UNCOVERING TRANSPORT BARRIERS IN GEOPHYSICAL FLOWS

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1 Background and Overview

A key component of dynamical systems theory is the search for dynamical structures that organize the global and long-term behavior of the system. Examples of such structures include periodic orbits, invariant manifolds, homoclinic orbits, and invariant tori. By performing appropriate local analyses (e.g. linearization, computation of normal forms, etc.) around these structures and studying how they all fit together, one aims to construct a global picture of the dynamics.

Comprehensive analytical methods for uncovering dynamical structures currently only apply when the associated vector field is either known for all time or has some well-defined temporal behavior (e.g. periodic, quasi-periodic). These methods are therefore of limited use for studying geophysical flows, where detailed knowledge of the vector (velocity) field is not available and complex time-dependence is the rule rather than the exception. The need to develop robust mathematical methods to identify key transport barriers in geophysical flows has never been more pressing, however, given their role in climate processes (e.g. algal blooms, ozone transport) and environmental disasters (e.g. Deepwater Horizon oil spill, Icelandic volcanic ash cloud, Fukushima nuclear disaster).

This report summarizes the material covered at the Banff workshop on *Uncovering Transport Barriers in Geophysical Flows*, highlighting the latest theoretical, computational and experimental advances, and laying the groundwork for future studies in the field. Each participant has provided a summary of the research they presented so that the reader can identify a particular focus topic of interest to them and get an overview of the standout issue that is being addressed by that researcher.

2 Summary of Presented Research

Accounting for windage in the identification and classification of FTLE ridges (*M. Allshouse*): Understanding the transport of contaminants on the surface of the ocean is aided by identifying regions of large Lagrangian deformation. Given that the FTLE field measures the local deformation, its ridges represent the locally maximum repelling structures in the flow. We have developed a numerical approach to identifying and refining FTLE ridges that enables their advection and classification of local deformation. Through application on a number of of analytic velocity fields, the ridge classification has been confirmed. Additionally, because the target application, ocean models, contains data at only discrete points in space and time, the methods were also tested on a discretized version of an analytic velocity field. The agreement between the discretized analysis and analysis of the analytic field confirms that the methods are sufficiently robust for application on oceanic simulations.

Using these techniques, we analyzed the ocean surface currents near the Ningaloo Reef along the Western Australia coastline, which contains a large fringing reef and significant offshore natural resources. A number of FTLE ridges are located through ridge tracking and refinement and are then classified. Because surface winds as well as ocean surface currents effect oil advection, a hybrid ocean-wind velocity field is created and analyzed. The resulting hybrid LCSs provide critical information for the transport of the oil that differs significantly from analysis of the ocean surface currents alone. In the example studied, accounting for wind results in a key transport feature, a hyperbolic saddle point, shifting closer to the Ningaloo shoreline. Qualitatively, the shift in the features position demonstrates that the attracting oil feature is closer to the fringing reef than pure surface current analysis indicates.

Explicit stable and unstable manifolds in a class of unsteady 2D and 3D flows (*Sanjeeva Balasuriya*): Transport barriers in unsteady flows are difficult to determine, particularly in three dimensions. A multitude of methods have been suggested for this, some of which are motivated by properties of stable and unstable manifolds for *steady* flows. Testing whether the methods are accurate is itself a nontrivial exercise, since there are few known models in which unsteady flow barriers are unambiguously known. Here, a class of unsteady Eulerian velocity fields in both 2D and 3D, in which stable and unstable manifolds are *explicitly* known, is introduced. The entity to which they decay in backwards and forwards time—a hyperbolic trajectory—is stated explicitly, and the fact that this trajectory is hyperbolic (i.e., it possesses both a stable and an unstable manifold) is proven rigorously using exponential dichotomies. The explicit nature of the expressions given for the stable and unstable manifolds offer a nice testbed for evaluating the relationships between the different types of methods which are in use to determine transport barriers, and genuine stable and unstable manifolds. The fact that this class of models possesses time variation which can be modified to the user's requirements (such as having oscillations, translation, rotations, axes re-orientation, etc, each occurring at time-scales which may be specified), enables testing of the ability of diagnostic methods to deal with different types of difficulties that a particular data set may have. The presence of genuinely three-dimensional models is another great advantage, as there is increasing interest in being able to determine transport barriers in true flows; quite a few of the methods which are in usage are either difficult or impossible to apply in three dimensions.

