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Stochastic approaches to Lagrangian coherent structures

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Abstract.

This Note discusses a connection between deterministic Lagrangian coherent structures (robust fluid parcels which move coherently in unsteady fluid flows according to a deterministic ordinary differential equation), and the incorporation of noise or stochasticity which leads to the Fokker–Planck equation (a partial differential equation governing a probability density function). The link between these is via a stochastic ordinary differential equation. It is argued that a closer investigation of the stochastic differential equation offers additional insights to both the other approaches, and in particular to uncertainty quantification in Lagrangian coherent structures.

§1. Lagrangian coherent structures

The 'Lagrangian coherent structure' problem typically takes the following form. For some geophysical (oceanic [9], atmospheric [42], extraterrestrial [22]) or laboratory-scale [12, 33] flow, fluid velocities u are obtained as observational/experimental data, usually on a spatiotemporal grid defined for positions $x \in \Omega \subset \mathbb{R}^n$ (typically, the dimension is $n = 2$ or 3) and times $t \in [0, T]$. The Lagrangian evolution of fluid particle positions x is then given by the *ordinary* differential equation

$$\frac{\mathrm{d}x}{\mathrm{d}t} = u\,(x, t)\ , \tag{1}$$

for which—given the fact that u is available as discrete data in a finite-time interval $[0, T]$—*numerical* methods are needed. Determining sets in Ω at time 0 which 'remain coherent' under some given criterion after

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evolution by (1) to time T will be referred to as 'the standard Lagrangian coherent structure problem' [7]. The adjective 'Lagrangian' in this case refers to the fluid-dynamical nomenclature of 'following fluid particles' as opposed to the 'Eulerian' framework of specifying flow properties as functions of (x, t). Influential observations [27] pointed to the inadequacy of using Eulerian information in determining coherent fluid regions which had a dominant influence on how fluid transport occurred, if u were nonautonomous. However, defining exactly what is meant in saying that a time-varying structure is 'coherent' in a Lagrangian sense is less clear. Thus, there are many approaches to this, each based on a particular interpretation of 'coherence.' Both theoretical (variational formulations [23, 25] and stable/unstable manifold approaches [2, 3] to define coherent structure boundaries) and numerical (stretching of fluid elements [44], entangling of trajectories [1], complexity of motion [29]) methods have been developed. In general, these methods tend to be *deterministic* in that they rely on advecting Ω according to (1), and then extracting sets at time 0 based on some specific information gleaned from such advection. Review and comparison articles on the extensive field of Lagrangian coherent structure methods are available [7, 21, 24].

An issue that is gradually coming to the fore is that *the velocity u in* (1) *is not known with certainty.* This is because in typical applications, u is obtained from experimental/observational data. Uncertainties therefore include measurement error, known situations in which the velocity measurements have large errors (e.g., regions of cloud cover when taking satellite observations of sea-surface heights in order to infer oceanic velocities), modeling errors in converting observations to velocities (as in using the geostrophic approximation to relate sea-surface height to a streamfunction [45]), as well as errors arising from interpolating data only available on a spatiotemporally discrete grid. The latter situation arises even when using velocity field from numerical simulations, since any computational fluid dynamics simulation itself has a finite resolution. How can subgrid processes, or velocity uncertainties, be encapsulated in Lagrangian coherent structure methods?

This Note highlights emerging approaches to this issue which are connected to stochastic differential equations. Furthermore, the relationship to a probability density function—whose evolution is governed by a corresponding Fokker–Planck equation [11, 16] or alternatively a Perron–Frobenius (transfer) operator [14, 15, 42]—is discussed.

