

The templex approach in Lagrangian Analysis

Gisela D. Charó,^{1,2} Christophe Letellier³ & Denisse Sciamarella^{2,4}

¹ CONICET – Universidad de Buenos Aires. Centro de Investigaciones del Mar y la Atmósfera (CIMA), C1428EGA CABA, Argentina.

² CNRS – IRD – CONICET – UBA. Institut Franco-Argentin d’Études sur le Climat et ses Impacts (IRL 3351 IFAECI), C1428EGA CABA, Argentina.

³ Rouen Normandie University — CORIA, Campus Universitaire du Madrillet, F-76800 Saint-Etienne du Rouvray, France.

⁴ CNRS – Centre National de la Recherche Scientifique, 75016 Paris, France.

denisse.sciamarella@cnr.fr

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Lagrangian analysis is central to understanding how fluid particles are organized in their time evolution. Of particular interest in geophysics are rotating fluids in the presence of a radial temperature gradient, similar to those that control the dynamics of the atmosphere and oceans on a planetary scale. The phenomenon can be studied with the help of simplified kinematic models, such as Shadden’s driven double gyre, which simulates oceanic patterns, or the Bickley Jet, which reproduces the dynamics of zonal jets in the atmosphere. The use of Branched Manifold Analysis through Homologies (BraMAH) has proven useful for detecting Lagrangian Coherent Sets (LCSs) from single particle time series [Charó et al., 2019, 2020, 2021]. Here we examine how the templex approach, introduced by Charó, Letellier and Sciamarella in 2022, improves the description of the dynamics of the different particle sets.

1 Introduction

The detection of coherent Lagrangian regions in fluids is central to understanding the dispersion of different chemical species in the atmosphere, the ultimate fate of an oil spill in the ocean, or the concentration structure of the ozone layer around the polar vortex. Despite the proliferation of methods over the last quarter century, as recorded in retrospectives such as the one provided in [Hadjighasem et al., 2017], identifying coherent Lagrangian regions from data remains a challenge.

Most theoretical approaches to the problem rely either on detailed knowledge of the velocity field, or else on the calculation of local gradients for fluid particle trajectories. In most practical applications, such requirements are impossible to satisfy, making these methods impractical. On the other hand, a comparative inspection of the results obtained with different methods reveals that the predictions can be highly dependent on the type of [Allshouse and Peacock, 2015] approach. It is thus an open problem on which the scientific community is actively and intensively working.

An important step towards a methodological solution for the detection of Lagrangian regions from sparse data was taken in [Charó et al., 2019, Charó et al., 2020, Charó et al., 2021]. The approach, called Branched Manifold Analysis through Homologies (BraMAH), describes the topological structure corresponding to the individual dynamics of the particle. The method is based on the principle establishing that the non-communicating (or weakly communicating) regions of a fluid have well-differentiated dynamics [Kelley et al., 2013].

One of the models used in [Charó et al., 2020] to test the BraMAH method is known as the Bickley jet and corresponds to a sinuous zonal jet flanked by counter-rotating vortices. The self-contained system of four coupled ordinary differential equations can be derived from an analytical expression for the current function. Its solutions reproduce Lagrangian patterns typically observed in the Gulf Stream or in the nocturnal polar jet perturbed by a finite number of Rossby waves. Virtual experiments using streaklines show (Figure 1.a) the formation of coherent

