# Estimating stable and unstable sets and their role as transport barriers in stochastic flows

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We consider the situation of a large-scale stationary flow subjected to small-scale fluctuations. Assuming that the stable and unstable manifolds of the large-scale flow are known, we quantify the mean behavior and stochastic fluctuations of particles close to the unperturbed stable and unstable manifolds and their evolution in time. The mean defines a smooth curve in physical space, while the variance provides a time- and space-dependent quantitative estimate where particles are likely to be found. This allows us to quantify transport properties such as the expected volume of mixing as the result of the stochastic fluctuations of the transport barriers. We corroborate our analytical findings with numerical simulations in both compressible and incompressible flow situations. We moreover demonstrate the intimate connection of our results with finite-time Lyapunov exponent fields, and with spatial mixing regions.

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#### I. INTRODUCTION

Lagrangian coherent structures [1-3] have a wellestablished importance in fluid flows. Loosely speaking, they consist of fluid regions which move "almost" coherently, and their boundaries act as transport barriers separating the inside of the structure from the outside, at least for some time. The boundaries of Lagrangian structures are analogs of stable and/or unstable manifolds. In applications these boundaries are identified using a variety of different techniques which take into account that data are usually only known for finite times [4,5]. The analysis of these time-varying boundaries (which, confusingly, are themselves sometimes referred to as Lagrangian coherent structures) between coherent fluid blobs has seen many recent applications, ranging from geophysical [6] to microfluidic [7] scales. Environmental applications include oil spills [8], garbage in the ocean [9], coral protection [10], plankton distribution [11], ozone depletion [12], transport of biological spores [13], and atmospheric wind hazards near airports [14]. Additional applications include determining a "skeleton for turbulence" [2,15], microfluidic mixing optimization [7], and fisheries [6]. In essentially all these applications, the velocity field is considered *deterministic*.

Most realistic flow situations are, however, typically of a *stochastic* nature, related to the uncertainties present in any data, model, or simulation [16–19]. The stochasticity naturally enters coarse-grained macroscopic degrees of freedom, that is, those which we observe, in a multiscale setting. Recent work has extended the classical deterministic framework of Eulerian partial differential equations for fluid flows to stochastic partial differential equations [20–25] where the stochasticity enters on

In this paper, we restrict to two-dimensional flows, motivated by the fact that oceanic flows are weakly two dimensional in that there is dominant flow on two-dimensional isopycnal surfaces [39]. Since these surfaces are not necessarily uniformly spaced, three-dimensional incompressibility does not translate to two-dimensional divergence-free velocity fields on each surface, and therefore we allow for general compressibility in our work. We consider the following idealized situation: We assume that there is a large-scale flow which is slowly varying in time and which can be viewed as steady for some characteristic time scale  $\tau_c$ . The large-scale flow is subjected to small-scale disturbances which we model as a stochastic forcing of the large-scale flow, along the lines described above. Let us assume that we have knowledge of the stable and/or unstable manifold of the deterministic large-scale flow from some coarse-grained measurements at some time  $t_1$ . Our aim here is to describe the effect of the stochasticity on the temporal evolution of these manifolds. More specifically: extending the notion of stable and unstable manifolds in this

the side of the Lagrangian particle dynamics. The stochasticity arises as the integrated effect of the fast small-scale degrees of freedom by the process of homogenization [25-28], and describes the effect of the unresolved fast processes onto the resolved slow degrees of freedom. Thus, there is a need to incorporate the effect of stochasticity into the deterministic approaches for understanding and quantifying transport between coherent structures. The natural extension from deterministic intuition may be to think of stable and unstable manifolds of the stochastic system to demarcate transport barriers. While there exists deep theory for defining stable and unstable manifolds in stochastic differential equations (usually falling under "random dynamical systems" approaches) [29-38], there is at present little insight on how such theory can be adapted to quantify transport barriers, and/or determine mixing across these.

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setting, and quantifying transport and mixing properties and their uncertainty.

The presence of stochasticity destroys the natural notions of stable and unstable manifolds, necessitating a definition of what a backward-time or forward-time flow barrier is. Following a recently developed idea for general curves in two-dimensional flows [40], our approach here is to study the statistics of the initial-time flow barrier over many realizations of the noise. For each realization we define stable and unstable sets which are determined by flowing in time the initially known locations of the stable and unstable manifolds. Depending on an interpretation of how the driving noise is implemented, these sets can take different forms. If the same noise realization is used across all initial conditions, we are in the classical domain of random dynamical systems, in which the stable and unstable sets are indeed smooth curves for each realization, and therefore can be termed (random) stable and unstable manifolds [29-38]. On the other hand, we introduce in this paper an alternative scenario, in which the noise realizations are nonuniform across initial positions. This corresponds to the viewpoint that each fluid particle is subject to a different noise realization. The stable and unstable sets in this case will consist of an uncountable collection of points which do not form a curve. The statistical behavior of the stable and unstable sets in either case is characterized by their *mean*, a smooth curve in space, and their *variance*. The former identifies the average location of particles, while the latter quantifies the width or uncertainty of the mean behavior. It is this uncertainty quantification of transport barriers, albeit in a simplified setting, that forms the main contribution of this article.

We remark that uncertainty quantification of propagating structures typically has two aspects: the uncertainty in the identification at the initial time, and the uncertainty engendered through propagation by uncertain velocities. We address here the latter aspect, assuming that the stable and unstable manifolds are known at some initial time. In identifying transport barriers (i.e., analogs of stable and unstable manifolds) over a finite-time duration, we note that this is nonunique even in deterministic flows [41]. This has led to the preponderance of different methods, often called "Lagrangian coherent structure" (LCS) methods, which continue to be developed to identify these (for reviews, see [1,3,41,42]). These methods include ridges of finite-time Lyapunov exponents (FTLEs) [1,43-50], curves or surfaces towards which there is extremal repulsion or attraction [1,51–56], sets which are "almost coherent" with respect to the operation of a transfer operator [57-61], identification of vorticity cores or oscillations [62,63], etc. Thus, the very definition of "transport barrier" at some finite time is ambiguous. If following finite-time Lyapunov exponent ideas, for example, one is seeking the infinite-time property of stable (unstable) manifolds as initial conditions which decay exponentially in forward (backward) times; however, in finite-time situations, any continuous function f of time t in a finite-time interval can be bounded in the form  $|f(t)| \leq Ae^{\lambda t}$ , where  $\lambda$  is any given positive constant, by choosing A appropriately. Thus, exponential stretching is no more than a *diagnostic* for determining (an analog of) a stable or unstable manifold; using ridges of finite-time Lyapunov exponents does not constitute a watertight way of defining

stable and unstable manifolds [50,51]. On the other hand, it has come to be expected that some types of transport barriers in finite-time flows (those which are analogous to stable and unstable manifolds) carry an exponential stretching signature. We verify this property in the first example that we consider, an incompressible flow in Sec. III, in validating our uncertainty theory for transport barriers under stochastic perturbations.

An advantage of our approach is that it enables a spatial quantification of the mixing imparted by the stochasticity, complementing the notion of partitioning space into regions which are dominantly coherent under noise [58,59,64,65]. The fluctuations around the mean curve lead to the potential for transport between regions which, in the absence of stochasticity, would be identified as separate physical regions. We argue that the variance (with respect to realizations of the noise) describes the leakiness between the regions separated by the mean curves. The leakiness is an averaged mean quantity and does not describe the behavior of a single particle but rather of an ensemble of particles. From a practical perspective, the crucial insight is that, under the assumption of ergodicity of the stochastic dynamical system, the variance is related to the relative volume of mass of an initial distribution of particles that will be leaking at a specified finite time. This quantity is important, for example, when estimating the spatial distribution of oil spills and knowledge of the time-dependent spatially varying variance around the mean curve can be used to assess the extent of further oil contamination. Our second example, focusing on Taylor-Green flow in Sec. IV, validates that our theory correctly identifies mixing regions and their evolution with time.

The paper is organized as follows. In Sec. II we present the theory for the time evolution of stochastically perturbed stable and unstable manifolds. This provides explicit analytical formulas for the mean of the stable and unstable sets as well as their variances. We show that the variance, as a measure of uncertainty, saturates under generic conditions. Section III applies the theory to an example of a compressible flow and presents numerical simulations illustrating the ability of our framework to capture the statistics of Lagrangian particle dynamics near stochastically perturbed stable and unstable manifolds. Moreover, we show that our analytical framework identifies structures which are aligned with FTLE ridges, with the ridge thickness variation being predicted by our theoretical variance. Section IV then treats an incompressible flow example, and shows how the ideas of transport barriers developed in the deterministic situation can be extended to the stochastic case. We show that the interchange of fluids across the transport barrier is spatially correlated to the variance of the stable and unstable sets. We conclude in Sec. V with a discussion and an outlook.