§2. Stochastic differential equation

A straightforward idea of modeling the velocity uncertainties described previously is to include them as perturbations in the velocity field, which are in some way *stochastic*. That is, the velocity field has some *dominant* smooth behavior (which is captured by the data), plus a small *stochastic* term which incorporates the range of uncertainties. This viewpoint implies the replacement of (1) with an appropriate *stochastic differential equation* [4, 5, 6, 8, 11, 16, 20]. A fairly general formulation for this could be [4, 6, 26]

$$\mathrm{d}x_t = u(x_t, t)\,\mathrm{d}t + \sigma(x_t, t)\,\mathrm{d}W_t\,, \tag{2}$$

in which W_t is n-dimensional Brownian noise in Ω, and σ is an $n \times n$ matrix, assumed small in some sense, which encodes the possibility that the stochasticity be modulated in a heterogenous anisotropic way. The potential for x-dependence in σ means that the noise is *multiplicative* [41], and here (2) will be thought of in an Itô (as opposed to Stratonovich) sense [39]. Thus, rather than deterministic trajectories $x(t)$ to (1), one can think of $t = 0$ conditions to (2) evolving as *random trajectories* x_t.

Stochastic ordinary differential equations of the form (2) are well-established in financial mathematics and stochastic integration theory [30, 36, 39, e.g.], but their usage in Lagrangian coherence is only emerging recently; hence, this Note.

How can one make sense of how individual random trajectories of (2) contribute collectively? Numerically, one can determine x_t using, say, an Euler–Maruyama algorithm [34]. By performing many simulations, the statistics of various scalar fields can then be numerically computed [4, 8, 20]. Such computational experiments have been performed for finite-time Lyapunov exponents [4, 6, 20] as well as so-called Lagrangian descriptors (taking a suitable average along trajectories) [8]. In these cases, σ is usually chosen to be proportional to the identity.

Another method to combine ensemble information is to seek theoretical means and variances resulting from (2), through the usage of Itô's isometry [31, 39]. With the assumption that σ is small, but that the velocity field need not be divergence-free, several such results have recently been developed in the context of two-dimensional unsteady flows operating over a finite time interval. The first is an expression for the'fattening' of a curve when advected according to (2) [4]. The second specializes to curves which have importance in Lagrangian coherent structures: unsteadily evolving flow barriers which demarcate distinct Lagrangian coherent structures [6]. The fuzziness of such flow barriers under stochasticity in the form (2) allows for a spatial characterisation of *mixing layers*

between coherent structures. The evolution of the spatial structure of these layers with time, as well as a limiting behavior, is determined [6]. The direct connection of this to *mixing* is verified by numerically evolving density fields initially supported on the coherent structures on the two sides of the mixing layer, and showing that their evolution obeys the predicted spatial characterization of the mixing layer. A third addresses (2) in the context of rigorously quantifying how sensitive each and every Lagrangian trajectory's final position x_T is to noise [5]. In this, the anisotropic variance of a scaled displacement from the deterministic location is defined as a field on Ω, which can then be related to a measure of *robustness* of sets [5]. Implications of this theory towards realistic data is ongoing, and shows promise for evaluating the interdependence between velocity measurement uncertainties, spatial resolution, and Lagrangian structures that can be resolved subject to these.

Building on the various approaches described in this section—-utilizing Monte Carlo simulations, stochastic calculus methods, or new approaches on (2)—seems to be a promising way forward in understanding the impact of noise and uncertainty on Lagrangian structures.

§3. Diffusion and the Fokker–Planck equation

Stochasticity at the microscopic level corresponds to diffusion at the macroscopic level. Thus, an alternative way of understanding 'coherence' associated with trajectories of the deterministic ordinary differential equation (1) is to consider instead an evolving density $\rho(x,t)$ governed by the advection–diffusion partial differential equation

$$\frac{D\rho}{dt} := \frac{\partial \rho}{\partial t} + u \cdot \nabla \rho = \nabla^2 \rho \,, \tag{3}$$

in which the left-hand side is the convective derivative (derivative following the flow) of (2). 'Coherence' can now be attributed to the structure of the evolving scalar field $\rho(x,t)$. For example, if there is a collection of closed contours of $\rho(x,t)$ at some time t which evolve without developing significant filamentation [24] then these might be construed as demarcating an unsteady coherent structure. Alternatively, material surfaces across which there is minimum diffusive flux might be taken as defining a boundary of a coherent structure [26].

