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

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ABSTRACT

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.

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. [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 [5,6,3]. In non-periodic time-dependent settings, finite-time hyperbolic material lines [7] and surfaces [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. [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

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Probabilistic Description of Dynamics
Transfer Operator
Almost-invariant Sets

Identifies which geometric structures are the strongest barriers to global mixing ↓

↑ Further informs the dynamics underlying almost-invariant sets

Geometric Description of Dynamics
Invariant Manifolds

Fig. 1. Connecting the probabilistic and the geometric approaches.

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

$$\dot{x} = F(x, t). \tag{1}$$

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

$$\frac{\mathrm{d}\phi_\tau}{\mathrm{d}\tau}(x_0, t_0)|_{\tau=0} = F(x_0, t_0), \quad \text{for all } x_0 \in M, t_0 \in \mathbb{R}. \tag{2}$$

If a trajectory is at $x_0 \in M$ at time t_0, then τ 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 $\phi_\tau(x) := \phi_\tau(x, 0) = \phi_\tau(x, t)\ \forall t \in \mathbb{R}$. In the fourth case study of a periodically driven velocity field we will directly apply these concepts to the time-dependent flow map $\phi_\tau(x, t)$.

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

Definition 2. Endow M with the Borel σ-algebra and let μ be a probability measure on M. We call μ an *invariant measure* for ϕ if $\mu(\phi_{-\tau}(A)) = \mu(A)$ for all measurable $A \subset M$ and all $\tau \in \mathbb{R}$.

Definition 3. Let μ be an invariant probability measure on M and $A \subset M$ a measurable set. We call μ an *ergodic measure* for ϕ if whenever $\phi_{-\tau}(A) = A$ for all $\tau \in \mathbb{R}$, then 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 Λ the "maximal invariant set". In fluid-like flows, $\Lambda = M$, the entire compact domain; for dissipative flows, $\Lambda \subset M$, for example, $\Lambda_0 := \bigcap_{\tau \geq 0} \phi_\tau(M)$ 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 $\Lambda \subsetneq M$ numerically appears to be a chaotic attractor. The flow numerically appears to preserve an ergodic physical invariant measure[1] μ. 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 $t \in \mathbb{R}$, 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 μ be preserved by ϕ. We will say that a set $A \subset M$ is *almost-invariant* over the interval $[0, \tau]$ if

$$\rho_{\mu,\tau}(A) := \frac{\mu(A \cap \phi_{-\tau}(A))}{\mu(A)} \approx 1. \tag{3}$$

If $A \subset M$ is *almost-invariant* over the interval $[0, \tau]$, then the probability (according to μ) of a trajectory leaving A at some time in $[0, \tau]$ and not returning to A at time τ is relatively small. Thus, almost-invariant sets can be considered as an alternative type of coherent structures in flows.

In the context of analysing a particular flow, we are interested in those sets that are *maximally* almost-invariant; that is, the ratio in Definition 4 is closest to unity. In order to maximise this ratio, one may construct an optimisation problem where the "variables" are sets [16,17]. However, even a spatially discretised version of this optimisation problem is combinatorially hard to solve, and in practice we adopt a heuristic approach to identifying large maximally almost-invariant sets. This heuristic approach utilises eigenfunctions of the Perron–Frobenius operator. The use of the Perron–Frobenius operator has many additional advantages as it is a global linear propagator for the flow and carries significant statistical information on ergodicity and mixing properties [33], and on invariant densities and rates of decay of correlations [33–35].

Definition 5. We define the *Perron–Frobenius operator* or *transfer operator* $\mathcal{P}_\tau : L^1(M) \circlearrowleft$ by

$$\mathcal{P}_\tau f(x) = f(\phi_{-\tau}(x)) \cdot |\det(D\phi_{-\tau}(x))|, \tag{4}$$

where $D\phi_\tau(x)$ is the Jacobian matrix corresponding to the spatial derivatives of ϕ_τ.