# **II. MANIFOLD UNCERTAINTY**

#### A. Stable and unstable sets

Let  $x \in \Omega$ , where  $\Omega$  is a two-dimensional connected open set. Let  $v : \Omega \to \mathbb{R}^2$  be (sufficiently) smooth, and consider the deterministic dynamical system

$$\dot{x} = v(x). \tag{1}$$



FIG. 1. Stable ( $\Gamma^s$ ) and unstable ( $\Gamma^u$ ) manifolds of the fixed point *a* of (1).

If v is a velocity field of a fluid, then solutions to (1) are flow trajectories. We restrict here to a slowly varying large-scale flow which can be considered as steady for times smaller than some characteristic time scale  $\tau_c$ . For such flows, (1) can be considered the leading-order approximation. Suppose (1) possesses a hyperbolic fixed point *a* to which is attached a one-dimensional stable manifold  $\Gamma^s$  and a one-dimensional unstable manifold  $\Gamma^{u}$  [66]. These are shown by the thick curves in Fig. 1, and are respectively parametrized by  $x^{s}(t)$  and  $x^{u}(t)$ , both solutions of (1). In deterministic systems (1) manifolds of this sort are specifically important since they are flow separators (flow barriers, transport barriers) in terms of particle trajectories. Consider, for example, a blob of fluid placed on top of the stable manifold  $\Gamma^s$  as shown in Fig. 1. As this blob evolves according to (1), it eventually gets close to a. At this point, it is strongly influenced by the unstable manifold  $\Gamma^{u}$ , and the blob gets stretched (exponentially fast) along  $\Gamma^{u}$ . Thus, particles in the blob which were on one side of  $\Gamma^s$  get stretched in one direction, while those on the other side of the blob are stretched in the other direction. In this sense,  $\Gamma^s$  is a flow separator in forward time. Similarly,  $\Gamma^{u}$  is a flow separator in backward time. We remark that these interpretations continue to hold when v is *unsteady*; in this instance a is not a fixed point, but a time-varying trajectory to which is attached stable and unstable manifolds. The flow-barrier property is well known, and is a fundamental reason why finite-time analogs of stable and unstable manifolds (e.g., strong ridges of finite-time Lyapunov exponent fields [3], curves to which there is maximal attraction [1], etc.) are investigated numerically as flow barriers in realistic flows.

We want to determine the intuitive counterparts to these, i.e., intuitive flow barriers, when the coarse-grained large-scale flow (1) is subjected to small-scale fluctuation. We model the resulting flow by a stochastically perturbed version of (1). We assume that the unstable and stable manifolds are known at some time  $t_1$ , and aim to determine their subsequent evolution and uncertainty up to some time t which is smaller than the characteristic time scale of the large-scale flow  $\tau_c$ . We will discuss this under two slightly different interpretations of the perturbing stochastic differential equation (SDE).

We first consider the Itô stochastic differential equation (SDE)

$$dy = v(y) dt + \varepsilon \sigma(y, t) dW_t$$
(2)

for  $y \in \Omega$  for initial condition  $y(t_1) = \zeta$ . Here,  $\varepsilon$  is a dimensionless parameter representing the size ( $|\varepsilon| \ll 1$ ) of the stochasticity,  $dW_t$  is two-dimensional Brownian motion, and  $\sigma$ is a 2×2 matrix with components  $\sigma_{ii}$ , in general both spatially and temporally dependent, incorporating anisotropic diffusion. In the form (2) above, the first term is the "drift" and the second the "diffusion" associated with the variable y. The SDE (2), if interpreted as the Lagrangian description of fluid parcels, assumes the same realization of noise  $W_t$  for all fluid particles. This model is what is usually studied in the framework of slow manifolds in random dynamical systems, which establishes the existence of smooth manifolds for each noise realization [29-38]. The manifolds can be initialized at time  $t_1$  by choosing a collection of initial conditions for the  $\zeta$ . The time t, until which we plan to describe the manifold evolution can be any value such that  $|t - t_1| \ll \tau_c$ , the characteristic timescale of the large-scale flow, to assure steadiness of the manifolds  $\Gamma^{u,s}$ . The unstable manifold is propagated forward in time with  $t > t_1$ whereas the stable manifold is propagated backward in time with  $t < t_1$ .

We also consider a slightly different viewpoint in which each initial condition is allowed to be driven by independent noise realizations. In particular, we consider

$$dy^{(\zeta)} = v(y^{(\zeta)}) dt + \varepsilon \,\sigma(y^{(\zeta)}, t) dW_t^{(\zeta)}, \tag{3}$$

where  $y^{(\zeta)}$  denotes conditioning on the initial value  $y(t_1) = \zeta$ , and the noise realization is independent with  $\mathbb{E}[W_t^{(\zeta)}W_s^{(\xi)}] = \delta(\zeta - \xi)\delta(t - s)$ . This is a broader modeling framework in which a correlation between the noise experienced by all particles, as in (2), is *not* assumed. A principal computational advantage of this viewpoint is the ability to efficiently capture many stochastic realizations simultaneously when doing a forward simulation in time. For brevity, we will call (2) an SDE driven by *uniform noise* and (3) driven by *nonuniform noise*, to refer to the fact that the noise realization used in each simulation is uniform or nonuniform in the initial condition, respectively. In the remainder we use the term "simulation" to express one implementation of (2) or (3) over a time interval, for a given collection of initial conditions.

The systems (2) and (3) can alternatively be thought of in the weak sense via the same corresponding Fokker-Planck equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = \frac{\varepsilon^2}{2} \nabla \cdot \nabla \cdot (\rho \, \sigma \, \sigma^\top), \tag{4}$$

which encodes how densities  $\rho(y,t)$  evolve under the flow [67].

Since solutions y to (2) or (3) are random processes, any entities analogous to stable and unstable manifolds of the deterministic system (1) are themselves random. There are well-established methods to account for stable and unstable manifold displacements due to *deterministic* perturbations using, for example, the Melnikov function [4]. Here, we extend this notion to stochastic perturbations.

We first consider stochastically perturbed unstable manifolds. For the deterministic flow,  $\Gamma^{u}$  is defined in terms of the set of points which approaches *a* as  $t \to -\infty$ . Thus, setting  $\sigma(y,t) = 0$  for  $t < t_{1}$  is a technical trick which enables the identification of the random unstable manifold at time  $t_{1}$  to be precisely  $\Gamma^{u}$ . Its continuation in time is then obtained by flowing *forward* in time from  $t_1$  onwards. To formalize the definition, we first note that the deterministic unstable manifold  $\Gamma^u$  can be parametrized as a solution  $x^u(t)$  of (1), where  $x^u(t) \rightarrow a$  as  $t \rightarrow -\infty$ . (This highlights the necessity of requiring infinite times in order to define the unstable manifold  $\Gamma^u$  in the standard way for deterministic systems.) Thus,  $\Gamma^u := \bigcup_{p \in \mathbb{R}} x^u(p)$ . The random unstable set  $G^u(t)$  is now defined by

$$G^{u}(t) := \bigcup_{p \in \mathbb{R}} \{ y^{u}(p,t) : y^{u}(p,t) \text{ solves } (2)/(3)$$
  
with  $y^{u}(p,t_{1}) = x^{u}(t_{1}-t+p) \}.$  (5)

The initial condition  $y^u(p,t_1) = x^u(t_1 - t + p)$  is chosen to ensure that the time-evolved state  $y^u(p,t)$  will be close to  $x^u(p)$ at time t [for the deterministic case with  $\sigma = 0$  we would have  $y^u(p,t) = x^u(p)$ ]. Upon varying the initial condition  $x^u(t_1 - t + p)$  over p, the full deterministic unstable manifold  $\Gamma^u$  is used as the initial condition at time  $t_1$ . Since points on  $\Gamma^u$  at  $t = t_1$  asymptote to a as  $t \to -\infty$  (because there is no stochasticity imposed when  $t < t_1$ ), so will points on  $G^u(t)$ for any t. Thus, our definition complies with the notion of pullback attractors (see for example [29]). We note moreover that definition (5) is generalizable to the situation where the ODE (1) is in  $\mathbb{R}^n$ , and the perturbed unstable set is associated with an (any-dimensional) unstable manifold of any invariant submanifold a, as long as the stochasticity is assumed to be zero for  $t < t_1$ .