Stable and unstable manifolds cannot as they stand be used effectively in flows in which the velocities are defined for finite-time only, since in defining these manifolds in unsteady (nonautornomous) flows, decay requirements as time goes to $\pm\infty$ are needed. As such, the finite-time analogues of (un)stable manifolds—for which there is not yet a universally accepted definition—need to be understood if making comparisons with realistic flows. The class of models is modified to create explicitly expressible finite-time versions of stable and unstable manifolds, to which there is attraction/repulsion over a user-defined time-interval. This enables the exact quantification of genuinely finite-time entities, which can be a fruitful testbed for evaluating the accuracy and efficacy of the diverse range of methods currently in use for locating transport barriers in unsteady flows. An extension of the models to non-hyperbolic situations—in which methods such as Lyapunov exponents fail—is also suggested.

Geodesic analysis of oceanic flows (*F. J. Beron-Vera*): Lagrangian Coherent Structures (LCS) are key material surfaces that shape global transport [9]. The geodesic LCS theory enables unified detection of all relevant LCS types in finite-time aperiodic two-dimensional flows in a frame-independent, directly invariant, and robust manner [7, 1, 8, 6, 5]. These are: hyperbolic LCS (generalized invariant manifolds or maximally attracting/repelling material lines); elliptic LCS (generalized invariant KAM tori or eddy boundaries); and parabolic LCS (generalized twistless KAM tori or jet core barriers). LCS in each type follow as null geodesics of a Lorentzian metric representing some form of material deformation characterized by the Cauchy–Green strain tensor. In particular, closed material curves forming elliptic LCS satisfy similar equations as closed light rays forming photon spheres. This enables a fascinating analogy between the notion of coherent material eddy and black hole in cosmology.

We reported on several applications of the geodesic LCS theory to oceanic flows: 1) hyperbolic LCS extracted from altimetry data revealed that the mesoscale circulation play an important role in shaping the transport near the surface of the ocean in the Gulf of Mexico [11]; 2) using hyperbolic LCS as a measure of model performance, data assimilation schemes in models were optimized [10]; 3) persistently attracting LCS cores in hyperbolic cores were found to predate the development of instabilities in the shape of the oil slick during the Deepwater Horizon spill [12]; 4) using satellite altimetry data, Agulhas rings were revealed and shown to preserve their shape for many months as they travel across the South Atlantic [1, 8]; 5) a time series of coherent transport of water in the South Atlantic was constructed using the whole record (1992–2013) of altimetric data revealing that coherent water transport represents an important contribution to the total meridional transport of water [13]; and 6) a parabolic LCS associated with the Gulf Stream was detected for the first time, confirming prior speculations that the Gulf Stream should behave as a barrier for cross-stream transport.

Lagrangian transport barriers in three-dimensional unsteady flows (*D. Blazevski & G. Haller*): Detecting barriers to, and facilitators of, transport is a fundamental problem in studying the behavior of trajectories in a dynamical system. Flows for steady (autonomous) or temporally periodic vector fields have been understood geometrically by finding structures governing transport such as KAM tori, stable manifolds, Cantori and chaotic regions. In contrast, the velocity fields in the ocean, atmosphere, fusion plasmas, etc. are temporally aperiodic and finite in time and classical dynamical systems theory does not apply

The approach taken is to study the impact they have on nearby trajectories. We modeled the behavior of trajectories near a co-dimension one surface of initial conditions (material surface) $\mathcal{M}(t_0)$ by studying how the linearized flow $DF_{t_0}^t$ acts on the normal n of $\mathcal{M}(t_0)$. We deduce that nearby trajectories can either expand or contract in the direction normal to $\mathcal{M}(t_0)$ or spread out in the direction tangent to $\mathcal{M}(t_0)$. This leads to the notions of *normal repulsion* and *tangential shear*.

Transport barriers are then classified as hyperbolic or elliptic Lagrangian Coherent Structures (LCS) if they generate maximal deformation of nearby trajectories in the direction normal or tangent to the barrier. For three-dimensional flows, we used this intuition to precisely define hyperbolic and elliptic LCS. We provided a numerical method to compute the barriers, and gave both analytic and numerical examples illustrating the theory. Especially interesting is that the elliptic LCS constructed are a way to define the boundary of a coherent Lagrangian vortex for a three-dimensional unsteady fluid flow. Current work is to use the theory to provide estimates of Lagrangian transport for geophysically relevant flows.