How is this connected to the stochastic differential equation (2)? The impact of evolving random trajectories of (2) generically results in a nonuniform distribution of trajectory densities $\rho(x,t)$ for $t \in [0,T]$. Standard stochastic techniques [35, 40, 43] enable the derivation that

this evolves according to

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = \frac{1}{2} \nabla \cdot \nabla \cdot \left(\rho \, \sigma \sigma^{\top} \right) , \tag{4}$$

which is the *Fokker–Planck equation* corresponding to the stochastic dynamics (2) [40]. In the simplest case where σ is proportional to the identity [11, 18, 32] and when the fluid is incompressible ($\nabla \cdot u = 0$), this collapses to the classical advection–diffusion equation. Preserving the (x, t)-dependence in σ is relevant, allowing for the possibility of modeling anisotropic diffusion which is further modulated by time and space.

While (2) and (4) may be considered equivalent, there are some practical differences in the *usage* of these two equations. Complicated σ causes considerable difficulties in analyzing, and in simulating, (4). (For example, lack of spatial periodicity will complicate using Fourier methods.) In contrast, such σ is easily incorporated into numerical simulations of (2) using, for example, the Euler-Maruyama algorithm [34]. Itô calculus [30], relevant to analyzing (2), forms an alternative methodology for addressing Lagrangian coherence information, contrasting with classical parabolic PDE methods required for (4). One interesting approach for the general Fokker–Planck equation (4) is by Haller et al [26], who develop a variational approach for determining surfaces across which there is the least diffusive flux (as a potential definition for demarcating a Lagrangian coherent structure). Another is by Denner et al [11], who (with σ being the identity) propose a method which can be numerically applied to (4) to investigate coherence.

Another direct comparison between (2) and (4) is that the probability density obtained from the collection of random trajectories of (2) all starting at the *same* initial position x_0, is equivalent to considering (4) with the initial density distribution $\rho(x, 0) = \delta(x - x_0)$, where $\delta(\cdot)$ is the Dirac-delta distribution. Thus, statistical information from the trajectories of (2) can be used to reach conclusions on the Fokker–Planck equation's evolution. The linearity of (4) may allow for amalgamation of this information for ensembles of trajectories with different x_0-vaiues.

§4. Perron–Frobenius transfer operator

Given a map M, the *Perron–Frobenius* or *transfer* operator $\mathfrak{P}$ encodes how probability densities are pushed forward by M [10]. If imagining M to be the deterministic flow map of the ordinary differential equation (1) from time 0 to T, an approximation for $\mathfrak{P}$ is obtainable by the *Ulam matrix* P with elements P_{ij}, by partitioning Ω into boxes

B_i and by deterministic evolution, determining the transition probabilities into boxes C_j in $M(\Omega)$. The Perron–Frobenius operator can be made compact by convolving with a diffusive kernel prior to and after applying M [11, 14]; this enables the extraction of singular values λ_k and corresponding singular vectors v_k of the approximant P. Thus $P^\top P v_k = \lambda_k^2 v_k$, with the singular vector v_k (a constant on each of the B_is) forming an approximation for a field on Ω. Consequently, the transfer operator satisfies $\mathfrak{P}^\top \mathfrak{P} v_k \approx \lambda_k^2 v_k$. Singular vectors associated with the largest (near unity) λ_ks therefore identify 'almost coherent' sets [14, 15, 42] in Ω, with the level of coherence quantified by λ_k. This method, popularized and extended by Froyland and collaborators, is a well-established method for the detection of coherent structures associated with Lagrangian trajectories if (1) [14, 15, 37, 42]. It is often viewed as *deterministic* because M is, and nice theoretical results related to the singular limit of diffusion approaching zero are available [15].