Depending on whether the stochastic system employs uniform noise as in (2) or nonuniform noise as in (3), the unstable set  $G^u(t)$  will have different characteristics. If the same noise realization is used for every initial point on the manifold for each forward-time simulation as in (2),  $G^u(t)$  will be a smooth curve for fixed time slice t. Indeed, in this situation, it is possible to define  $G^u(t)$  as the random unstable *manifold* for (2), and there are many results which establish its smoothnesss in more generality [29,30,33–38]. We show in Fig. 2(a) a schematic for  $G^u(t)$  (green curve) at a time instance t, in this situation.

On the other hand, if we use (3) to define the random unstable set  $G^{u}(t)$ , then it will not be smooth because each

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initial point  $x^{u}(t_{1} - t + p)$  experiences a different noise realization in a forward-time simulation. We display in Fig. 2(b) a schematic of the set  $G^{u}(t)$  in this case, bearing in mind that this is a finite representation of the uncountable number of points comprising  $G^{u}(t)$ . We note that while the random unstable set associated with uniform noise using (2) could be defined for infinite-time stochasticity using alternative methods [29-31,33-38], it cannot be extended to infinite times in an obvious way for nonuniform noise using (3). Moreover, the actual computational construction of stochastic slow manifolds in the sense of [29] for the uniform noise case (2) is based on noise convolutions which involve unknown anticipating future noise terms. The most lucid construction is provided by a normal form transformation [32,68] but requires knowledge of future unknown noise which may be heuristically replaced by additive noise terms. The restriction to a finite value of t circumvents this problem, suggesting a straightforward computational construction which works equally well for describing the statistics associated with random unstable sets for uniform and for nonuniform noise.

Next, we provide an analogous definition for the finite-time random stable set  $G^{s}(t)$  for  $t < t_{1}$ . The stable manifold  $\Gamma^{s}$ is defined at time  $t = t_{1}$  for the deterministic flow (1) by  $\Gamma^{s} := \bigcup_{p \in \mathbb{R}} x^{s}(p)$ , in which  $x^{s}(t)$  is a solution to (1) obeying  $x^{s}(t) \to a$  as  $t \to \infty$ . For the stochastic flow (2), we take  $\Gamma^{s}$ as an "initial" condition at time  $t_{1}$ , and run (2) backwards in time to time t. This requires viewing the SDEs (2) and (3) as backward stochastic differential equations which, like their forward counterparts, have well-defined solutions over a finite time under certain smoothness assumptions [69]. Using this backwards time approach, the random stable set  $G^{s}(t)$  is the set of points which asymptotically approaches a as  $t \to \infty$ . We therefore define the *random stable set*  $G^{s}(t)$  by

$$G^{s}(t) := \bigcup_{p \in \mathbb{R}} \{ y^{s}(p,t) : y^{s}(p,t) \text{ solves } (2)/(3)$$
with  $y^{s}(p,t_{1}) = x^{s}(t_{1}-t+p) \}.$  (6)

The set  $G^{s}(t)$  will be either a smooth random stable manifold, or an uncountable collection of points depending on whether the noise is uniform as in (2) or nonuniform as in (3).



FIG. 2. Illustration of the geometry of the finite-time random unstable set  $G^u(t)$  (green curve) in a time slice t and the deterministic unstable manifold  $\Gamma^u$  (dashed yellow curve). (a) For the SDE (2) with uniform noise,  $G^u(t)$  is a smooth curve. (b) For the SDE (3) with nonuniform noise  $G^u(t)$ , is an uncountable collection of random points.

#### B. Uncertainty of stable and unstable sets

The random stable and unstable sets differ for each realization of noise. To enable a statistical description of this variation, we characterize their mean and variance with respect to realizations of the driving Brownian noise. We first examine the uncertainty associated with the unstable set  $G^u(t)$ . While the geometric nature of the sets  $G^u(t)$  is inherently different for uniform and nonuniform noise (cf. Fig. 2), our theory applies to *either* case. To define the displacement from the deterministic manifold  $\Gamma^u$ , we fix  $p \in \mathbb{R}$ , and let

$$\hat{n}^{u}(p) := \frac{v^{\perp}(x^{u}(p))}{|v(x^{u}(p))|} \tag{7}$$

be the unit normal vector to  $\Gamma^{u}$  at the location  $x^{u}(p)$ . Here, the  $\perp$  operation on vectors in  $\mathbb{R}^{2}$  denotes rotation by  $+\pi/2$ , that is,

$$h^{\perp} := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} h. \tag{8}$$

Let  $t > t_1$  be finite. For  $y^u(p,t) \in G^u(t)$ , we define the random normal displacement by

$$N^{u}(p,t) := [y^{u}(p,t) - x^{u}(p)] \cdot \hat{n}^{u}(p)$$
(9)

which represents the normal displacement of  $G^{u}(t)$  with respect to  $\Gamma^{u}$ , at locations parametrized by p, and at times  $t > t_1$ . The reader is referred to Fig. 2 for a geometric depiction of the displacement.

We now look at the statistics of the displacement in terms of averaging over different realizations of the driving noise. To elucidate the leading order behavior of  $N^u$ , we consider the random variable

$$\tilde{N}^{u}(p,t) := \lim_{\varepsilon \to 0} \frac{N^{u}(p,t)}{\varepsilon}.$$
 (10)

By adapting the stochastic curve theory of [40], we show in Appendix A that the leading-order expectation of the normal displacement is zero, i.e.,

$$E[\tilde{N}^{u}(p,t)] = 0 \quad \text{for all } p, \tag{11}$$

where the expectation value is taken with respect to all Brownian driving paths. This relies on Itô's lemma [70,71] being applied to (2) to determine the evolution equation for the random variable  $y^{u}(p,t)$  to first order. The mean over realizations of the unstable set  $G^{u}(t)$  is therefore the deterministic unstable manifold  $\Gamma^{u}$ , independent of t.

Next, we define the standard deviation, a measure for the uncertainty, of the leading-order normal displacement by

$$w^{u}(p,t) := \sqrt{\operatorname{Var}[\tilde{N}^{u}(p,t)]}.$$
(12)

Appendix A shows that the methods of [40] (which rely on the Itô isometry [70,71]) can be adapted to obtain

$$w^{u}(p,t) = \frac{\left[\int_{t_{1}}^{t} e^{2\int_{\tau}^{t} [\nabla \cdot v](x^{u}(\xi-t+p))d\xi} \left| \sigma^{\mathsf{T}}(x^{u}(\tau-t+p),\tau)v^{\perp}(x^{u}(\tau-t+p))\right|^{2}d\tau\right]^{1/2}}{|v(x^{u}(p))|},$$
(13)

in which  $\sigma^{\top}$  is the transpose of the matrix  $\sigma$ . Thus,  $\varepsilon w^{u}(p,t)$  gives an expression for the leading-order uncertainty of the normal displacement between  $G^{u}(t)$  and  $\Gamma^{u}$  at a location p, and at a time instance t. In contrast with the random variable  $N^{u}(p,t)$ ,  $w^{u}(p,t)$  is smooth in p even for nonuniform noise as in (3). We note that the expressions (11) and (13) work for *either of the interpretations (2) or (3)* because in deriving the expressions, p is considered fixed (see Appendix A).

The uncertainty (13) associated with the unstable set monotonically increases with time t, representing the accumulation of stochastic effects as time progresses. However, under generic conditions ( $\sigma$  is bounded), we show in Appendix B that as t increases,  $w^u(p,t)$  approaches a constant value at any particular point  $x^u(p)$  on  $\Gamma^u$ , and does so exponentially fast. The saturation of the uncertainty of the flow barrier is related to approaching the invariant density of the corresponding Fokker-Planck system (4). If the time required to reach statistical equilibrium is less that the characteristic timescale  $\tau_c$  of the large-scale flow, we may set in our formulas  $t \to \infty$ . We numerically verify that this saturation occurs rapidly in the Taylor-Green example we analyze in Sec. IV.