Differential geometry perspective of shape coherence and curvature evolution by finite-time nonhyperbolic splitting (*Erik Bollt & Tian Ma*): Mixing, and coherence are fundamental issues at the heart of understanding fluid dynamics and other non- autonomous dynamical systems. Only recently has the notion of coherence come to a more rigorous footing, and particularly within the recent advances of finite-time studies of nonautonomous dynamical systems. The term coherence" relates regions with distinct properties as becoming an important fundamental subject of fluid dynamics. We define shape coherent sets which we relate to measure of coherence in differentiable dynamical systems from which we will show that tangency of finite time stable foliations (related to a forward time perspective) and finite time unstable foliations (related to a backwards time" perspective) serve a central role. Motivated by the idea that some sets may preserve their shape in finite-time, we relate the boundaries of shape coherent sets to the nonhyperbolic splitting angle of the finite-time stable and unstable foliations which leads to slowly changing curvatures. This perspective is agreeable with the recent theory of geodesics derived from a variational principle of geodesics. We develop zero-angle curvers, meaning nonhyperbolic splitting, by continuation methods in terms of the implicit function theorem, from which follows a simple ODE description of the boundaries of shape coherent sets.

While this work represents a new direction in describing coherent sets, and a firm foundation based on our definition of shape coherence, it is likely that the other popular current methods for constructing coherent sets, 1) based on coherent pairs using transfer operators, 2) minimizing growth of arc length toward the theory of geodesics, both may produce sets whose boundaries have slow changing curvature, and are therefore shape coherent. We will investigate this possible equivalence in the future, as well there may be a way to formulate the minimization of curvature growth as a variational problem directly, in analogy to how the geodesic curve theory was developed, although likely with complicated involvement second derivatives. Finally, we remark that fundamentally the study of coherence and specifically shape coherent sets here, is in some sense the complement to study transport, and mixing which occurs in the hyperbolic-like mixing sets. These are fundamentally complementary questions on complement sets.

Mesochronic analysis: computation and interpretation (*M. Budisic & I. Mezic*): Mesochronic analysis (from Greek, *meso-*, middle-, mean-; *chronos,* time) is a study of a dynamical system $\dot{x} = \mathbf{u}(t, x)$ based on averages of observables along trajectories. A common name for such an average in fluid flows is the *Lagrangian average* of scalar or vector fields. If the velocity field $\mathbf{u}$ is chosen as the observable, its Lagrangian average $\tilde{\mathbf{u}}(p)$ along the segment $t \in [0, T]$ of trajectory $x_p(t)$, originating at a point p, is affinely related to the flow map $p \mapsto x_p(T)$.

Consequently, the Jacobian matrix $J_{\tilde{\mathbf{u}}}$, termed *mesochronic Jacobian*, can be used to characterize deformation of the material released at point p and advected for duration $[0, T]$. Qualitatively, possible deformations in planar incompressible flows fall into three types: hyperbolic (stretching, with or without reflection), elliptic (rigid rotation), and parabolic (translation). A single quantity, $\det J_{\tilde{\mathbf{u}}}$, can be used to determine the class of deformation. A paper by Mezić et al. (Science, 2010) demonstrated that regions of hyperbolic mesochronic deformation in the model of Gulf of Mexico corresponded to directions followed by the oil slick in the aftermath of the Deepwater Horizon Spill.

In an effort to provide intuition about mesochronic analysis, we have demonstrated the analysis is a nonzero-time extension of the Okubo-Weiss criterion. Furthermore, in a joint work with S. Siegmund and T.S. Doan, we showed that 3D flows can be classified into several deformation categories, where two quantities, the determinant and trace of the cofactor of $J_{\tilde{\mathbf{u}}}$, are needed. Preliminary numerical results for a 3D ABC flow show that vortices in the flow tend to be classified as non-hyperbolic, while the chaotic zone is classified as non-rotationally hyperbolic; these conclusions cannot be reached from the instantaneous Okubo-Weiss-Chong analysis for the same flow, yet they correspond to intuition about these structures.

Moving forward, we are numerically exploring how deformation partitions interact with material lines in the flow, how the choice of reference vs. co-moving frame affects the classification, and how deformation quantifiers change with the choice of time interval. We expect that these numerical results will inform a more rigorous investigation of the same questions in the future.