In the above implementation, there is usually no explicit reference to a stochastic ordinary differential equation. However, the Perron–Frobenius operator is also often mentioned as the solution operator $\mathfrak{P}'$ of a Fokker–Planck equation [11, 16, 18]; specifically, $\mathfrak{P}'\rho(x,0) = \rho(x,T)$. Since the Fokker–Planck equation (4) is generated from the stochastic differential equation (2), this Perron–Frobenius operator $\mathfrak{P}'$ captures the *continuing* impact of uncertainties in the velocity field over the *entire* time duration $t \in [0,T]$. This is different from the understanding of the transfer operator $\mathfrak{P}$ in the most commonly known deterministic Lagrangian coherent structure approaches [14, 15, 37, 42]. However, it *is* a method for incorporating the uncertainty in the velocity field, and singular vectors of $\mathfrak{P}'$ give similar information on coherence [11] to those of $\mathfrak{P}$, albeit with a different interpretation of diffusion.

It should be pointed out that even with a deterministic u, if it were only known on a spatio-temporal grid, there is uncertainty in u at the subgrid level. When performing advection numerically, implicit or explicit interpolation usually occurs between gridpoints. These values, therefore, are in reality not known exactly. A possible modeling approach is to apply the stochastic differential equation (2) with a σ matrix which is zero at the gridpoints, but *unknown* off these gridpoints. Thus, (2) and its Fokker–Planck equation (4) may be apply even if the velocity is known with infinite accuracy, if only known on a discrete grid.

It is worth summarizing the two different Perron–Frobenius operator interpretations that have been discussed, within the context of the Fokker–Planck equation (4) and the corresponding stochastic differential equation (2). In both cases, consider an initial condition x_0 for (2).

(1) $\mathfrak{P}$: The impact of a diffusive kernel prior to advection is associated with applying (2) and (4) with $\sigma \equiv 0$. In other words, rather than (2), the understanding is that the deterministic advection (1) is in operation, while the Fokker–Planck equation (4) collapses to the pure advection/transport equation $\partial\rho/\partial t + \nabla \cdot (\rho u) = 0$. However, the initial condition $\rho(x, 0)$ is then not a Dirac mass at x_0, but is a diffused version of this.

(2) $\mathfrak{P}'$: The impact of velocity uncertainties can be modeled by applying (2) and (4) with $\sigma \neq 0$, but with the initial condition to the Fokker–Planck equation being $\rho(x, 0) = \delta(x - x_0)$. This applies if there is genuine uncertainty in u (measurement error, say), or if u is only known at gridpoints.

Additionally, to evaluate the impact across *all* initial conditions x_0 (in terms of a field on Ω), a broadening of the above understanding will be necessary.

The two transfer operators approaches above have a nice connection to how *uncertainties in data impact Lagrangian predictions*, which can have profound consequences (e.g., attributing uncertainties to the movement of coherent weather systems). Uncertainties in the prediction of any model can arise because of two main reasons: (i) uncertainty in initial position, and (ii) uncertainty in the model. These are quite naturally connected to $\mathfrak{P}$ and $\mathfrak{P}'$ respectively, because the former reflects diffusion imparted on the initial condition $\delta(x - x_0)$ but evolved with no noise, while the latter has an exact initial condition subject to a noisy evolution. Can these two effects be *combined* within the Fokker–Planck framework by having a diffused initial condition (rather than $\delta(x - x_0)$) at each point x_0, and also letting σ be nonzero (but chosen in a reasonable way to model system noise, e.g., having it zero at gridpoints but nonzero elsewhere to model resolution error)? Alternatively, is there an advantage to thinking of $\mathfrak{P}$ and $\mathfrak{P}'$ in terms of the stochastic differential equation (2), where the former might be associated with a weighting of initial conditions?

§5. Concluding remarks

This Note discusses the link between deterministic advection (which reflects the 'standard' Lagrangian coherent structure methodology) as given in (1), and the Fokker–Planck equation (4). The relationship is via the stochastic equation (2), which hitherto has only seen limited attention from this community. It is suggested that analyzing the stochastic ordinary differential equation (2) may offer considerable new insight into Lagrangian coherence, noise and diffusion.

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References

[1] M. Allshouse and J.-L. Thiffeault, Detecting coherent structures using braids, *Physica D*, **241** (2012), 95–105.