The limit  $p \rightarrow -\infty$  in (13) provides the uncertainty at the saddle point *a*. This limit is computed exactly as described in Sec. 3.5 of [72], where a similar limit is computed for a comparable expression (this argument is similar in spirit to

that presented in Appendix B for the limit  $t \to \infty$  as well). We find that

$$w^{u}(-\infty,t) = e^{\lambda_{s}t} \left( \int_{t_{1}}^{t} e^{-2\lambda_{s}\tau} \left| \sigma^{\mathsf{T}}(a,\tau) \hat{e}_{u}^{\perp} \right|^{2} d\tau \right)^{1/2}, \quad (14)$$

and this uncertainty is measured in the direction  $\hat{e}_u^{\perp}$  from *a* [i.e.,  $\hat{n}^u(p) \rightarrow \hat{e}_u^{\perp}$  as  $p \rightarrow -\infty$ ]. The vectors  $\hat{e}_s$  and  $\hat{e}_u$  are the normalized eigenvectors of the Jacobian matrix  $\nabla v(a)$  with corresponding eigenvalues  $\lambda_s < 0$  and  $\lambda_u > 0$ , tangential to the stable and unstable manifolds at *a*, respectively. The appearance of the *complementary* eigenvalue  $\lambda_s$  when considering an uncertainty of the unstable manifold in the  $v_u^{\perp}$  direction is to be noted.

Let us return to the general expression (13) for the uncertainty  $w^{u}(p,t)$ . There are two simplifications which occur under regularly considered cases:

(i) If the fluid is incompressible with  $\nabla \cdot v = 0$ , the entire exponential factor in (13) simplifies to 1.

(ii) If the diffusion is isotropic and independent of space and time, then  $\sigma = \text{Id}$  (but let us suppose it retains the appropriate dimensions). This allows the  $\sigma$  term to be discarded from (13). Moreover, since  $|v^{\perp}| = |v|$ , the  $\perp$  symbol on the v in the integrand can be removed.

If *both* the above simplifications are in operation, then the uncertainty formula (13) reduces to the particularly simple

form

$$w^{u}(p,t) = \frac{\left[\int_{t_{1}}^{t} |v(x^{u}(\tau - t + p))|^{2} d\tau\right]^{1/2}}{|v(x^{u}(p))|}.$$
 (15)

This is the temporal  $L^2$  norm of the quantity  $|v(x^u(\tau - t + p))|/|v(x^u(p))|$ , which represents the fractional speed at a time-varying point in relation to that at the final point  $x^u(p)$  (occurring at  $\tau = t$ ). The along-manifold velocity variations therefore impact the across-manifold uncertainties; an intuitive explanation is that the along-manifold velocity variation is directly linked to that across the manifold because of incompressibility.

If only simplification (ii) applies, the uncertainty at a [Eq. (14)] is explicitly integrated to give

$$w^{\mu}(-\infty,t) = e^{\lambda_s t} \left(\frac{e^{-2\lambda_s t} - e^{-2\lambda_s t_1}}{-2\lambda_s}\right)^{1/2}, \qquad (16)$$

and if additionally  $\nabla \cdot v = 0$ , the condition  $\lambda_s = -\lambda_u$  can be applied.

The general expression for the standard deviation (13) allows for the definition of uncertainty regions around  $\Gamma^{u}$ . At any time instance *t*, we define

$$R^{u}_{\alpha}(t) := \bigcup_{p} \{ x^{u}(p) + \alpha r \varepsilon \, w^{u}(p,t) \hat{n}^{u}(p) : r \in [-1,1] \}.$$
(17)

The parameter  $\alpha$  represents how many standard deviations around  $\Gamma^u$  the region is, and therefore  $R^u_{\alpha}$  defines a region of uncertainty of the stochastic unstable sets  $G^u(t)$ , to leading order in  $\varepsilon$ . While there is no obvious reason to expect that the unstable sets are normally distributed around the unstable manifold  $\Gamma^{u}$  (indeed, in our numerical simulations they are not), a choice  $\alpha = 2$  (which would represent a 95% confidence interval for an assumed normal distribution) appears reasonable for capturing the bulk of the uncertainty.

An analogous characterization is possible for the displacement of the random stable set  $G^{s}(t)$ . We define

$$\hat{n}^{s}(p) := \frac{v^{\perp}(x^{s}(p))}{|v(x^{s}(p))|}$$
(18)

and for  $t < t_1$  consider

$$N^{s}(p,t) := [y^{s}(p,t) - x^{s}(p)] \cdot \hat{n}^{s}(p).$$
(19)

As before, we expect  $E[N^s(p,t)] = O(\varepsilon)$ , motivating the definition

$$\tilde{N}^{s}(p,t) := \lim_{\varepsilon \to 0} \frac{N^{s}(p,t)}{\varepsilon}.$$
(20)

The proofs for the unstable manifold furnished in Appendix A go through for the stable manifold with no substantive change. In particular,

$$E[\tilde{N}^{s}(p,t)] = 0 \quad \text{for all } p, \tag{21}$$

implying that the mean of the stable sets over different realizations of the Brownian driving noise is given by the stable manifold  $\Gamma^s$ . The standard deviation defined by

$$w^{s}(p,t) := \sqrt{\operatorname{Var}[\tilde{N}^{s}(p,t)]}$$
(22)

yields the uncertainty measure

$$w^{s}(p,t) = \frac{\left[\int_{t}^{t} e^{2\int_{\tau}^{t} [\nabla \cdot v](x^{s}(\xi-t+p))d\xi} \left| \sigma^{\top}(x^{s}(\tau-t+p),\tau)v^{\perp}(x^{s}(\tau-t+p))\right|^{2}d\tau \right]^{1/2}}{|v(x^{s}(p))|}.$$
(23)

Our previous discussions on simplifications under incompressibility and isotropic diffusion for  $w^u$  apply equally for (23). Moreover, saturation of  $w^s(p,t)$  is to be expected as  $t \to -\infty$  for bounded  $\sigma$ . The uncertainty at *a* in the direction  $\hat{e}_s^{\perp}$  is obtained by taking the limit  $p \to \infty$  in (23), which leads to

$$w^{s}(\infty,t) = e^{\lambda_{u}t} \left( \int_{t}^{t_{1}} e^{-2\lambda_{u}\tau} |\sigma^{\top}(a,\tau)\hat{e}_{s}^{\perp}|^{2} d\tau \right)^{1/2}.$$
 (24)

The corresponding expression under  $\sigma = \text{Id is}$ 

$$w^{s}(\infty,t) = e^{\lambda_{u}t} \left(\frac{e^{-2\lambda_{u}t} - e^{-2\lambda_{u}t_{1}}}{2\lambda_{u}}\right)^{1/2}.$$
 (25)

In general, the region of uncertainty is

$$R^{s}_{\alpha}(t) := \bigcup_{p} \{ x^{s}(p) + \alpha r \varepsilon \ w^{s}(p,t) \hat{n}^{s}(p) : r \in [-1,1] \}, \quad (26)$$

which quantifies the fuzziness of the stable manifold when subjected to a (small) stochastic perturbation.

In the next two sections, we consider two specific examples. In the first example in Sec. III, we examine the perturbations to the stable manifold for uniform and nonuniform noises as in (2) and (3) for a velocity which is not area preserving. Our

focus here is directly on the manifolds and their uncertainty, but we will also compare our uncertainty measures to the spatial structure of a noise-averaged exponential stretching measure. In the second example, we study a stochastically perturbed area-preserving flow and show how our analytical expressions can be used to quantify fluid transport across stochastic Lagrangian structures. Specifically, this example relates our measures to spatial mixing regions near the stable manifold.

## III. STOCHASTIC SETS RESPECT EXPONENTIAL STRETCHING: A COMPRESSIBLE EXAMPLE

The deterministic base flow we consider for this example is given by

$$\dot{x}_1 = -4x_1 + x_1^2 \\ \dot{x}_2 = 3x_2 - x_2^2$$
(27)

which is *not* area preserving. The part of the phase plane of interest to us is shown in Fig. 3. The focus shall be on the stochastic perturbation to the stable manifold  $\Gamma^s$  of (0,0) as shown in green. The relevant parametric representation for this, as a solution to (27), is

$$x^{s}(p) = \begin{pmatrix} 4/(1+e^{4p})\\ 0 \end{pmatrix}; \quad p \in \mathbb{R}.$$



FIG. 3. The phase plane of (27), with the stable manifold of interest  $\Gamma^s$  shown in green.