If f is the density of an absolutely continuous probability measure ν (so that $d\nu/dx = f$), then $\mathcal{P}_\tau f$ is the density of the probability measure $\nu \circ \phi_{-\tau}$.[2] Fixed points of $\mathcal{P}_\tau$ represent densities that are invariant under the action of $\phi_{-\tau}$. If, for example, the flow ϕ is area preserving then $f \equiv 1$ is a fixed point of $\mathcal{P}_\tau$ for all τ. In the autonomous setting, if Lebesgue measure is also ergodic for $x \mapsto \phi_\tau(x)$ for a particular τ, then $f \equiv 1$ is the unique density fixed by $\mathcal{P}_\tau$ Theorem 4.2.2 [33]. If, on the other hand, Lebesgue measure is not ergodic, then $\mathcal{P}_\tau$ will have two or more fixed densities of the form $(1/m(A))\chi_A$ where A is invariant under ϕ (see e.g. the proof of Theorem 4.2.2 [33]). We illustrate these basic concepts in the following simple example.

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

$$\begin{aligned} \dot{x} &= -\pi \sin(\pi x)\cos(\pi y) \\ \dot{y} &= \pi \cos(\pi x)\sin(\pi y) \end{aligned} \tag{5}$$

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

[1] We will say that the autonomous flow $\phi_\tau(x)$ possesses a *unique physical measure* μ if $\mu_x = \mu$ for Lebesgue almost all $x \in M$, where $\mu_x := \lim_{\tau\to\infty} \frac{1}{\tau} \int_0^\tau \delta_{\phi_s(x)}\, ds$, and a weak* limit is meant.

[2] This is the natural action of ϕ_τ on a measure ν. Suppose that ν (and f) has its support concentrated on a set A; that is, $\nu(A) = 1$ (and $\int_A f\, dm = 1$). Then $\nu \circ \phi_{-\tau}(\phi_\tau(A)) = 1$ and $\mathcal{P}_\tau f$ has support on $\phi_\tau(A)$.

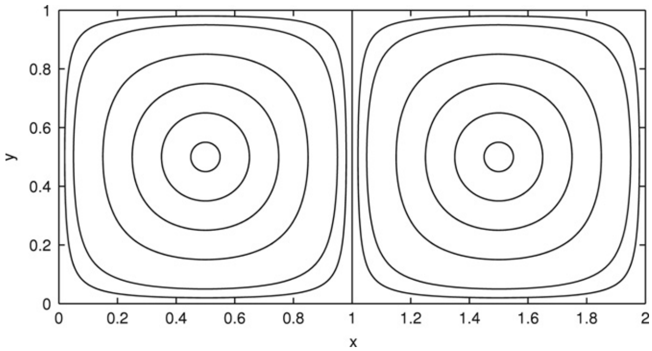

Fig. 2. Typical trajectories in the autonomous double-gyre flow.

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 $\chi_{[0,1]\times[0,1]}$ and $\chi_{[1,2]\times[0,1]}$ are both fixed under $\mathcal{P}_\tau$ for all τ.

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 $\{B_1,\dots,B_n\}$ (usually a fine grid of boxes) and applies the projection $\pi_n : L^1(M)\to \mathrm{sp}\{\chi_{B_1},\dots,\chi_{B_n}\}$ defined by

$$\pi_n f = \sum_{i=1}^{n}\left(\frac{1}{m(B_i)}\int_{B_i} f\,\mathrm{d}m\right)\chi_{B_i} \tag{6}$$

to $\mathcal{P}_\tau$ to form $\pi_n\mathcal{P}_\tau$. The action of $\mathcal{P}_\tau$ on $\mathrm{sp}\{\chi_{B_1},\dots,\chi_{B_n}\}$ is given by the matrix[3]

$$P_{n,\tau,ij} = \frac{m(B_i\cap\phi_{-\tau}(B_j))}{m(B_i)}. \tag{7}$$

The matrix $P_{n,\tau}$ is stochastic and therefore has a spectral radius of one and has at least one fixed point[4] p_n (satisfying $p_nP_{n,\tau} = p_n$ 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 τ, $x \mapsto \phi_\tau(x)$ preserves an ergodic invariant probability measure μ that is absolutely continuous with respect to Lebesgue measure, then $P_{n,\tau}$ is eventually positive,[5] 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 of $\mathcal{P}_\tau$ is constructed by setting