Transport barriers and coherent structures in mean-field Hamiltonian systems (*D. del-Castillo-Negrete*): Broadly speaking one can distinguish two different classes of transport problems: the study of passive scalars which are transported by the flow without affecting it, and the study of active scalars that modify the flow while being transported. In general, in an active transport problem the advected field determines the velocity field through a dynamical constrain. Because of this, active transport is also called self-consistent transport. If in addition the Lagrangian trajectories of individual fluid elements exhibit sensitive dependence on initial condition, the transport is called self-consistent chaotic transport. Many important problems including the problem of potential vorticity mixing and homogenization in geophysical flows, the problem of magnetic confinement in fusion plasmas, and the magnetic dynamo problem fall in the category of self-consistent chaotic transport problems. In this study we discussed three reduced, mean-field models of self-consistent chaotic transport in fluids and plasmas. In the fluid dynamics context the transported field is the vorticity and the self-consistency condition is the vorticity-velocity coupling. The first two models, the vorticity defect model and the single wave model, are constructed by successive simplifications of the vorticity-velocity coupling. The third model is an area preserving self-consistent map obtained by a space-time discretization of the single wave model. In the plasma physics context the transported field is the electron distribution function in phase space and the self-consistency condition is the Poisson equation. This electron plasma problem is closely related to the vorticity mixing problem. Also, the single wave model is analogous to models used in the study of globally coupled oscillator systems, and to Hamiltonian mean-field models used in statistical mechanics [2].

Of particular interest was the study of coherent structures and self-consistent transport in the context of the previously described mean-field models. Numerical simulations in the finite-N and in the $N \to \infty$ kinetic limit, where N is the number of particles, show the existence of coherent, rotating dipole states. We approximate the dipole as two macroparticles (one hole and one clump) and consider the $N = 2$ limit of the model.We show that this limit has a family of symmetric, rotating integrable solutions described by a one-degree-of-freedom nontwist Hamiltonian. A perturbative solution of the nontwist Hamiltonian provides an accurate description of the mean field and rotation period of the dipole. The coherence of the dipole is explained in terms of a parametric resonance between the rotation frequency of the macroparticles and the oscillation frequency of the self-consistent mean field. This resonance creates islands of integrability that shield the dipole from regions of chaotic transport. For a class of initial conditions, the mean field exhibits an elliptic-hyperbolic bifurcation that leads to the filamentation, chaotic mixing and eventual destruction of the dipole [3].

We also discussed recent results on transport barriers and coherent structures in mean-field coupled many degrees-of-freedom area preserving maps. We presented a model in which the different degrees of freedom are coupled through a mean-field that evolves self-consistently. Based on the linear stability of period one and period-two orbits of the coupled maps, we constructed coherent states in which the degrees of freedom are synchronized and the mean-field stays nearly fixed. Nontwist systems exhibit global bifurcations in phase space known as separatrix reconnection. We showed that the mean-field coupling leads to dynamic, self-consistent reconnection in which transport across invariant curves can take place in the absence of chaos due to changes in the topology of the separatrices. In the context of self-consistent chaotic transport, we studied two novel problems: suppression of diffusion and breakup of the shearless curve. For both problems, we constructed macroscopic effective diffusion models with time-dependent diffusivities. Self-consistent transport near criticality was also studied, and it was shown that the threshold for global transport as function of time is a fat-fractal Cantor-type set [4].

Transfer operator methods for discovering transport barriers in geophysical flows (*G. Froyland*): Finite-time transport of time-dependent or nonautonomous chaotic dynamical systems has been the subject of intense study over the past decade. Existing techniques to analyze transport have evolved from classical geometric theory of invariant manifolds, where codimension 1 invariant manifolds are impenetrable transport barriers. We have taken a very different approach based on spectral information contained in a finite-time transfer (or PerronFrobenius) operator. This technique automatically identifies regions of state space that are maximally coherent or nondispersive over a specific time interval in the presence of an underlying chaotic system. These regions, called coherent sets, are robust to perturbation and are carried along by the chaotic flow with little transport between the coherent sets and the rest of state space. Thus, these coherent sets are ordered skeletons of the time-dependent dynamics, around which the chaotic dynamics occurs relatively independently over the finite time considered.

We have developed the theory behind an optimization problem to determine these coherent sets and describe in detail a numerical implementation. On the theoretical side we introduce a new analytic transfer operator construction that enables the calculation of finite-time coherent sets. This new construction also elucidates the role of diffusion in the calculation and we show how properties such as the spectral gap and the regularity of singular vectors scale with noise amplitude. On the numerical side, the approach is very simple to implement, requiring only singular vector computations of a matrix of transitions induced by the dynamics. We have tested our new methodology on two and three-dimensional analyses of ECMWF reanalysis data to map the Antarctic polar vortex, and on two and three-dimensional ocean models and satellite-derived vector fields to track Agulhas rings over periods up to 26 months. Our studies have demonstrated how the strongest transport barriers vary with time duration and make connections with the geometry of invariant manifolds. The methods can be seamlessly applied to dynamical systems with both advective and diffusive components.

