (a) Application of the set-oriented FTLE approach using flow times $\tau = \pm 5$ on the ABC flow model with dark values highlighting invariant manifolds. The scalar field gives an indication of dynamically distinct regions. (b) Extremal values in the eigenvector $v_i$ of $R_\tau, n = 262144$, in the ABC flow indicate the existence of (numerically almost-)invariant sets.
Finally, to further demonstrate the power of the transfer operator approach we show that the individual 3D invariant sets are easily extracted by simply displaying those grid sets with $\nu^2_{c,i}$ values in the appropriate ranges. The results are shown in Fig. 6(b). Thus the set-oriented transfer operator method combined with thresholding also provides a convenient framework to visualise and extract invariant sets. To extract further invariant sets, one may use information from other eigenvectors $\nu^k_i$, see Remark 3.

6. Case Study II — Autonomous dissipative 3D flow (Lorenz flow)

The Lorenz flow [31]

\[
\begin{align*}
\dot{x} &= \sigma (y - x) \\
\dot{y} &= \rho x - y - xz \\
\dot{z} &= -\beta z + xy
\end{align*}
\]

arose as a model of convection rolls in climatology. It is well known as a simple model of a continuous-time dynamical system that can exhibit chaotic dynamics. We choose the classical parameters $\sigma = 10, \beta = \frac{8}{3}, \rho = 28$ for which the system is known to possess a chaotic attractor $\Lambda$ with an SBR measure $\mu$ [54].

First, we approximate the chaotic attractor observed in the Lorenz system using a set-oriented subdivision scheme; for details on such computations we refer to [48-50]. We obtain an approximation of the attractor $\hat{A}$ consisting of $n = 19978$ equally sized boxes. These boxes will also be the basis for approximating the transfer operator $\hat{\Sigma}$, where we choose $\tau = 0.2$. As with the ABC flow we use 1000 points per box to obtain the $n \times n$ matrix $P_n$ with its leading left eigenvector $p_n$ and then compute $\hat{P}_n$ and $R_n$. The largest eigenvalues of $R_n$ are found to be $\lambda_1 = 1, \lambda_2 = 0.9853, \lambda_3 = 0.9801, \lambda_4 = 0.9702, \lambda_5 = 0.9666, \lambda_6 = 0.9641$. As the Lorenz flow is transitive on $\Lambda$, we should not be able to identify any open invariant sets, in contrast to the ABC flow. Thus the features contained in the second eigenvector $\nu^2_n$ should correspond to almost-invariant sets rather than invariant sets. The second eigenvector $\nu^2_n$ is shown in Fig. 8(a).

Applying the thresholding ansatz to $\nu^2_n$ while varying $c$, we find that $\min(\rho_0(\Lambda^c_+), \rho_0(\Lambda^c_-))$ has a global maximum at $c = 0$, with $\rho_0(\Lambda^c_+)$ $= 0.9419 = \rho_0(\Lambda^c_-)$ and $\mu(\Lambda^c_+)$ $= 0.5 = \mu(\Lambda^c_-)$, see Fig. 7. Inserting $\lambda_2 = 0.9853$ into Eq. (14) gives a theoretical lower bound of $0.8285$ and an upper bound of $0.9927$. So the thresholding heuristics produce sets $\Lambda^c_+, \Lambda^c_-, c = 0$, with values $\rho(\Lambda^c_-) = 0.9419$ close to the theoretical upper bound.

The partition into two sets obtained via thresholding is shown in Fig. 8(b). Note that the symmetry in the Lorenz flow not only affects the geometry of the attractor but it also carries over to the transfer operator and, hence, the resulting partition into almost-invariant sets; see [55] for an analysis of symmetries and Perron–Frobenius operators.

In Fig. 8(c) we have also included part of the stable manifold of the hyperbolic fixed point at the origin, approximated using set-oriented continuation methods (see [48-50] for details). The intersection between the attractor and the stable manifold of the origin determines a large part of the boundary between the two almost-invariant sets, but because of the mutual geometry of the manifolds they can only form a partial boundary. For a more detailed visualisation of the interaction of the Lorenz manifold and attractor under parameter variation we refer to [56].