[2] S. Balasuriya, A tangential displacement theory for locating perturbed saddles and their manifolds, *SIAM J. Appl. Dyn. Sys.*, **10** (2011), 1100–1126.

[3] S. Balasuriya, *Barriers and transport in unsteady flows*: *a Melnikov approach*, volume 21 of *Mathematical Modeling and Computation*, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, 2016.

[4] S. Balasuriya, Stochastic uncertainty of advected curves in finite-time unsteady flows, *Phys. Rev. E*, **95** (2017), 062201.

[5] S. Balasuriya, Stochastic sensitivity: A computable Lagrangian uncertainty measure for unsteady flows, *SIAM Review, in press*, (2020).

[6] S. Balasuriya and G. Gottwald, Estimating stable and unstable sets and their role as transport barriers in stochastic flows, *Phys. Rev. E*, **98** (2018), 013106.

[7] S. Balasuriya, N. Ouellette and I. Rypina, Generalized Lagrangian coherent structures, *Physica D*, **372** (2018), 31–51.

[8] F. Balibrea-Iniesta, C. Lopesino, S. Wiggins and A. Mancho, Lagrangian descriptors for stochastic differential equations: a tool for revealing the phase portrait of stochastic dynamical systems, *Intern. J. Bifurc. Chaos*, **26** (2016), 1630036.

[9] J. Bettencourt, V. Rossi, E. Hernández-Garcia, M. Marta-Almeida and C. López, Characterization of the structure and cross-shore transport porperties of a coastal upwelling filament using three-dimensional finite-size Lyapunov exponents, *J. Geophys. Res. Oceans*, **122** (2017), 7433–7448.

[10] M. Dellnitz and O. Junge, On the approximation of complicated dynamical behavior, *SIAM J. Numer. Anal.*, **36** (1999) 491–515.

[11] A. Denner, O. Junge and D. Matthes, Computing coherent sets using the Fokker–Planck equation, *J. Comp. Dyn.*, **3** (2016) 163–177.

[12] L. Fang, S. Balasuriya and N. Ouellette, Local linearity, coherent structures, and scale-to-scale coupling in two-dimensional flows, *Phys. Rev. Fluids*, **4** (2019) 014501.

[13] G. Froyland, Finite approximation of Sinai-Bowen-Ruelle measure for Anosov systems in two dimensions, *Random Comput. Dyn.*, **3** (1995), 251–264.

[14] G. Froyland, An analytical framework for identifying finite-time coherent sets in time-dependent dynamical systems, *Physica D*, **250** (2013), 1–19.

[15] G. Froyland, Dynamic isoperimetry and the geometry of Lagrangian coherent structures, *Nonlinearity*, **28** (2015), 3587–3622.

[16] G. Froyland and P. Koltai, Estimating long-term behavior of periodically driven flows without trajectory integration, *Nonlinearity*, **30** (2017), 1948–1986.

[17] G. Froyland and K. Padberg-Gehle, Finite-time entropy: A probabilistic approach for measuring nonlinear stretching, *Physica D*, **241** (2012), 1612–1628.

[18] G. Froyland and N. Santitissadeekorn, Optimal mixing enhancement, *SIAM J. Appl. Math.*, **77** (2017) 1444–1470.

[19] J. Guckenheimer and P. Holmes, *Nonlinear oscillations, dynamical systems, and bifurcations of vector fields*, Springer, New York, 1983.

[20] H. Guo, W. He, T. Peterka, H.-W. Shen, S. Collis and J. Helmus, Finite-time Lyapunov exponents and Lagrangian coherent structures in uncertain unsteady flows, *IEEE Trans. Visual. Comp. Graphics*, **22** (2016), 1672–1682.

[21] A. Hadjighasem, M. Farazmand, D. Blazevski, G. Froyland and G. Haller, A critical comparison of Lagrangian methods for coherent structure detection, *Chaos*, **27** (2017), 053104.

[22] A. Hadjighasem and G. Haller, Geodesic transport barriers in Jupiter's atmosphere: a video-based analysis, *SIAM Review*, **58** (2016), 69–89.

