# Extraction and Prediction of Coherent Patterns in Incompressible Flows through Space-Time Koopman Analysis

Dimitrios Giannakis*
*Courant Institute of Mathematical Sciences, New York University, New York, New York, USA*

Summary. We present a method for detecting and predicting the evolution of coherent spatiotemporal patterns in incompressible time-dependent fluid flows. Our approach is based on representations of the Koopman and Perron-Frobenius governing the evolution of observables and probability measures on Lagrangian tracers in a smooth orthonormal basis learned from velocity field data through the diffusion maps algorithm. These operators are defined on the product space between the phase space for the velocity field evolution and the spatial domain in which the flow takes place, and as a result their eigenfunctions correspond to global space-time coherent patterns under the flow. Moreover, used in conjunction with Leja interpolation of matrix exponentials, our data-driven representation enables the simulation of the evolution of observables and probability densities.

## Introduction

The formation of coherent patterns is a ubiquitous phenomenon in fluid flows [1] which has received considerable attention in the engineering, mathematical, and physical sciences. In this work, we develop an operator-theoretic, data-driven framework for identification and prediction of such patterns generated by time-dependent, incompressible flows with ergodic dynamics. The evolution of Lagrangian tracers in such systems has a natural skew-product structure on the product between the fluid flow's phase space and the physical domain where the tracers move, along with the associated Koopman and Perron-Frobenius operators governing the evolution of observables and probability measures. While Koopman and Perron-Frobenius operators have been extensively used for identification of coherent sets in dynamical systems [2, 3], it appears that this skew-product structure has not been previously exploited in data-driven techniques.

## Operator-theoretic formulation for skew-product systems

We model a time-dependent incompressible fluid flow on a domain $X$ as a mapping $F : A \mapsto \mathfrak{X}$ from the state space $A$ of an ergodic dynamical system to the space $\mathfrak{X}$ of divergence-free (with respect to Lebesgue measure) vector fields on $X$. On $A$, the dynamics is described by a mapping $\Phi_t : A \mapsto A$, $t \in \mathbb{R}$, preserving an ergodic probability measure $\alpha$, and to each state $a$ there corresponds a velocity field $v = F(a) \in \mathfrak{X}$ generating the (non-autonomous) evolution of tracers. In particular, the motion of Lagrangian tracers is governed by the family of maps $\Psi_t : A \times X \mapsto X$ such that $\Psi_t(a, x)$ corresponds to the position of a tracer at time $t$ released from the point $x$ when the underlying flow state is $a$. Note that $\Psi_t$ satisfies the cocycle property, $\Psi_s(\Phi_t(a), \Psi_t(a, x)) = \Psi_{s+t}(a, x)$. Given a collection of time-ordered velocity field snapshots $\{v_0, v_1, \dots, v_{N-1}\}$, $v_n = F(\Phi_{n\tau} a_0)$, taken at a fixed time interval $\tau$, and assuming no a priori knowledge of the dynamics $(A, \Phi_t)$ or availability of tracer trajectories, our objectives are to (i) identify coherent spatiotemporal patterns associated with the motion of passive tracers in $X$; (ii) predict the evolution of observables and probability densities defined on the tracers. Our approach for addressing these objectives relies on data-driven approximations of Koopman and Perron-Frobenius operators characterizing the evolution of observables and probability measures on the product space $M = A \times X$. Intuitively, we think of $M$ as a "space-time manifold" with $X$ playing the role of physical space where the motion of tracers takes place and $A$ the role of "time" where the velocity field evolves. On $M$, the dynamics is autonomous (though not necessarily ergodic), and is governed by the flow $\Omega_t : M \mapsto M$, $t \in \mathbb{R}$, having the skew product form $\Omega_t(a, x) = (\Phi_t(a), \Psi_t(a, x))$. Moreover, this flow preserves the product measure $\mu = \alpha \times \lambda_X$. Associated with $\Omega_t$ is a group of Koopman operators $\{W_t\}$, $t \in \mathbb{R}$, governing the evolution of observables in $L^2(M, \mu)$ via composition with $\Omega_t$, i.e., $W_t f = f \circ \Omega_t$. This group is generated by a vector field $w = \frac{dW_t}{dt}\big|_{t=0}$ on $M$, which acts as a skew-adjoint operator on observables in $L^2(M, \mu)$.