$$h_n := \sum_{i=1}^{n}\frac{p_{n,i}}{m(B_i)}\chi_{B_i}. \tag{8}$$

A corresponding approximate invariant probability measure is defined by

$$\mu_n(A) := \int_A h_n\,\mathrm{d}m. \tag{9}$$

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, $i=1,\dots,n$, we will define a set of N test points $x_{i,1},\dots,x_{i,N}$ and numerically integrate trajectories to obtain $\phi_\tau(x_{i,k})$, $k=1,\dots,N$. Then

$$P_{n;\tau,ij} \approx \frac{\#\{k : x_{i,k}\in B_i,\ \phi_\tau(x_{i,k})\in B_j\}}{N}. \tag{10}$$

The flow time τ should be chosen long enough so that most test points leave their partition set of origin, otherwise at the resolution given by the partition $\{B_1,\dots,B_n\}$, the approximate operator appears similar to the identity operator (i.e. $P_{n,\tau}\approx \mathrm{Id}_{n\times n}$). There is no upper limit on τ, however, if ϕ acts to separate nearby points, clearly the longer τ 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 $\mathcal{C}_n := \{A\subset M : A=\bigcup_{i\in I} B_i, I\subset\{1,\dots,n\}\}$. We will search for sets in $\mathcal{C}_n$ that maximise $\rho_{\mu,\tau}$. In practice, we use the following discretised version of ρ:

$$\rho_{n,\tau}(A) := \frac{\sum_{i,j\in I} p_{n,i}P_{n,\tau,ij}}{\sum_{i\in I} p_{n,i}}. \tag{11}$$

We now describe a heuristic method for identifying sets in $\mathcal{C}_n$ for which $\rho_{n,\tau}$ 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-reversible version of $P_{n,\tau}$ by

$$R_{n,\tau} := (P_{n,\tau}+\hat{P}_{n,\tau})/2, \tag{12}$$

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

$$\hat{P}_{n,\tau,ij} = p_{n,j}P_{n,\tau,ji}/p_{n,i}. \tag{13}$$

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 $\rho_{n,\tau}(A)\approx 1$ forces the existence of an eigenvalue of $R_{n,\tau}$ close to 1 and vice versa.

Proposition 1. *Let λ_2 denote the second largest eigenvalue of $R_{n,\tau}$ and $A=\bigcup_{i\in I}B_i$, $I\subset\{1,\dots,n\}$.*

$$1-\sqrt{2(1-\lambda_2)} \le \max_{A\in\mathcal{C}_n,\ \sum_{i\in I}p_{n,i}\le 1/2}\rho_{n,\tau}(A) \le \frac{1+\lambda_2}{2}. \tag{14}$$

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 $v^2_{n,\tau}$ be the right eigenvector of $R_{n,\tau}$ corresponding to the second largest eigenvalue λ_2 and define the sets

$$A^+ := \bigcup_{i:v^2_{n,\tau,i}\ge 0} B_i,\qquad A^- := \bigcup_{i:v^2_{n,\tau,i}<0} B_i. \tag{15}$$

The pair A^+, A^- partition M into two sets between which we expect little communication of trajectories. This heuristic was originally proposed[6] by Dellnitz and Junge [15,14].

[3] For simplicity of exposition, we will assume throughout that $m(B_i)=m(B_j)$ for all $i\ne j$. If this is not the case, the expression on the RHS of (7) should have $m(B_j)$ 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 $m(B_i)$, $i=1\dots,n$ on the diagonal.

[4] We assume that p_n provides a good estimate of an invariant measure μ via the density h_n(8); see [35] and the references therein for details. As μ does not depend on τ, in practice p_n has negligible time dependence. We will therefore drop the τ dependence for p_n and its corresponding density h_n.

[5] A matrix P is eventually positive if there exists a finite positive integer k such that $P^k>0$.

[6] Dellnitz and Junge [14] used the left eigenvector $v^2_{n,\tau}$ of $P_{n,\tau}$ corresponding to the second largest eigenvalue λ_2 of $P_{n,\tau}$, and based their heuristic on a perturbation argument; see [14] for details.