Practical concerns of using FTLE with experimental data (*M. Green*): Using Lagrangian techniques to find transport barriers and vortex boundaries in complex, aperiodic flows necessitates a careful consideration of the spatial and temporal resolution of the data to be analyzed. In particular, if two-dimensional velocity fields obtained using particle image velocimetry are used to investigate complex three-dimensional flows, significant information may not be captured. To illustrate this, we calculate planar FTLE fields from three-dimensional direct numerical simulation results of a fully turbulent channel (3D FTLE), and then repeat the calculation using only the in-plane velocities (2D FTLE). The resultant FTLE fields degrade in way that cannot be attributed to a simple spatial or temporal filter. In some regions, where the dominant vorticity is perpendicular to the plane of interest, the 2D FTLE may perform well. However, in those regions where we know the dominant vorticity is parallel to the plane of interest, whole structures are simply not captured by the 2D FTLE, compared with the 3D FTLE.

To demonstrate the effects of poor time resolution, simulated 3D experiments were also done by artificially degrading the time resolution of the velocity data, such as using only every tenth or only every fiftieth data set and recreating intermediate velocity fields with linear or cubic interpolation. The resultant 3D FTLE fields progressively worsen by changing shape and appearing to ”smear” in the streamwise direction, indicative of the poorly resolved intermediate velocity fields. We were able to correct for this with a simple model to recreate intermediate velocity fields: Taylor’s Hypothesis. If intermediate velocity fields are created by shifting the given velocity fields in the streamwise direction along the mean velocity profile of the turbulent channel, the resultant 3D FTLE are much more similar to the those from the fully resolved data.

Both spatial and temporal resolution problems in experimental velocity fields can cause major errors in the resulting FTLE fields. We propose that with some fundamental understanding about the flow field of interest, such as local vorticity direction or relevant length and time scales, some of the pitfalls maybe avoided. In some cases, this maybe by avoiding FTLE where it is not appropriate, and in others, low-dimensional models of the flow field can be used to make up for the lack of resolution.

Geodesic theory of transport barriers (*G. Haller*): Detecting transport barriers is important in a number of areas, including geophysical flows plasma fusion, reactive flows and molecular dynamics . For steady and temporally periodic flow models, available dynamical systems theory identifies invariant manifolds that act as phase space barriers. Even in this well-understood setting, however, only specific examples of de facto barriers have been found. Indeed, even for steady flows, no general approach to defining and locating transport barriers has been available. A commonly used definition of barriers as surfaces of zero transverse flux is inadequate, because any randomly chosen surface of trajectories admits zero normal flux.

In a series of publications, our group has developed a general theory of transport barriers in two-dimensional non-autonomous dynamical systems with general time dependence. The barriers are sought as material curves that act as exceptional locations of coherence in the deformation field. We express this coherence requirement by seeking stationary curves of the averaged stretching functional and the averaged shearing functional defined on material lines. In other words, we look for special material curves where we see no leading order change in the average straining or shearing of their nearby neighbors. This unusual lack of variability imposes observed coherence in tracer evolution.

The above approach leads to involved calculus of variations problems with no immediately clear solutions. However, both shearless and stretchless barriers can be shown to be solutions of appropriately defined geodesic problems. Specifically, they both are geodesics of appropriately defined Lorentzian metrics derived from the flow deformation gradient. These geodesics can be explicitly computed as trajectories of ordinary differential equations, yielding transport barriers as explicitly parametrized smooth curves in the flow.

We show applications of these mathematical results to various geophysical flow data sets, some obtained from mathematical models, others from satellite observations of sea-surface height. This enables us to identify, among other things, sharp Lagrangian jet cores for the Kuroshio current, and super-coherent mesoscale eddies in the Southern Ocean. We are also able to forecast impending large-scale instabilities in observed pollution patterns, such as the Deep Water Horizon oil spill.

Clustering on the surface ocean (*J. Olascoaga*): Observations indicate a tendency of floating material in the ocean to cluster within coherent material eddies. The floating material in question include drifting buoys, sargassum, and chlorophyll. These observations are consisting with extensive results from 2-d turbulence DNS. Consistent with this we consider inertial (particle's finite-size) effects in a 2-d incompressible setting to provided a plausible explanation for the observed behavior in the ocean.