The analytical formula (23) for the uncertainty measure  $w^s$  along the stable curve requires the calculation of the quantities

$$v(x^{s}(\tau - t + p)) = \begin{pmatrix} -16e^{4(\tau - t + p)}/(1 + e^{4(\tau - t + p)})^{2} \\ 0 \end{pmatrix}$$

and

 $x_{2}$ 

$$[\nabla \cdot v](x^{s}(\tau - t + p)) = -1 + \frac{8}{1 + e^{4(\tau - t + p)}}.$$

After some algebra (not shown), the leading-order uncertainty of the stable manifold (23) reduces to

$$w^{s}(p,t) = e^{3t} \left\{ \int_{t}^{t_{1}} e^{-6\tau} \left[ \sigma_{21}^{2} \left( \frac{4}{1 + e^{4(\tau - t + p)}}, 0, \tau \right) + \sigma_{22}^{2} \left( \frac{4}{1 + e^{4(\tau - t + p)}}, 0, \tau \right) \right] d\tau \right\}^{1/2}, \quad (28)$$

where  $\sigma_{ij}$  represent the components of the diffusion matrix. For the computations in this section, we choose

$$\sigma_{11} = 1, \ \sigma_{12} = 0, \ \sigma_{21} = x_2 - 1$$
 and  
 $\sigma_{22} = 3\sin(2\pi x_1)e^{0.8x_1}$ 

which support a nontrivial dependency along the deterministic stable manifold  $x_2 = 0$ .

We will now study the stable set  $G^s(t)$  with  $t_1 = 2$ . To numerically solve the SDEs (2) and (3), we employ the Euler-Maruyama scheme [73,74]. There are two competing issues in choosing  $\varepsilon$  and the time step  $\Delta t$  for the numerical simulations:  $\varepsilon \sqrt{\Delta t}$  must be much smaller than  $\Delta t$  (i.e.,  $|\varepsilon| \ll \sqrt{\Delta t}$ ) to ensure that the stochasticity appears as a perturbation, while  $\Delta t$  must itself be small for better accuracy of the method. In the following, we use  $\varepsilon = 0.02$  and  $\Delta t = 0.01$  unless otherwise specified.

Let us first compute the stable curve  $G^{s}(t = 0)$  for the system (27) driven by uniform noise, in which each initial condition is propagated with the same realization of the noise as in (2). To do so, we seed 4000 particles along  $y_2 = 0$ , equally spaced between  $x_1 = 0$  and 0.004 at time  $t_1 = 2$ , and advect (2) backward in time to t = 0. The stable curve  $G^{s}(0)$  (green) associated with one single simulation is shown in Fig. 4(a). We now show that the average behavior of the stable curves  $G^{s}(t)$  with respect to different realizations of the noise is well described by our theory, where the mean is given by  $\Gamma^s$  [up to  $O(\varepsilon^2)$  and the standard deviation by  $w^s(p,t)$ . In Fig. 4(b), we present a histogram using 100 000 independent simulations (each seeded with 4000 initial particles), formed by counting the proportion of the  $4 \times 10^8$  points within each bin of size  $(0.0525 \times 0.01)$  in the displayed domain at time t = 0. It is clearly seen that the contour lines of the histogram align well with the regions  $R^s_{\alpha}(0)$  of the uncertainty.

We next numerically generate the random stable set  $G^{s}(t = 0)$  for the system (27) driven by nonuniform noise, as in the class of SDEs (3). Figure 5(a) shows  $G^{s}(t = 0)$  obtained for a single simulation; it is now a collection of points as opposed to



FIG. 4. Smooth stable set  $G^s(t = 0)$  of the stochastic flow associated with (27) driven by uniform noise with  $\varepsilon = 0.02$  from time  $t_1 = 2$ . (a) Single simulation (green). (b) Histogram from 100 000 simulations. The black curves depict the  $\alpha = 1$  (thick dashed line),  $\alpha = 2$  (thin dashed line), and  $\alpha = 3$  (dotted line) standard deviation envelopes  $R^s_{\alpha}(t = 0)$  [cf. (26) using the analytical expression (28) for  $w^s(p,t)$ ].



FIG. 5. Stable set  $G^s(t = 0)$  of the stochastic flow associated with (3) driven by nonuniform noise with  $\varepsilon = 0.02$  from time  $t_1 = 2$ . (a) Single simulation (green dots). (b) Histogram from 1000 simulations. The black curves depict the  $\alpha = 1$  (thick dashed line),  $\alpha = 2$  (thin dashed line), and  $\alpha = 3$  (dotted line) standard deviation regions  $R_{\alpha}^s(t = 0)$  [cf. (26) using the analytical expression (28) for  $w^s(p,t)$ ].

the smooth curve depicted in Fig. 4(a). The histogram over realizations of the noise is shown in Fig. 5(b) and resembles the histogram obtained for the SDE (2) driven by uniform noise shown in Fig. 4(b). Note that the average is taken here only with 1000 realizations whereas in the uniform nosie case we used 100 000 realizations. As the Fokker-Planck equation (4) is identical for the two SDEs (2) and (3), we can interpret the simulation of the nonuniform noise case (3) as an effective computational tool to determine the statistical behavior of an ensemble of realizations of the noise for the uniform noise case (2).

Our theory gives the mean and standard deviations of the instantaneous normal distance  $N^s$  of the stable curve  $G^s(t)$ to the stable manifold  $\Gamma^{s}$  [cf. (19)]. We now numerically verify these expressions, validating also that these expressions are correct to order  $\varepsilon$ . To determine the statistics of scatter around the point (1.5,0) on the stable manifold at time t = 0, we advect backwards from time  $t_1 = 2$  from the point  $(0.000\,696\,8,0)$ . This is the point from which (1.5,0) maps under deterministic advection from t = 0 to  $t_1 = 2$ , and is associated with p = 0.12771. Since we are considering only one initial condition, the systems (2) and (3) are equivalent for this experiment. The quantity  $N^s$  (in this case  $N^s = x_2$ because  $\hat{n}^s$  is the unit vector in the  $x_2$  direction) is computed for each of  $M = 10^4$  simulations. The empirical probability density function  $f(N^s)$  is shown in Fig. 6 for several values of  $\varepsilon$  together with a normal probability density function with the mean and variance given by our theoretical predictions; the mean is zero according to (21) and the standard deviation  $\varepsilon w^{s}(0.12771,0)$  is computed from (23). The simulations also illustrate the interesting fact that the actual density function clearly does not converge to a Gaussian; in all our simulations we observed a sharper peak at zero. The spread of the density, however, clearly exhibits convergence as  $\varepsilon \to 0$ . Our theory provides an  $O(\varepsilon)$  expression for the standard deviation, and thus this value should be accurate up to  $O(\varepsilon^2)$ . We explore this in Fig. 6(d), where we use M simulations for each  $\varepsilon$  to plot the

logarithm of the error

$$E = \left| \sqrt{\frac{1}{M} \sum_{j=1}^{M} \left( x_2^{(j)}(0) \right)^2 - \varepsilon w^s(0.12771, 0)} \right|$$
(29)

between the theoretical and numerical standard deviations against  $\varepsilon$ , where  $x_2^{(j)}(0)$  is the  $x_2$  coordinate at time t = 0 of the *j*th ensemble member with initial condition  $x_1(t_1) = 0.12771$  and  $x_2 = 0$ . In this region, the error appears to go as  $\varepsilon^{2.5}$ , confirming the scaling  $O(\varepsilon^2)$  as discussed above.