In addition we approximated low-period unstable periodic orbits (using estimates on the periods by [57]). The lowest period symmetric unstable periodic orbit (period $T = 1.558652$, see [57]) and its stable manifold determine another large part of the boundary between the two almost-invariant sets, see Fig. 8(d). The complete boundary between the two almost-invariant sets appears to be determined by both the unstable equilibrium point and this unstable periodic orbit and their stable manifolds.
An explanation for why this lowest period symmetric unstable periodic orbit and its stable manifold\(^{8}\) should form part of the boundary between the two identified almost-invariant sets is as follows. If we focus our attention on the right-hand wing in Fig. 8(d) we see that trajectories starting in the dark region ("outside" the periodic orbit) will be injected into the dark region on the left-hand wing ("inside" the periodic orbit). Meanwhile, trajectories that begin in the light region on the right-hand wing near to the light/dark boundary will be ejected into the light region on the left wing. Thus, at least on the wings, the periodic orbit acts as a dividing line separating the two almost-invariant sets. Away from this periodic orbit, the boundary of the almost-invariant sets is determined by the stable manifold of the equilibrium point at the origin.

In Fig. 8(c) we demonstrate how a typical trajectory starting close to the stable manifold of the origin behaves: it first follows the outside of the left wing of the attractor in a clockwise direction and then switches to the right-hand wing and spirals for a long time around the equilibrium point in the right wing before switching to the left wing again. This switching behaviour is described by the two almost-invariant sets: the trajectory follows the light set for a long time before moving to the darker set. We note that trajectories can move between the inner and outer parts of the wings of the attractor. The manifolds determine the paths a trajectory may take and consequently the likelihood and possible location of transitions between certain regions in the attractor. In fact, transitions between the two identified almost-invariant sets may only occur through the part of the common boundary that is not comprised of invariant manifolds. This part of the common boundary is the "exit boundary" we discussed in Section 4.6.

In Fig. 9(a) we view a slice of the attractor and its intersections with the stable manifold of the origin. This manifold alone determines only part of the boundary between the two almost-invariant sets as already described above. In Fig. 9(b) additionally the stable manifold of the periodic orbit described above (see Fig. 8(d)) is shown. This visualisation in Fig. 9(b) supports the observation that the combination of these manifolds largely explains the formation of the two almost-invariant sets and the transport mechanism between them.

When considering a finer covering of the Lorenz attractor (\(n = 636544\) boxes)\(^{9}\) the geometry of the two almost-invariant sets becomes more detailed; see Fig. 10. Here the boundary appears to be determined not only by the stable manifolds of the equilibrium and lowest period periodic orbit but also of the next simplest symmetric unstable periodic orbit (period \(T = 3.084277\), see [57]).

---

\(^{8}\) Note that the periodic orbit corresponds to the curve of intersection of its stable manifold with the covering of the attractor.

\(^{9}\) Computational results for this setup: \(\lambda_2 = 0.9875, \mu_{n}(A_0^{-}) = 0.95\) and \(\mu_{s}(A_0^{-}) = 0.5\).
Fig. 9. Slice through the attractor at $z = 27$ and intersections with stable manifolds (computed via a set-oriented continuation scheme). (a) Stable manifold of the origin determines part of the boundary between almost-invariant sets as in Fig. 8(c). (b) The combination of stable manifolds of the origin and of a low-period periodic orbit (see Fig. 8(d)) agrees well with the almost-invariant decomposition.

Fig. 10. A finer box partition is used for the approximation of the attractor and $P_{\tau}, \tau = 0.2$. (a)–(b) The boundaries of the almost-invariant sets appear to be composed of parts of the stable manifolds of the origin and of low-period unstable periodic orbits (periods $T = 1.558652$ and $T = 3.084277$, see [57]). For clarity only the orbits themselves are shown.