More precisely, we consider the minimal Maxey-Riley set describing the motion of an inertial particle. We find that appropriate choices of inertial particle decay time and fluid to inertial particle density ratio provide reasonable matches with observations. Specifically, LCS extracted from the Maxey-Riley set, referred to as inertial LCS or iLCS, are found to be consistent with patterns formed by: drifting buoys in the Pacific Ocean and the Gulf of Mexico; sargassum distributions in the North Atlantic; and chlorophyll distributions in the South Atlantic. Our preliminary work has neglected the effects of the Earth's rotation. Ongoing work is showing that these are important and must be accounted for to reduce differences with observed behavior in the ocean.

Connecting spectral dynamics to coherent structures (*Nicholas T. Ouellette*): The past few decades have seen an explosion of proposed tools for identifying coherent structures in fluid flows, based on a broad range of assumptions. Some of these approaches, such as thresholding of the velocity or vorticity field, are quite simple, but may not produce meaningful results. Other methods, such as those rooted in the Lagrangian description of fluid mechanics, are potentially much more powerful, although at the cost of being more subtle and less obviously connected to flow visualization. In almost every case, however, methods for identifying coherent structures only take advantage of kinematic information such as the flow velocity field or its gradients. By neglecting the rich dynamical structure present in turbulent flows, such as the well-understood transport of energy and momentum between motion on different length and time scales, we may be artificially limiting our ability to find dynamically relevant and predictive coherent structures in complex fluid flows.

To make progress towards the goal of linking a coherent-structures analysis with the dynamical properties of the flow field, we have developed and implemented an analysis method known as a filter-space technique that allows us to measure the transfer of energy and enstrophy between scales in a spatially localized way. These fluxes can then be studied either statically in space or along the Lagrangian paths of fluid elements. We have demonstrated this analysis on experimental data sets measured in a laboratory quasi-two-dimensional weakly turbulent fluid flow, where the entire velocity field and its gradients can be measured using particle-tracking velocimetry. This study has so far produced two primary results: first, that the spectral energy flux is correlated along fluid-element trajectories for times that can be as long as the velocity itself [**?**]; and second, that the same transport barriers that organize the mixing in the flow field, known as Lagrangian Coherent Structures, also partition the field into regions that show distinct spectral dynamics [**?**].

In the future, it will be fascinating to continue to incorporate the spectral dynamics of the flow with coherent-structures tools. In particular, transfer and Koopman operator methods are very promising candidates where the energy flux can be linked with existing kinematic information, as are mesochronic analysis methods.

Chaotic Advection in a Steady, Three-dimensional, Ekman-Driven Eddy: Part I (*L. Pratt, I. Rypina, T.Özgökmen, and P. Yang)*: The ocean is filled with eddies of all sizes. Of great interest to the current oceanographic community are submesoscale eddies, with horizontal scales of hundreds of meters to tens of kilometers, and depths up to 100 meters. In addition to the horizontal swirl circulation, clockwise or counterclockwise, that defines the eddy, there is often an overturning circulation, with water upwelling in the center and downwelling at the edges, or vice versa. Oceanographers are interested in how heat, oxygen, nutrients and other scalar quantities are circulated and mixed though an eddy. The existence of barriers to transport and mixing are is therefore a central focus of inquiry.