We next compute the finite-time Lyapunov exponent (FTLE) field, whose strong ridges help identify stable manifolds in the deterministic setting. Forward-time FTLE fields are the relevant diagnostics for stable manifolds since particles on the stable manifold will be exponentially stretched apart by the complementary unstable manifold attached to (0,0)as visible in Fig. 3. The FTLEs at a time t are the finitetime averages of the maximum expansion rate for a pair of particles propagated by (2) over the time interval  $[t,t_1]$ (see, for example, [3] on the computation of FTLEs). Monte Carlo methods for FTLE fields are now emerging as a tool in stochastic situations [18,19,75–79]. Following these ideas, we seed  $200 \times 400$  particles in the same domain displayed in Fig. 4 at time t = 0. The particles are then advected forward in time with the dynamics (2) to time  $t_1 = 2$ , and the resulting FTLE field is computed. Figure 7(a) shows a clear ridge of the FTLE field, indicative of the stable manifold curve  $G^{s}(t = 0)$ . Exactly as for deterministic flows, this sharp ridge is an indication that for that particular realization of noise, the stable curve is smooth. Since recent work legitimizes taking the expectation over many simulations [79], in Fig. 7(b) we show the averaged FTLE field across 100 000 simulations, of which (a) is one. The statistical spread of the stretching fields displays a "fattening" associated with the uncertainty of the stable set. We have used a nonlinear scaling on the color bar to

![](_page_8_Figure_2.jpeg)

FIG. 6. (a)–(c) Analysis of the normal statistics of  $N^s = x_2$  at the (1.5,0) for the stochastic flow associated with (27) driven by uniform noise from time  $t_1 = 2$  to t = 0, for the values (a)  $\varepsilon = 0.02$ , (b)  $\varepsilon = 0.007$ , and (c)  $\varepsilon = 0.002$ . Shown is the empirical probability density function  $f(N^s)$  of the simulation (red circles) using  $M = 10^4$  simulations, and a reference normal probability density function with variance given by the theoretical values  $\varepsilon w^s(0.12771,0)$  as computed from (23) and mean zero as computed from (21) (blue curves). (d) The error *E* in the standard deviation versus  $\varepsilon$  in these simulations (red circles), in a log-log plot. The slope obtained by linear regression is 2.48.

![](_page_8_Figure_4.jpeg)

FIG. 7. The forward FTLE field computed at time t = 0 for the stochastic flow associated with (27) driven by uniform noise until time  $t_1 = 2$ , using identical conditions and notation as in Fig. 4. (a) One single simulation, and (b) the mean of 100 000 simulations using a nonlinearly scaled color bar. The black curves depict the  $\alpha = 1$  (thick dashed line),  $\alpha = 2$  (thin dashed line), and  $\alpha = 3$  (dotted line) standard deviation regions  $R_{\alpha}^{s}(t = 0)$  [cf. (26) using the analytical expression (28) for  $w^{s}(p,t)$ ].

elucidate the variation in the (rarely visited) outer flanges, for an effective comparison with the theory even up to the three standard-deviation level. Our theoretical regions  $R^s_{\alpha}(0)$  capture the undulating nature of the averaged FTLE field excellently, implying that the spatial structure of the exponential stretching statistics is well recovered by our theory.

We remark that performing the FTLE calculation using the nonuniform model (3) does not make sense because the presence of *different* noise realizations in adjacent trajectories generates a flow map which is not smooth. The spatial gradients of the flow map then acquire large values which are additional to those arising from exponential separation.

### IV. STOCHASTIC SETS GOVERN TRANSPORT: TAYLOR-GREEN FLOW

The previous example illustrated that the theory for the uncertainty of stochastic stable sets was consistent with both the actual stochastic evolution of a curve positioned on the stable manifold  $\Gamma^s$  at some final time, as well as the distribution of exponential stretching as quantified by FTLEs. We now explore the implications associated with the uncertainties to quantitatively understand *transport* across the deterministic flow barriers.

The deterministic base flow we examine here is the areapreserving Taylor-Green flow [4], also known as planar cellular flow:

$$\dot{x}_1 = -\sin(\pi x_1)\cos(\pi x_2) \dot{x}_2 = \cos(\pi x_1)\sin(\pi x_2)$$
(30)

Its phase portrait, which consists of a periodic array of counterrotating vortices, is depicted in Fig. 8. We wish to relate the uncertainty of the heteroclinic manifold (shown in green in Fig. 8) with the transport occurring between the upper and lower cells under stochastic perturbations. Particles within the cells get fed into the transport region by coming in towards the point (1,0) and then getting pulled along by this heteroclinic manifold; hence for the study of how particles are advected in forward time and diffuse across these two cells, it is their location with respect to the *unstable manifold*  $\Gamma^{u}$  which is pertinent.

w

![](_page_9_Figure_9.jpeg)

FIG. 8. The phase plane of the Taylor-Green flow (30), with the transport barrier between the upper and lower cells shown in green.

We note that here  $\nabla \cdot v = 0$ , and moreover

$$x^{u}(p) = \begin{pmatrix} \frac{2}{\pi} \tan^{-1}(e^{-\pi p}) \\ 0 \end{pmatrix}$$

and

1

$$v(x^{u}(\tau - t + p)) = \begin{pmatrix} -2\operatorname{sech}[\pi(\tau - t + p)] \\ 0 \end{pmatrix}$$

For general  $\sigma$ , performing the algebra on (13) leads to

$${}^{u}(p,t) = \frac{\left(\int_{t_{1}}^{t} \operatorname{sech}^{2}[\pi(\tau-t+p)] \left[\sigma_{21}^{2}(x_{1}(\tau-t+p),0,\tau) + \sigma_{22}^{2}(x_{1}(\tau-t+p),0,\tau)\right] d\tau\right)^{1/2}}{\operatorname{sech}(\pi p)},$$
(31)

where

$$x_1(p) := \frac{2}{\pi} \tan^{-1}(e^{-\pi p})$$
(32)

is the relationship between the  $x_1$  coordinate along  $\Gamma^u$  and its p parametrization.

We examine the case  $\sigma = \text{Id}$ , in which case (31) can be integrated explicitly to yield

$$w^{u}(p,t) = \cosh(\pi p) \left( \frac{\tanh[\pi p] - \tanh[\pi(t_{1} - t + p)]}{\pi} \right)^{1/2}.$$

After using the relationship (32) to represent  $w^u$  in terms of the location  $x_1 \in (0,1]$  along  $\Gamma^u$  rather than p, the *explicit* uncertainty measure is evaluated as

$$\tilde{w}^{u}(x_{1},t) := w^{u}(p,t) = \frac{1}{\sqrt{\pi \{ \coth [\pi (t-t_{1})] - \cos (\pi x_{1}) \}}} .$$
(33)

This is not zero as  $x_1 \rightarrow 1$ , and the limiting value coincides with the unstable manifold uncertainty expression  $w^u(-\infty,t)$ "at saddle-point" given in (14). However,  $\tilde{w}^u$  becomes unbounded as  $x_1 \rightarrow 0^+$ , influenced by the stable manifold at (0,0). This can be understood by realizing that any small perturbation near  $x_1 \gtrsim 0$  will be impacted by the strong exponential stretching in backward time due to the unstable manifold. Another interesting observation is that  $\tilde{w}^u$  in (33) is monotonically increasing in *t* at each fixed location  $x_1$  (representing an increase in uncertainty with time), but saturates rapidly to

$$\tilde{w}^{u}(x_{1},\infty) = \frac{1}{\sqrt{2\pi}} \csc\left(\frac{\pi x_{1}}{2}\right),\tag{34}$$

defining a *long-term uncertainty* with respect to the location  $x_1$  on  $\Gamma^u$ . This is a special case of the expected convergence to a limiting long-term uncertainty as shown in Appendix B. The existence of a constant limiting long-term uncertainty reflects the fact that the number of particles leaving a cell equals on average the number of particles entering a cell, allowing for a statistical equilibrium.

We now relate these expressions for the uncertainty to mixing. Specifically, we focus on the fact that, in the absence of stochasticity, the unstable manifold  $\Gamma^u$  forms a flow barrier between the upper and lower cells in Fig. 8. Fluid which swirls around in each cell and approaches  $x_2 = 0$  from near  $x_1 = 1$ remains separated by  $\Gamma^u$  as it travels near  $x_2 = 0$ . The inclusion of stochasticity destroys the "flow barrier," thereby causing mixing between the fluids of the upper and lower cells. The spatial distribution of this mixing is directly controlled by the uncertainty regions  $R^u_{\alpha}$  given by our theory, as we now verify. For our numerical verification, we seed the entirety of the upper cell with a uniform grid of  $1000 \times 2000$  particles at time  $t_1 = 0$ , and advect it with the stochastically perturbed flow (with  $\sigma = \text{Id and } \varepsilon = 0.1$ ), using the Euler-Maruyama scheme with  $\Delta t = 0.01$ . To obtain an efficient statistical description, we choose the SDE driven by nonuniform noise (3) rather than (2)driven by uniform noise, and perform only one simulation. In effect, we perform a Monte Carlo approximation of the Fokker-Planck equation (4) with the initial density being the Lebesgue measure on the two cells. [We cross validated this computation by directly simulating the Fokker-Planck equation (4) using a spectral scheme with Crank-Nicolson time stepping, using as our initial density each of (i) uniform density in the top cell, (ii) uniform density in the bottom cell, and (iii) Dirac density supported on  $\Gamma^u$  (not shown).]