An explanation for this is as follows. In our earlier discussion referring to Fig. 8(d) we pointed out that trajectories beginning in the light region in the right-hand wing near to the light/dark boundary were immediately ejected to the outer light region in the left-hand wing. However, the existence of the periodic orbit in Fig. 10(b) demonstrates that this is not true for all such points. In fact, points sitting on or nearby the “interior curve” of the periodic orbit shown in Fig. 10(b) flow (after winding twice around the right-hand wing) into the “interior” of the shorter periodic orbit shown in Fig. 8(d). This finer structure is picked up by the transfer operator and is the darker coloured loop in the interior of the right-hand wing shown in Fig. 10(a). Most of the darker coloured points on this thin curve quickly find their way into the large dark coloured outer portion of the right-hand wing and are then ejected into the large dark coloured inner portion of the left-hand wing.

To conclude we point out that the transfer operator approach determines maximally almost-invariant sets. Ranking is possible with respect to the corresponding eigenvalues which also bound the invariance ratios of the sets of interest. We find that the boundaries between the maximally almost-invariant sets in the Lorenz system are composed of parts of the stable manifold of unstable objects (i.e. fixed point, low-period periodic orbits), allowing a more detailed understanding about the transport mechanisms between almost-invariant sets. However, a decomposition into almost-invariant sets solely based on the knowledge of the geometric objects is problematic because there are many possible candidate objects and since transitivity precludes open invariant sets, combinations of stable and unstable manifolds can at best form partial boundaries for almost-invariant sets.

7. Case Study III — Autonomous dissipative 3D flow (Chua circuit)

The Chua flow is another example of an autonomous dissipative 3D system. It arose as a model of a simple electric circuit and is described by the following set of ordinary differential equations:

$$\begin{align*}
\dot{x} &= \alpha \left( y - m_0 x - \frac{1}{3} m_1 x^3 \right) \\
\dot{y} &= x - y + z \\
\dot{z} &= -\beta y
\end{align*}$$

with $\alpha = 18, \beta = 33, m_0 = -0.2, m_1 = 0.01$.

For the analysis of the maximal invariant set, we approximate the global unstable manifold of the origin using a set-oriented continuation method, see again [48–50] for details. Numerical integration of trajectories suggests that this manifold supports a
unique physical measure $\mu$. As a result we obtain a covering of the numerically observed chaotic attractor $A$, consisting of $n = 76034$ boxes. Integrating 1000 uniformly distributed points per box for time $\tau = 0.2$ we build $P_n$ and $R_n$ as described earlier. The leading eigenvalues of $R_n$ are $\lambda_1 = 0.9915, 10$, $\lambda_2 = 0.9839$, $\lambda_3 = 0.9785$, $\lambda_4 = 0.9756$, $\lambda_5 = 0.9754$, $\lambda_6 = 0.9741$. The eigenvector $v_1^2$ is shown in Fig. 11(a).

Thresholding using $v_1^2$ and varying $c$ as described above results in a global maximum of $\min(\rho_0(A_0^c), \rho_0(A_0^{c+}))$ for $c = 0$. For this value we obtain $\rho_0(A_0^c) = \rho_0(A_0^{c+}) = 0.9524$ and $\mu_0(A_0^c) = \mu_0(A_0^{c+}) = 0.5$, with the two sets shown in Fig. 11(b). This value is again close to the theoretical upper bound of 0.9920, whereas the lower bound is 0.8206. Note that as in the Lorenz flow the symmetry of the attractor naturally carries over to the almost-invariant sets.

The geometry of the stable manifold of the origin is even more complicated than in the Lorenz system. Therefore we demonstrate the interaction of the manifold with the almost-invariant sets by showing only its intersection with the numerical approximation of the attractor, see Fig. 11(b). This is obtained by extracting regions with high expansion rate values $\delta_i(B_i)$ for $i = 1, \ldots, n_i$ with $n_i > n$, corresponding to a finer covering of the attractor (for visualisation purposes only). The expansion rate field is computed for flow time $\tau = 1$. In Fig. 11(b) we see that the stable manifold of the origin approximated as described above forms a partial boundary of the almost-invariant sets. In Fig. 11(c) we show the primary intersection of the stable manifold (approximated via a set-oriented continuation method) on a fixed slice $z = 0$, confirming our observations. We note that as in the Lorenz system low-period unstable periodic orbits and their stable manifolds will most likely explain further parts of the boundary between the two almost-invariant sets.