### Identification of coherent spatiotemporal patterns

We identify coherent spatiotemporal patterns in time-dependent fluid flows through approximate eigenfunctions of the Koopman generator $w$ at small corresponding eigenvalue and Dirichlet energy (roughness). In particular, our approach is based on a Galerkin method for the eigenvalue problem for $w$ (with a small amount of self-adjoint diffusion added for regularization) formulated in a data-driven orthonormal basis of $L^2(M, \mu)$ acquired from the velocity field data using the diffusion maps algorithm [4]. A variant of this technique was developed in [5] in the case of ergodic systems; here we extend this methodology to the skew-product systems governing the evolution of Lagrangian tracers. To motivate our approach, consider the eigenvalue problem $w(\psi) = \lambda\psi$, and suppose that this problem has a nonconstant solution $\psi \in L^2(M, \mu)$ at eigenvalue $\lambda = 0$. Because $W_t\psi = e^{t\lambda}\psi = \psi$, such an eigenfunction is preserved on tracers. Moreover, the level sets $\zeta_c = \{(a, x) \in M \mid \psi(a, x) = c\}$ of $\psi$ create an ergodic quotient [2] of $M$; that is, a partition into codimension 1 invariant sets on which tracers on $M$ are trapped. In particular, if $(a, x) \in \zeta_c$ then $\Omega_t(a, x) \in \zeta_c$ for all $t \in \mathbb{R}$ since $\psi(\Omega_t(a, x)) = \psi(a, x)$. If $w$ has eigenfunctions with nonzero corresponding eigenvalues, then these eigenfunctions also provide a useful notion of coherent spatiotemporal patterns that vary periodically on the tracers.

While theoretically attractive, this approach for coherent pattern identification lacks a crucial feature, namely an operator enforcing smoothness. That is, even in simple dynamical systems with pure point spectrum, there exist eigenfunctions

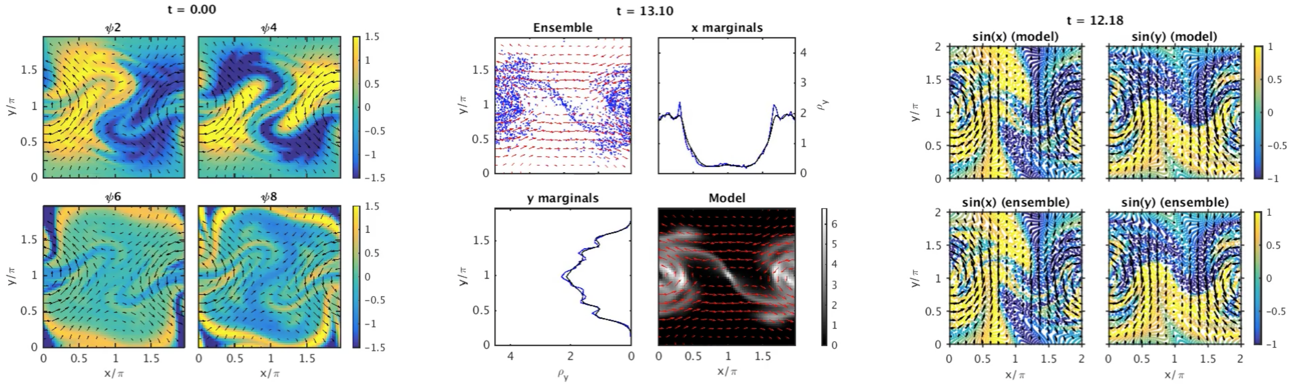


Figure 1: Illustration of our operator-theoretic framework for skew-product systems in the case of a time-periodic flow featuring a shifting vortex with a Gaussian streamfunction in a two-dimensional periodic domain. Left-hand panels: Snapshots of coherent spatiotemporal patterns associated with regularized Koopman eigenfunctions with small Dirichlet energy. Middle panels: A comparison of the time evolution of an initially Gaussian probability density under the time-dependent flow as simulated by our nonparametric model with an ensemble of Lagrangian tracers evolved with the full model. Right-hand panels: Evolution of tracer positions with our nonparametric model compared to a simulation with the full model.