Since our focus is on particles which escape into the lower cell, we use periodic boundary conditions for  $x_1 \in [0,1]$  to ensure that particles escaping from the left and right sides are fed back into the cell. We focus on a mixing zone near  $x_2 = 0$ , in particular choosing the region  $(x_1, x_2) \in [0.1, 0.9] \times$ [-0.1, 0.1] (we exclude regions near  $x_1 = 0$  and 1 to minimize periodic boundary condition effects). We bin this region into boxes of width 0.025 and height 0.005. We show in Fig. 9(a) the histogram of the particles at time t = 2 which were initially at  $t_1 = 0$  in the upper cell. The dashed blue curves are the  $\alpha = 1$  (thick) and  $\alpha = 2$  (thin) standard deviation envelopes of  $R^{u}_{\alpha}(t)$  computed using (33); that is, the curves  $x_{2} = \pm \varepsilon \tilde{w}(x_{1},t)$ (thick) and  $x_2 = \pm 2\varepsilon \tilde{w}(x_1,t)$  (thin). These curves, which demarcate the uncertainty around the mean of the unstable set, align well with the density contour lines of the simulation. The larger density in the upper-right region is associated with regions well divorced from the mixing region, that is outside the uncertainty region  $R^{u}_{\alpha}(t)$ . The "leakage" of the

![](_page_10_Figure_7.jpeg)

FIG. 9. Mixing characterization of Taylor–Green flow from time  $t_1 = 0$  to t = 2, using uniformly seeded particles in the upper and lower cells. In all cases, the blue dashed lines depict the  $\alpha = 1$  (thick) and  $\alpha = 2$  (thin) standard deviation envelopes  $R_{\alpha}^{u}(t)$  computed using (33). (a) Upper fluid histogram, (b) Lower fluid histogram, (c) Histogram of the covariance function  $c_i(t = 2)$  as given in (35).

upper fluid into the lower cell is seen to be spatially correlated with the fact that the uncertainty region  $R^u_{\alpha}(t)$  extrudes into the lower cell. Moreover, the fact that the uncertainty region  $R^u_{\alpha}(t)$  also ventures into the upper cell is displayed by the fact that there is a smaller density in the region defined by  $R^u_{\alpha}(t)$ about  $x_2 = 0$  in comparison to regions well above  $x_2 = 0$ . Figure 9(b) is a similar histogram, but now of the *lower* fluid, i.e., particles seeded uniformly in the lower cell at time  $t_1 = 0$ , and advected stochastically until t = 2. Once again, the ability of the uncertainty regions of the unstable set to describe the probability density function of the fluid particles is apparent.

To further quantify *mixing* between the cells, we define a covariance-like quantity as follows. Let  $u_i$  and  $l_i$  represent the number of "upper" and "lower" fluid particles which are in bin i at time t, and  $\bar{u}$  and  $\bar{l}$  be the average number of particles in each bin, with the average taken over all the bins in our mixing zone. Then, we define the covariance function

for each cell *i*. One or the other of the two terms in (35) is close to zero in regions in which only one of the fluid types dominate, and therefore  $c_i$  is expected to be small in such regions. In contrast,  $c_i$  will be larger in regions in which *both* fluid types are present, i.e., regions of strong mixing between upper and lower fluids. The histogram of  $c_i(2)$  is shown in Fig. 9(c). As expected, the spatial distribution of the mixing measure  $c_i$ indeed strongly correlates with the uncertainty envelopes of the unstable set. The dashed blue curves identifying  $R_{\alpha=1}^{u}(t)$  align with these contours of the covariance. That is, we have verified that the uncertainty measure  $R_{\alpha}^{u}(t)$  quantifies the spatial mixing regions between cells.

Next, we analyze the temporal evolution of the mixing. Figure 10 shows the covariance function  $c_i(t)$  as a function of the final time t. The solid green curves drawn in each figure are the curves  $x_2 = \pm \varepsilon \tilde{w}^u(x_1, \infty)$ , with the saturated variance of the unstable set  $\tilde{w}^u(x_1, \infty)$  as given in (34). At each time pictured in Fig. 10, the blue dashed curves  $R^u_{\alpha}(t)$ 

![](_page_11_Figure_6.jpeg)

FIG. 10. Mixing characterization of Taylor-Green flow from time  $t_1 = 0$ , using the contours of the covariance  $c_i(t)$  [cf. (35)], with parameters and curve descriptions as in Fig. 9. The final times for the figures are (a) t = 0.1, (b) t = 0.4, (c) t = 1, and (d) t = 7. The solid green curve represents the saturated uncertainty as defined by (34), to which  $R^u_{\alpha=1}(t)$  is seen to converge as t increases.

![](_page_12_Figure_2.jpeg)

FIG. 11. Exactly as in Fig. 10, the covariance  $c_i(t)$  is shown for the temporally and spatially varying diffusion  $\sigma$  as defined in (36) rather than  $\sigma = \text{Id}$ . The final times are (a) t = 0.1, (b) t = 0.4, (c) t = 1, and (d) t = 7.

(for each *t*) describe the spatial variation of the covariance (35) remarkably well. As time increases, the increase in uncertainty is captured by the fact that the blue dashed curves are progressing outwards. However, this increase in uncertainty saturates rapidly with time. Specifically,  $R_{\alpha=1}^{u}(t)$  appears to have converged by t = 1 to the green curves, which mark the saturation. Moreover, the dominant characteristics of the covariance contours at t = 1 are not very different from those at t = 7, and in both these situations the thick blue dashed curves associated with  $R_{\alpha=1}^{u}(t)$  are virtually indistinguishable from the solid green curve representing the saturated variance around the unstable manifold  $\Gamma^{u}$ .

Finally, we illustrate that our theory also describes the spatial mixing for diffusion matrices which are temporally and spatially varying. We choose here

$$\sigma_{11} = 1, \ \sigma_{12} = 0, \ \sigma_{21} = 0, \sigma_{22} = \operatorname{sech}(x_1 - \frac{1}{2})\cos(5\pi x_1)\tanh(t) \bigg\}.$$
 (36)

In this case, an explicit expression as in (34) for the saturated uncertainty cannot be given. However, it can be numerically computed using (31) for  $t \gg 1$ . Figure 11 displays the covariance field  $c_i(t)$ . The highly mixing region expands from being compressed near  $x_2 = 0$  at t = 0.1, and saturates as expected (at a slower rate than for  $\sigma = \text{Id}$ ). The spatial variation of the uncertainty region  $R_{\alpha}(t)$  at each time t, and its temporal evolution describes the numerically observed spatial mixing remarkably well.

#### V. DISCUSSION AND OUTLOOK

We have developed a framework to study the effect of small stochastic noise on the transport and mixing properties of twodimensional fluid flow situations. We considered the idealized situations of a well-defined slowly varying large-scale flow subjected to small-scale noise, where we have access to the associated stable or unstable manifolds at some fixed time. We extended the notion of stable and unstable invariant manifolds to noisy stable and unstable sets, by tracking the evolution respectively in backward and forward time. These sets are smooth curves for stochastic dynamical systems which employ the same noise realization for each initial condition, but are an uncountable collection of points when each initial condition is evolved with its own Brownian noise driver. The mean and variance of the displacement of these curves from the associated deterministic stable and unstable manifolds at any finite time are calculated in the presence of small noise. The mean displacement is, to leading order in the noise parameter, zero, consistent with the heuristic expectation that the mean stable and unstable sets remain close to their deterministic counterparts. The variance is a measure of the fuzziness of these stable and unstable sets and quantifies how different realizations of the noise vary around the mean. As such, we provide an easily expressible theoretical quantification of statistical properties of the random stable and unstable manifolds. The theory can also be applied for an *unsteady* velocity field v(x,t) as long as we are able to identify the stable and unstable manifolds at a given time  $t_1$ . In other words, the theory works to quantify the uncertainty due to propagation, assuming that at an initial time, the manifold is known.

We validate in numerical simulations that the coherent sets identified by the mean of the stable and unstable sets coincide with the ridges of the FTLEs. Whereas this is well established in the deterministic context, the application of FTLEs in the stochastic, or equivalently diffusive [18,77,78], context is less well explored. Moreover the variance theory that we developed was shown to capture the spatial structure of the averaged FTLE field, thereby providing an explicit method for ascribing an uncertainty in the location of ridges.