In Fig. 11(d) we have separated the two almost-invariant sets to make the complicated interior structure of the attractor visible. The spiral pattern is also seen in Fig. 11(c) and appears to largely determine the shape of the attractor. Again the almost-invariant set decomposition provides high-level information on the macroscopic dynamics of the underlying dynamical system.

8. Case Study IV — Periodically driven 2D flow (Double-Gyre)

We consider the time-dependent system of differential equations [11]

\[
\begin{align*}
\dot{x} &= -\pi A \sin(\pi f(x, t)) \cos(\pi y) \\
\dot{y} &= \pi A \cos(\pi f(x, t)) \sin(\pi y) \frac{df}{dx}(x, t),
\end{align*}
\]

where $f(x, t) = \epsilon \sin(\omega t) x^2 + (1 - 2\epsilon \sin(\omega t)) x$.

For $\epsilon = 0$, (32) corresponds to the autonomous double-gyre (5) on $M = [0, 2] \times [0, 1]$. For small $\epsilon \neq 0$ the instantaneous separation point moves along the $x$-axis with a period $\frac{2\pi}{\omega}$. For $t = 0$ the
Fig. 12. Second eigenvector $v^2_n(t)$ of $R_n(t)$, $n = 131072$, for different choices of $t$ in the double-gyre flow.

An initial decomposition: Regular and chaotic regions

Thresholding with $v^2_n := v^2_{n,1}(0)$ while varying $c$, we find $\min\{v^2_n(A^1), \rho_1(A^1)\}$ has two global maxima at $c = \pm 0.0013$; see Fig. 13(a). For $c = -0.0013$ we obtain $\rho_1(A^1) = 0.9960$ and $\rho(A^1) = 0.9992$ with $\mu(A^1) = 0.1611$ and $\mu(A^1) = 0.8389$, for $c = 0.0013$ it is $\rho(A^1) = 0.9992$ and $\rho(A^1) = 0.9960$ with $\mu(A^1) = 0.8389$ and $\mu(A^1) = 0.1611$. The resulting two sets for some $c = \pm 0.0013$ are one of the egg-shaped regions in Fig. 13(a) and its complement, respectively. A three-set partition as shown in Fig. 13(a) is obtained choosing $A_1 = \cup_{c+0.0013 < c < c} B_i$, $A_2 = \cup_{c+0.0013 < c} B_i$, $A_3 = \cup_{c+0.0013 > c} B_i$, where $c = 0.0013$. Here $A_1$ (dark) and $A_2$ (light) correspond to the two eggs with $\rho(A_1) = 0.9960$, $\mu(A_1) = 0.9961$ and $\rho(A_2) = 0.9981$, $\mu(A_2) = 0.6778$.

We now begin to analyse the system using standard geometrical constructions. We will see that the sets $A_1$, $A_2$, and $A_3$ are in fact invariant sets. Firstly, we note that for all $t$ there are hyperbolic fixed points of the Poincaré maps $g_t$ in the corners of the rectangle $M$ with invariant manifolds located within the rectangle boundaries. These fixed points and their manifolds are independent of $t$.