[23] G. Haller, A variational theory of hyperbolic Lagrangian Coherent Structures, *Physica D*, **240** (2011), 574–598.

[24] G. Haller, Lagrangian Coherent Structures, *Annu. Rev. Fluid Mech.*, **47** (2015), 137–162.

[25] G. Haller and F. Beron-Vera, Geodesic theory of transport barriers in two-dimensional flows, *Physica D*, **241** (2012), 1680–1702.

[26] G. Haller, D. Karrasch and F. Kogelbauer, Material barriers to diffusive and stochastic transport, *Proc. Nat. Acad. Sci.*, **115** (2018), 9074–9079.

[27] G. Haller and G. Yuan, Lagrangian coherent structures and mixing in two-dimensional turbulence, *Physica D*, **147** (2000), 352–370.

[28] H. Hwang, J. Jang and J. Jung, On the kinetic Fokker–Planck equation in a half-space with absorbing barriers, *Indiana Univ. Math. J.*, **64** (2015), 1767–1804.

[29] K. Ide, D. Small and S. Wiggins, Distinguished hyperbolic trajectories in time dependent fluid flows: Analytical and computational approach for velocity fields defined as data sets, *Nonlin. Proc. Geophys.*, **9** (2002), 237–263.

[30] K. Itô, Stochastic integral, *Proc. Imp. Acad.*, **20** (1944), 519–524.

[31] G. Kallianpur and P. Sundar, *Stochastic analysis and diffusion processes*, Oxford University Press, Oxford, 2014.
[32] D. Karrasch and J. Keller, A geometric heat-flow theory of Lagrangian coherent structures, *submitted*, (2018).
[33] D. Kelley and N. Ouellette, Onset of three-dimensionality in electromagnetically forced thin-layer flow, *Phys. Fluids*, **23** (2011), 045103.
[34] P. Kloeden, E. Platen and H. Schurz, *Numerical solution of SDE through computer experiments*, Universitext. Springer-Verlag, Berlin, 1994.
[35] B. Matkowsky, Singular perturbations, stochastic differential equations, and applications, In: *Singular Perturbations and Asymptotices*, (Eds. R. Meyer and S. Parter), pages 109–147, Academic Press, 1980.
[36] R. Merton, Lifetime portfolio selection under uncertainty: the continuous time case, *Rev. Econom. Statist.*, **51** (1969), 247–257.
[37] P. Miron, F. Beron-Vera, M. Olascoaga, J. Sheinbaum, P. Pérez-Brunius and G. Froyland, Lagrangian dynamic geography of the Gulf of Mexico, *Scientific Reports*, **7** (2017), 7021.
[38] F. Nier, Boundary conditions and subelliptic estimates for geometric Kramers–Fokker–Planck operators on manifolds with boundaries, *Mem. Amer. Math. Soc.*, **252** (2018), 1–145.
[39] B. Øksendahl, *Stochastic differential equations*, Springer, 4 edition, 1995.
[40] H. Risken, *The Fokker–Planck equation: Methods of solution and applications*, Springer, New York, 1984.
[41] J. Sancho, M. San Miguel, S. Katz and J. Gunton, Analytical and numerical studies of multiplicative noise, *Phys. Rev. A*, **26** (1982), 1589–1609.
[42] N. Santitissadeekorn, G. Froyland and A. Monahan, Optimally coherent sets in geophysical flows: a new approach to deliminating the stratospheric polar vortex, *Phys. Rev. E*, **82** (2010), 056311.
[43] Z. Schuss, Singular perturbation methods in stochastic differential equations of mathematical physics, *SIAM Review*, **22** (1980), 119–155.
[44] S. Shadden, F. Lekien and J. Marsden, Definitions and properties of Lagrangian coherent structures from Lyapunov exponents in two-dimensional aperiodic flows, *Physica D*, **212** (2005), 271–304.
[45] D. Stammer, Global characteristics of ocean variability estimated from regional TOPEX/POSEIDON altimeter measurements, *J. Phys. Oceanography*, **27** (1997), 1743–1769.

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