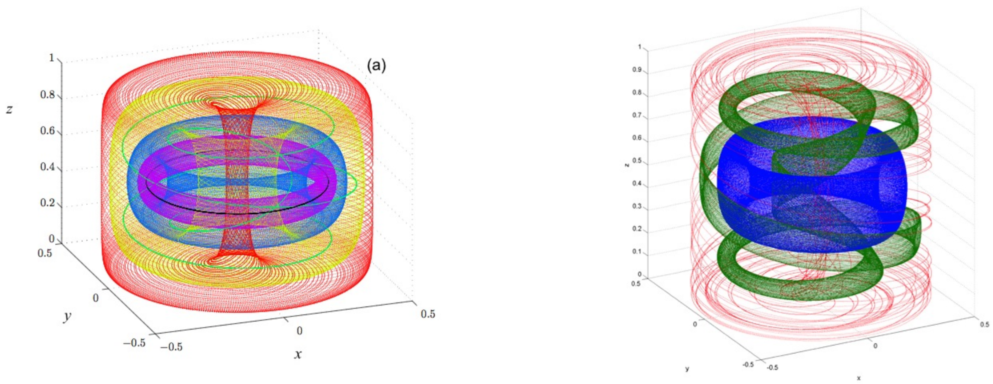
As an idealization of a submesoscale eddy, we consider a fully three-dimensional Navier-Stokes flow in a rotating cylinder. This idealization of an isolated ocean eddy is driven from above by a surface stress and has both horizontal swirl and overturning. If the flow is steady and has axial symmetry, it can be shown that each fluid parcel remains on a doughnut-shaped surface, a torus, as it circulates through the eddy (Fig. 1(a)). These tori can be thought of as barriers and some of them are destroyed when a symmetry-breaking disturbance is introduced. In regions where the barriers are broken the parcel trajectories become chaotic and the fluid in this region becomes well mixed (outer region in Fig. 1(b)). Chaos is induced either by resonance or by the breakup of the central axis streamline into stable and unstable manifolds in 3D. If the disturbance is not too large, some barriers remain (green and blue objects in Fig. 1(b)). We identify several distinct regimes of Lagrangian behavior and map these out in terms of the Ekman and Rossby numbers. We also use Eulerian constraints such as the Taylor-Proudman theorem to motivate the differences. We document a dramatic increase in the stirring rate when chaos is present and find some surprising trends. A formula for the resonance width is derived, and this and a version of the KAM theorem are used to interpret our findings.

A companion talk by the same authors documents similar behavior in a time-periodic flow. The intent is to build gradually towards a realistic simulation of an ocean eddy.

Geophysical transport structure and ecology: challenges and opportunities (*S. Ross*): Techniques uncovering transport barriers and structures in environmental flows are poised to make a considerable impact on the field of ecology. Here we discuss some results relevant for real-time analysis and prediction of geophysical transport structures, which have arisen from applications to fluid-borne microbial ecology. Focusing on aeroecology, we consider challenges involved in forecasting atmospheric Lagrangian coherent structures, including the effect of subgrid turbulence and ensemble averaging. We also consider notions that may be relevant in an ecological context, such as persistent barriers which may lead to the most diverse populations (in terms of origins) sampled sequentially at a geographically fixed location.

We find that forecasts of attracting LCSs exhibit less divergence from the archive-based LCSs than the repelling features. This result is important since attracting LCSs are the backbone of long-lived features in moving fluids. We also show under what circumstances one can trust the forecast results if one merely wants to know if an LCS passed over a region and does not need to precisely know the passage time.

Even with diffusion included, the LCSs play a role in structuring and bifurcating the probability distribution. Second, the uncertainty of the forecast FTLE fields is analyzed using ensemble forecasting. Unavoidable errors of the forecast velocity data due to the chaotic dynamics of the atmosphere is the salient reason for



(a) (b)

Figure 1: (a) For steady, axisymmetric flow in the idealized eddy, each fluid trajectory remains on a particular torus. The entire eddy is foliated with tori. (b) When the symmetry is broken, some of the tori are also broken and chaos results (red trajectory). However some barriers may remain, such as the blue torus and the twisted green torus. Fluid cannot cross these surfaces, and passive chemical or biological tracers are therefore blocked by them.

errors of the flow maps from which the FTLE fields are determined. The common practice for uncertainty analysis is to apply ensemble forecasting and here this approach is extended to FTLE field calculations. Previous work has shown an association between LCS passage and fluctuations in microbial populations and we find that ensemble FTLE forecasts are sufficient to predict such passages one day ahead of time with an accuracy of about 2 hours.

Coherent structure identification using flow map composition and spectral interpolation (*C. W. Rowley, S. Brunton, D. M. Luchtenburg, and M. O. Williams*): The flow map is the fundamental object that determines mixing characteristics of flows; it is used in virtually all methods for analyzing coherent structures, including calculation of finite-time Lyapunov exponents, and in approximating transfer operators such as the Perron-Frobenius or Koopman operators. We have developed an efficient method for approximating the the long-time flow map associated with an uncertain, time-varying velocity field, and can be used to greatly speed up computations of flow maps (often by factors of 1000 or more). The method can be used to efficiently compute finite-time Lyapunov exponents, or to approximate the evolution of probability density functions for systems with uncertain initial conditions or parameters. Short-time flow maps are approximated using polynomial basis functions, and are then composed to form a long-time flow map. Thus, the degree of the polynomial approximation grows exponentially in the number of compositions, while the number of coefficients needed to represent the short-time flow maps grows only linearly in the number of compositions. The long-time flow map is then used to compute stochastic quantities, which are shown to be correlated to coherent structures in the velocity field.