In the vicinity of the instantaneous separation point, each Poincaré map $g_t$ exhibits two hyperbolic fixed points, which give rise to the complicated manifold structure in the rectangle interior. Their location depends on $t$. For $t = 0$ the fixed points of the map $g_0$ are located in $x_{0,1} \approx (1.08079, 0)$ and $x_{0,1} \approx (0.91921, 1)$; for $t = 0.5$ at $x_{0,5} \approx (0.91921, 0)$ and $x_{0,5} \approx (1.08079, 1)$. Fig. 13(b) schematically illustrates the situation for $t = 0$. The unstable manifold of $x_{0,1}$ is located within the $x$-axis and forms a heteroclinic connection with the corner fixed points. One branch of the stable manifold is part of the heteroclinic tangle in the rectangle interior. For $x_{0,5}$ the stable manifold is contained in the upper rectangle boundary and one branch of its unstable manifold transversely intersects the stable manifold of $x_{0,1}$. These non-trivial hyperbolic fixed points of $g_t$ (i.e. periodic orbits for the full system) and the resulting heteroclinic tangle form the basis of complicated dynamics: one obtains a mixed phase space structure exhibiting a chaotic sea and families of tori as shown in Fig. 13(c), a familiar picture of periodically driven Hamiltonian systems.

We now extend the geometric analysis by attempting to find LCS via the expansion rate approach. We find that long integration time intervals (here $t = 10$) are necessary to discern structures of interest. In Fig. 14 boxes $B_i$ are coloured according to $\max(\delta(B_i, t), \delta(B_i, t))$ with extremal values in the scalar field highlighting LCS corresponding to stable and unstable invariant manifolds of hyperbolic periodic orbits of the flow and thus hyperbolic fixed points of the Poincaré maps $g_t$. Here we have chosen $t = 0$ and $t = 0.5$ to illustrate the time dependence.

If one compares the manifolds, see Fig. 14(a), with the partition in Fig. 13(a) one sees that the boundaries between the invariant sets perfectly match the innermost highlighted structures in Fig. 14(a) on the left and right halves of $M$, see also Fig. 13(d). However, these ridges in Fig. 14 ($t = 0$) corresponding to the boundaries of $A_1$ and $A_2$ are not characterised by particularly high values in the expansion rates fields in Fig. 14(a). Thus the highest expansion rates do not necessarily determine boundaries of sets that are maximally invariant or almost-invariant. This again shows the difficulty to define and rank sets solely on the basis of geometric information.

Almost-invariant sets in the chaotic region and comparison with lobe dynamics

As described above and demonstrated in Fig. 13(c), the initial partition into invariant sets appears to be a natural decomposition of phase space into regular and chaotic regions. To be able to find less obvious almost-invariant sets we restrict our box covering to the chaotic region. For this we first remove the sets identified as a
Fig. 13. (a) Partition into three (approximate) invariant sets. (b) Schematic illustration of the dynamics of the flow map $g_0$ with hyperbolic fixed points (black dots) on the rectangle boundaries and their stable and unstable manifolds. (c) The dynamically distinct regions in phase space obtained by plotting typical trajectories and the partition into invariant sets show good correspondence. The regular regions in phase space appear to be composed of families of invariant tori. (d) Boundaries of the invariant sets are determined by invariant manifolds of the hyperbolic periodic orbits. However, it is neither the primary segments of the manifolds nor parts with particularly high values in the FTLE that play the most important role (see Fig. 14).

Fig. 14. Expansion rates for the periodically driven double-gyre system: approximation of the stable and unstable manifolds of periodic orbits using the set-oriented expansion approach ($t = 0, \tau = 10$). Boxes $B_i$ are coloured according to $\max(\delta_+(B_i, t), \delta_-(B_i, t))$.

Fig. 15. (a) Zoom on maxima of the thresholding curve $\tau_{\epsilon, 1}^2(0)$ of $K_{n, 1}(0), n = 131072$. (a) Thresholding curve for reduced covering, $n = 84204, c = 0$ is the global maximum.
global maximum in the thresholding approach (i.e. the egg-shaped regions in Fig. 13(a)). We repeat this step and remove the eight regular islands circling the central regular regions (see Fig. 13(c)). As a result we arrive at a reduced covering consisting of $n = 84204$ boxes. Fixing $t = 0$ for the remainder of this section, we obtain the matrix $R_n$ for this reduced covering by restricting the full matrix $R_{n,1}(0)$ to the relevant entries.