From a practical perspective, our formulas quantify the expected transport of Lagrangian tracers across stochastically perturbed transport barriers. In particular, we use the variance of stable and unstable sets around their mean to determine the physical region in space which on average will be mixed at a given time. These well-defined mixing regions  $R_{\alpha}(t)$  allow us to specify, via  $\alpha$ , the probability of finding mixing and leakage across the mean of the stable and unstable sets. This can be used to determine, for example, the possible extent of environmental pollution such as oil spills, together with an uncertainty quantification based on any given model for the diffusivity matrix  $\sigma$ .

The analytical expressions we found require knowledge about the deterministic vector field as well as the diffusive behavior (for example, by means of eddy dispersion, drifter separation, or alternative model for stochasticity [80–83]). Conversely, information about the extent of the mixing region and the fuzziness of the transport barriers may allow us to find estimates on the diffusion tensor given only measurements of the mean flow and the mixing region. This can be used to cross validate the estimation of the diffusion tensor by oceanographers using eddy dispersion or drifter separation. Although this does not allow for the determination of each individual component of the diffusion tensor, the estimation of the variance allows for the estimation of the diffusivity across the mean stable and unstable curves. In the case presented in Sec. IV, the formula (31) for the width of the transport barrier allows to determine, for example,  $\sigma_{12}^2 + \sigma_{22}^2$ .

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# APPENDIX A: PROOF OF THE EXPECTATION AND UNCERTAINTY EXPRESSIONS (11) AND (13)

It will be necessary to first describe the results obtained in [40] in the notation of this paper. The idea in [40] is to determine the difference between an advected curve of

 $\dot{x} = v(x,t)$ 

and

(A1)

$$dy = v(y,t)dt + \varepsilon\sigma(y,t)dW_t$$
(A2)

from the time  $t_1$  to a general time t. The initial condition (at time  $t_1$ ) for both equations is a curve C given parametrically by  $x(q,t_1)$  where q is a parameter, and *any* parametric representation is permitted. Let x(q,t) represent the final advected curve at time t according to the deterministic advection (A1), and y(q,t) be the stochastically advected curve according to (A2), subject to the condition  $y(q,t_1) = x(q,t_1)$ . From this point onwards, we treat q as *fixed*. Define a moving normal on the deterministic curve at a general time  $\tau \in [t_1,t]$  by

$$\hat{n}(q,\tau) := \frac{\partial x(q,\tau)}{\partial q} \middle/ \left| \frac{\partial x(q,\tau)}{\partial q} \right|$$

and the normal displacement at time t by

 $N(q,t) := [y(q,t) - x(q,t)] \cdot \hat{n}(q,t).$ 

Then, using an application of Itô's lemma, it was shown in [40] that

$$N(q,t) = \frac{\varepsilon \int_{t_1}^t e^{\int_{\tau}^t [\nabla \cdot v](x(q,\xi),\xi)d\xi} \left( \left[ \frac{\partial x(q,\tau)}{\partial q} \right]^{\perp} \right)_{\sigma}^{\top} (x(q,\tau),\tau) dW_{\tau}}{\left| \frac{\partial x(q,t)}{\partial q} \right|},$$

to leading order in  $\varepsilon$ . It is immediately clear that  $E[N(q,t)]/\varepsilon = 0$  since the integrand is of a deterministic function with respect to Brownian motion and yields zero [70,71], and thus (11) will result. Moreover, it is shown in [40] with the help of the Itô isometry [70,71] that

$$\sqrt{\operatorname{Var}[N(q,t)]} = \frac{\varepsilon \left(\int_{t_1}^t e^{2\int_{\tau}^t [\nabla \cdot v](x(q,\xi),\xi)d\xi} \left| \sigma^{\top}(x(q,\tau),\tau) \left(\frac{\partial x(q,\tau)}{\partial q}\right)^{\perp} \right|^2 d\tau \right)^{1/2}}{\left| \frac{\partial x(q,t)}{\partial q} \right|}$$
(A3)

to leading order in  $\varepsilon$ . The task is to now convert (A3) into (13) since slightly different conditions are in operation in this paper. The first is that v is steady; this is easily implemented by simply neglecting the second argument of v. The more subtle issue is to decide on the proper parametrization for C [which is parametrized by q in the form  $x(q,t_1)$ ], which in the present context must be the unstable manifold  $\Gamma^u$ . We know that the trajectory  $x^u(p)$  parametrizes  $\Gamma^u$ , and so we define for  $\tau \in [t_1,t]$ 

$$x(q,\tau) := x^u(\tau - t + p). \tag{A4}$$

Therefore,  $x(q,t_1) = x^u(t_1 - t + p)$ , and thus we set  $q = p + t_1 - t$  as the (linear) relationship between the q and the p parametrizations. In fact, this is the reason why  $x^u$  in the definition for  $G^u$  in (5) is associated with the argument  $t_1 - t + p$ , i.e., q. Differentiating (A4), we get

$$\frac{\partial x(q,\tau)}{\partial q} = \frac{\partial x^u(\tau - t + p)}{\partial p} = v(x^u(\tau - t + p))$$

where we have used the fact that  $x^u$  is a solution to (1). Therefore,  $\partial x/\partial q$  can simply be replaced by v (with appropriate arguments as obtained from the above expression) in (A3). Because of the definition (10), what is shown in (13) is the  $O(\varepsilon)$  term of (A3), and thereby (13) has been derived. We note in particular that this works at each fixed p.

The results of (21) and (23) associated with stochastic perturbations to the stable manifold  $\Gamma^s$  are similarly derived; here the main difference is that the curve C is  $\Gamma^s$  instead and we need to propagate backward in time. Hence, we take  $x(q,\tau) = x^s(\tau - t + p)$  for  $\tau < t_1$ , and we relate the parameters by  $q = p + t_1 - t$  because  $x(q,t_1) = x^s(t_1 - t + p)$ .

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# APPENDIX B: SATURATION OF UNCERTAINTY EXPRESSION (13)

Here, we provide a quick heuristic justification for our claim that if the diffusion matrix  $\sigma$  is bounded, the uncertainty (13) saturates as *t* increases. In examining (13) at large *t*, we observe that  $x^u(\tau - t + p) \rightarrow a$ . Indeed, for large *t* it is true that

$$x^{u}(\tau - t + p) \sim a + c e^{\lambda_{u}(\tau - t + p)} \hat{e}_{u}$$

for some constant *c* (reflecting a choice of the parametrization along  $\Gamma^{u}$ ). Then,  $v(x^{u}(\tau - t + p))$  is simply the  $\tau$  derivative of this, and so

$$v(x^u(\tau-t+p)) \sim c\lambda_u e^{\lambda_u(\tau-t+p)} \hat{e}_u.$$

Next, we observe that as  $t \to \infty$ ,  $\nabla \cdot v \to \lambda_s + \lambda_u$ , which is the value at the fixed point *a*. Inserting all these approximations into (13) yields

$$w^{u}(p,t) \sim \frac{\sqrt{\int_{t_{1}}^{t} e^{2(\lambda_{s}+\lambda_{u})(t-\tau)} |\sigma^{\top}(x^{u},\tau)c\lambda_{u}e^{\lambda_{u}(\tau-t+p)}\hat{e}_{u}^{\perp}|^{2}d\tau}{|v(x^{u}(p))|} \sim \frac{c\lambda_{u}e^{\lambda_{u}p}\sqrt{e^{2\lambda_{s}t}\int_{t_{1}}^{t} e^{-2\lambda_{s}\tau} |\sigma^{\top}(x^{u}(\tau-t+p),\tau)\hat{e}_{u}^{\perp}|^{2}d\tau}}{c\lambda_{u}e^{\lambda_{u}p}} \leqslant K\sqrt{e^{2\lambda_{s}t}\int_{t_{1}}^{t} e^{-2\lambda_{s}\tau}d\tau} = K\sqrt{\frac{1-e^{2\lambda_{s}(t-t_{1})}}{-2\lambda_{s}}}.$$
 (B1)

In the above formal computations, we have assumed a bound K for  $\sigma$ , and demonstrated that  $w^u(p,t)$  remains bounded as t increases (note the exponential decay because  $\lambda_s < 0$ ). In general  $w^u(p,t)$  will saturate towards a p-dependent value arising from the presence of  $x^u(\tau - t + p)$  in the integrand.

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