Another class of methods for analyzing coherent structures involves transfer operators, such as the Perron-Frobenius or Koopman operators. For instance, eigenfunctions of these operators provide information about asymptotically invariant sets, and various other methods (for instance, developed by G. Froyland and collaborators) provide information about finite-time coherent sets. In this work, we develop a method for obtaining such transfer operators, and information about their eigenmodes, directly from data, using an algorithm called Dynamic Mode Decomposition. The method is illustrated through several examples, for both linear and nonlinear systems, and indeed the approximate eigenmodes closely agree with analytically determined modes.

A software pipeline for LCS computation (*S. Shadden*): We have developed software elements that for users encompass an easy to use toolkit to compute and visualize Lagrangian coherent structures (LCSs) in a variety of applications, and for developers provide a modular infrastructure amenable to further customization and technological advances. The key challenges in developing a community tool for LCS computation are (1) to seamlessly handle wide-ranging input data, (2) to integrate LCS computation with familiar visualization software, (3) to provide efficient computation that leverages modern multi- and many-core architectures, and to accommodate theoretical and computational advances in the field. The software pipeline is developed using Visualization Toolkit (VTK) libraries and standards, which enables us to leverage a wealth of existing data handling and processing functionality, and to build from mature and broadly supported toolkit using modern software engineering practices. The pipeline consists of various filters that together provide a complete pipeline for loading fluid mechanics data, processing the data to compute LCS, and exporting the results for visualization. The filters are designed to be modular to enable customization of filters, or addition or replacement of filters in the pipeline. We also are working on parallel implementation of flow map computation on GPUs. We consider basic strategies for parallelization, and recent performance improvements achieved through algorithms designed to efficiently handle GPU memory constraints. We finally consider an open source framework to promote community use and participation.

Moving walls accelerate mixing (*J.L. Thiffeault)*: In many engineering applications, a viscous fluid must be blended with a substance, referred to as a passive scalar. This is generally called mixing, and it is well known that stirring greatly enhances this process. In fact, even if turbulence is unavailable (because of low Reynolds number or delicate substances), it is possible to mix rapidly by the process of chaotic advection. This involves the chaotic stretching of fluid particles by the flow, and the subsequent increase in concentration gradients of the substance to be mixed. The increased gradients facilitate the action of molecular diffusion, and homogeneity ensues. The net process (chaotic advection together with diffusion) is known as chaotic mixing.

The quantity that is often tracked in mixing problems is the variance of the concentration of the scalar. The variance is the spatial integral of the squared deviation from the mean concentration, and measures therefore the intensity of concentration fluctuations. The reasoning is that the variance tends to zero as the concentration is homogenized. Simple arguments suggest that the concentration variance should decay exponentially with time. In an idealized scenario the fluid particles are stretched exponentially and folded by the flow, yielding a characteristic filamentary structure. The filaments then achieves an equilibrium width where diffusion balances stretching. Subsequently, the concentration field for that particle decays exponentially at the rate of stretching. An average over rates of stretching then gives the overall decay rate of the variance. In many cases the decay rate of the variance is determined in a less local manner, but the decay is still exponential.

This basic exponential-decay picture is appealing, but it is complicated by the presence of walls. In that case, several authors have suggested that the no-slip boundary condition and the presence of separatrices on the walls slow down mixing: the decay rate is algebraic rather than exponential. Recent experiments have confirmed this, and also showed that for a significant period of time the rate of decay of variance is dramatically reduced, even away from the walls, due to the entrainment of unmixed material into the central mixing region. We have shown that if the situation is such that mixing is slowed down by no-slip walls, then this can be cured by moving the wall in such a way as to destroy the separatrices. This creates closed orbits near the wall, effectively insulating the central mixing region from the wall. The rate of decay of the concentration variance becomes exponential rather than algebraic. The price to pay is that the thin region of closed orbits remains poorly mixed. Of course, in some applications moving or spinning the outer wall of a container is not practical, so we also consider other mechanisms for creating closed orbits near the wall.

3 Workshop Outcomes

From the extended range of research covered in the previous section it is clear that this is a fast moving field with many research directions to pursue. Some key topics to address in the coming years are to look for synergies between the different approaches that have been developed, to coordinate and develop computational tools for uncovering key Lagrangian transport structures, and to investigate the practicality and robustness when employing these approaches for real world applications using noisy and imperfect real-world data sets.

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