Using the second eigenvector of $R_n$, $n = 84204$, we obtain two almost-invariant sets corresponding to the global maximum in the respective thresholding curve at $c = 0$ (see Fig. 15(b)). The resulting partition into two almost-invariant sets is shown in Fig. 16(a).

Extending this partition to the full box covering we arrive at the same partition as if we considered a partition based on the $c = 0$ threshold in the second eigenvector of $R_n$ for the full problem ($n = 131072$). That partition is shown in Fig. 16(b). It is characterised by $\rho(A^{−1}−) = 0.9903, \mu(A^{−1}−) = 0.5$, which is a clear local maximum in the original thresholding curve (see Fig. 15(a)). In the following we return to the full domain.

We can now look at the properties of the partition for $c = 0$. Its boundaries do not exactly match the invariant manifolds for $x_{\text{left}}$ and $x_{\text{right}}$, but appear to cut just through the centres of the primary lobes. We also performed identical calculations at times $t = 0.2, 0.5$, and 0.8 and find that for these $t$, the partition boundaries also cut through the centres of the lobe positions at these times.

To further illuminate this result, let us consider the dynamics of (32) as an autonomous flow on the time-expanded space $(x, y, t) \in [0, 2] \times [0, 1] \times S^1$. In the time-expanded space, the surfaces $W_{\text{exp}}^{(1)} \equiv \{(W^1(x_{\text{left}}^0), t), 0 \leq t < 1\}$ and $W_{\text{exp}}^{(2)} \equiv \{(W^2(x_{\text{right}}^0), t), 0 \leq t < 1\}$ are invariant manifolds and thus represent impenetrable barriers to the autonomous flow on $[0, 2] \times [0, 1] \times S^1$. As the Poincaré map for $t = 0$ shows a chaotic regime, it is clearly impossible to form a non-invariant set with boundary comprised solely of portions of the surfaces $W_{\text{exp}}^{(1)}$ and $W_{\text{exp}}^{(2)}$. Such a set would necessarily be invariant, contradicting the chaotic regime and the observed transport between the left and right of the rectangle. Our transfer operator approach instead identifies a pair of almost-invariant sets whose common boundary is not comprised of invariant manifolds. The common boundary is thus a large “exit boundary” that is aligned to the dynamics in such a way that the transfer of mass through the exit boundary is very small.

Let us observe how the two sets in Fig. 16 interact over the boundary: first we consider the images of the boundary box centre points (black) under one iteration of the Poincaré map confirming that the boundary curve is nearly invariant (Fig. 16(a)–(b)). As a second method of visualisation we use our transition matrices $P_n$ and $P_n$. We define row vectors $u, w \in \mathbb{R}^n$ ($n = 131072$) and set $u^0 \equiv 1$, $w^0 \equiv 1$ if $B_i \subset A^+$ (i.e. initialise a uniform density in the light set) and compute $u^k \equiv w^0P_n^k$ and $w^k \equiv w^0\hat{P}_n^k$. The non-zero entries of $u^k$ correspond to boxes that contain terminal points from a $k$-fold propagation of the set $A^+$ by the Markov chain governed by $P_n$, likewise for $w^k$ and $\hat{P}_n$, $u^t$ and $w^t$ are shown in Fig. 17(c)–(d) (colouring from 0 (dark) to 1 (light)), where for clarity we also overlaid the boundary between the two almost-invariant sets. Obviously there is – as expected and observed – hardly any transport between the two sets.

Under further iteration we observe that $u^k$ converges towards the unstable manifold of $x_{\text{left}}^0$ and $w^k$ towards the stable manifold of $x_{\text{right}}^0$, see Fig. 18.

The existence of a heteroclinic tangle formed by the intersections of the stable and unstable manifolds (see Fig. 13(b)) suggests that transport between these particular almost-invariant sets can be explained in terms of lobe dynamics: computing $u_{\text{lobe}}$ based on this new constructed partition we can clearly follow the lobe mechanism (see Fig. 19, colouring from 0 (dark) to 1 (light)). Exactly one lobe volume is exchanged between the two sets for each iterate of the Poincaré return map, see also [13] for a related study.