of $w$ with arbitrarily small eigenvalue (frequency) but arbitrarily large roughness. To eliminate such pathological eigenfunctions, instead of using the raw generator we identify coherent patterns through the eigenfunctions of the regularized operator $L = w - \epsilon\Delta$, where $\Delta$ is a Laplace-Beltrami operator associated with a Riemannian metric on $M$ whose volume form is equal to the invariant measure $\mu$. This operator is self-adjoint on $L^2(M, \mu)$ and can be represented efficiently in the data-driven basis of [5] by a diagonal matrix. Moreover, due to the skew-product form of the dynamics, $w$ decomposes into $w = u + v$ where $u$ is the generator of the ergodic dynamics $\Phi_t$ on $A$ and $v$ the state-dependent vector field in $\mathfrak{X}$. Both of these operators can be represented by matrices in a tensor-product basis for $L^2(M, \mu)$, leading to Galerkin scheme for the eigenvalue problem for $L$. Moreover, the diffusion basis also allows for computation of Dirichlet energies of the eigenfunctions (using the diffusion eigenvalues). Ordering the eigenfunctions of $L$ in order of increasing Dirichlet energy, we thus identify coherent patterns with high smoothness on the product manifold $M$. Snapshots of such patterns for a periodic vortical flow in a two-dimensional periodic domain resembling a blinking vortex flow are displayed in the left-hand panels in Figure 1.

**Prediction of observables and probability densities**

Prediction of observables and probability densities on Lagrangian tracers has many important practical applications. For instance, in the framework studied here a probability measure $\nu_0$ on $M$ can be used to characterize uncertainty in both position in the physical domain $X$ as well as the sate of the time-dependent flow in $A$. Such a probability measure is transported at time $t$ to a measure $\nu_t = \Omega_{t*}\nu_0 = \nu_0 \circ \Omega_t^{-1}$. Assuming that the time-dependent measure $\nu_t$ has smooth density $\rho_t$ relative to the invariant measure $\mu$, we can compute this density through the adjoint (Perron-Frobenius) group $\{W_t^*\}$, i.e., $\rho_t = W_t^*\rho$. Here, we approximate $\rho_t$ using the exponential representation of this group, $W_t^* = e^{-tw}$, in conjunction with our finite-dimensional approximation of the generator $w$ in the diffusion maps basis. Numerically, this amounts to computing the action of a matrix exponential associated with the generator on column vectors containing the expansion coefficients of $\rho_t$ in the data-driven basis. To that end, we employ Leja interpolation algorithms [6] which approximate matrix exponentials via a polynomial interpolant—this method evaluates the action of a matrix exponentials on vectors without explicit evaluation of the exponential itself (which is important for computational efficiency), and also allows for large stepsizes without encountering stability issues. A comparison of $\rho_t$ (marginalized over $A$ for visualization) as simulated by our method with a Monte Carlo simulation using the perfect model is shown in the middle panels in Figure 1. We also construct an analogous scheme to approximate the action of the Koopman group on observables on tracers. In particular, given an observable $f \in L^2(M, \mu)$, then $W_t f = e^{tw} f$ corresponds to a time-shifted observable evaluated along the tracer trajectories. For instance, in the case of a doubly periodic domain $X$, observables of interest could be $f_1(x) = e^{ix_1}$ and $f_2(x) = e^{ix_2}$, where $(x_1, x_2)$ are the canonical coordinates of the point $x \in X$. In particular, knowledge of $W_t f_1$ and $W_t f_2$ is sufficient to uniquely determine the tracer positions at time $t$ starting from arbitrary positions in $X$ and velocity field states in $A$. This capability is illustrated in the right-hand panels in Figure 1.

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