While one can easily construct a manifold based partition in the spirit of lobe dynamics as shown in Fig. 19(a) (see also [13]), it is not possible to consistently extend this partition to the time-expanded domain in a way that the common boundary (i) varies continuously in space from time slice to time slice, and (ii) is comprised wholly of unstable/stable manifolds in each time slice. If such a partition existed, it would contradict the observed transport between the left and right halves of the 2D domain. Any separating surface in the time-expanded domain must therefore contain an “exit boundary” that allows the transport of exactly one lobe volume over one period. Any such-part-manifold based partition with leakage of one lobe volume yields $\rho(A^+) = 0.9899, \mu(A^+) = 0.5024$ and $\rho(A^−) = 0.9898, \mu(A^−) = 0.4976$. The invariance ratios are not as high as for the original partition based on the second eigenvector $v_0^t$ of $R_n$. Thus such an “exit boundary”, while possibly relatively small in area, is less well adapted to the dynamics and incurs more mass transport in one period than the transport across the larger exit boundary identified by our transfer operator approach.

In summary, our heuristic ansatz using the second eigenvector $v_2^t$ of $R_n$ appears to find a partition that is close to the one based on a primary manifold intersection. However, the partition defined by $v_2^t$ experiences less leakage. It achieves this by running the boundary directly through the middle of the lobes, reducing the exchange of particles by around 5% compared to the geometrically based partition.

12 Note that this quantity is obtained iteratively by matrix multiplications.
Fig. 17. (a) Images (light) of boundary boxes (dark) under one iteration of Poincaré map $g_0$. The boundary curve appears to be nearly invariant. (b) Zoom onto the lower part of the rectangle. (c) $u^1$ with the partition boundary overlaid (black). (d) $w^1$ with the partition boundary overlaid (black).

Fig. 18. (a) $u^3$ is very close to the unstable manifold of the hyperbolic fixed $x^2_{00}$ of $g_0$. (b) $w^3$ is very close to the stable manifold of the hyperbolic fixed $x^1_{00}$.

Fig. 19. (a) Manifold based partition. (b) $u^1_{\log}$ gives a clear indication of the lobe dynamics. The primary exchange of particles is via the central lobes.

9. Conclusion

We have demonstrated in a variety of settings that maximally dynamically isolated regions (almost-invariant sets) may be efficiently identified via transfer operator calculations. The selection algorithm we proposed for determining almost-invariant sets, based upon maximising the coherence or dynamical isolation, consistently revealed that maximally coherent almost-invariant sets possess boundaries that are formed from segments of stable and unstable manifolds. We demonstrated that a combination of a geometrical analysis via invariant manifolds and a probabilistic analysis via almost-invariant sets yielded a much richer understanding of the global dynamics of systems. On the one hand, the almost-invariant set analysis developed a skeleton of major
coherent structures for the system and ranked these according to coherency. This skeleton then clearly indicated which invariant manifolds were the greatest inhibitors to mixing. On the other hand, the invariant manifolds more clearly delineated the boundaries of the almost-invariant regions and further informed the dynamical mechanisms by which transport occurs to and from the almost-invariant sets.

Our final example of a periodically driven flow showed that this correspondence between almost-invariant sets and invariant manifolds may not be universal, and that classical theory such as lobe dynamics need not correspond to maximal transport barriers. In future work we will study the dynamical reasons behind this.

Finally, we mention that the transfer operator approach has also proved to be capable of detecting long residence regions in real world systems, such as gyres in ocean flows [30]. Future work will include the extension of the transfer operator framework to detect and approximate coherent structures in nonautonomous systems. Initial results for 1D discrete time systems [58] and continuous time systems [59] have been developed. These techniques allow the detection and analysis of coherent structures in aperiodically driven fluids, including dynamic structures such as eddies in ocean flows or hurricanes in atmospheric flows.

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