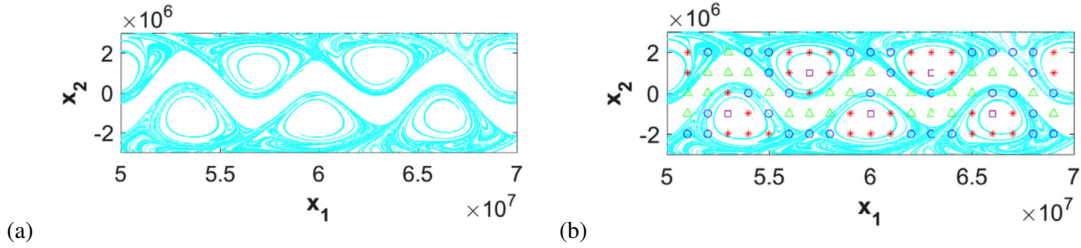


Fig. 1: Lagrangian Coherent Sets (LCSs) in the Bickley Jet. (a) Streaklines for injection points located at $x_1 = 1 \times 10^6$ m , $x_{21} = [-4 : 0.05 : -2] \times 10^6$ m and $x_{22} = [2 : 0.05 : 4] \times 10^6$, (b) topological grid where triangles, circles, squares and asterisks correspond to the different topologies obtained for particles advected from that position. Source: [Charó et al., 2020].

Lagrangian regions that can be studied topologically from an ensemble of scattered particles (Figure 1.b).

Introduced as a toy model for a two adjacent oceanic gyres enclosed by land, the unsteady or driven Double-Gyre (DDG) flow has a prominent role in the development of a variety of diagnostics associated with transport and mixing [Balasuriya et al., 2018]. The model can be seen as a simplification of a pattern that occurs frequently in geophysical flows [Shadden et al., 2005], or as a canonical example of complex transport in non-autonomous flows [Sulalitha Priyankara et al., 2017]. The system presents chaotic transport between two counter-rotating gyres [Sulalitha Priyankara et al., 2017], making it a simple and interesting testbench for methods designed to capture transport dynamics over a finite time [Allshouse and Peacock, 2015]. The laminar mixing properties of the DDG system, in the absence of diffusion, include the existence of persistent barriers to transport. Such flow ‘separators’ define sets of fluid particles that share a common dynamics.

As with the Bickley jet, BraMAH can be used to sort DDG particles according to their individual behavior. Coloring particles according to the BraMAH class they belong to provides a clear picture of how the LCSs are organised and move in the fluid domain [Charó et al., 2021]. The next section will revisit the BraMAH methodology when applied to this example. The subsequent section will use the templex concept, introduced in [Charó et al., 2022], to provide a more detailed description of the Lagrangian dynamics in each of the DDG regions.

2 LCS detection using cell complexes

In this section, we show how traditional algebraic topology can help to understand transport in fluid flows. The DDG, defined below, will be used as testbench. Its streamfunction defines a cellular flow with boundaries free of shear stresses.

$$\Psi(x, y, t) = A \sin(\pi f(x, t)) \sin(\pi y) \quad (1)$$

with

$$f(x, t) = \eta \sin(\omega t)x^2 + [1 - 2\eta \sin(\omega t)]x \quad (2)$$

defining the forcing term. Without the driving term $u = \eta \sin(\omega t)$, this is a flow with two degrees of freedom ($d_f = 2$), given by x and y . The usual parameter values are $A = 0.1$, $\eta = 0.1$ and $\omega = \pi/5$. Because $u = -\partial\psi/\partial y$, $v = \partial\psi/\partial x$, the flow is nondivergent at all times, $\partial u/\partial x + \partial v/\partial y = 0$. The driving term u as the solution to the second-order differential equation

$$\ddot{u} + \omega^2 u = 0 \quad (3)$$

with the following initial conditions

$$\begin{cases} u_0 = 0 \\ v_0 = \omega\eta. \end{cases} \quad (4)$$

The dynamical system under consideration is hence a the set of four ordinary differential equations:

$$\begin{cases} \dot{x} = -A\pi \sin\left(\pi\left[ux^2 + (1-2u)x\right]\right) \cos(\pi y) \\ \dot{y} = A\pi\left(2u\left[x-1\right] + 1\right) \\ \quad \times \cos\left(\pi\left[ux^2 + (1-2u)x\right]\right) \sin(\pi y) \\ \dot{u} = v \\ \dot{v} = -\omega^2 u \end{cases} \quad (5)$$

where the driving term u is explicitly described.

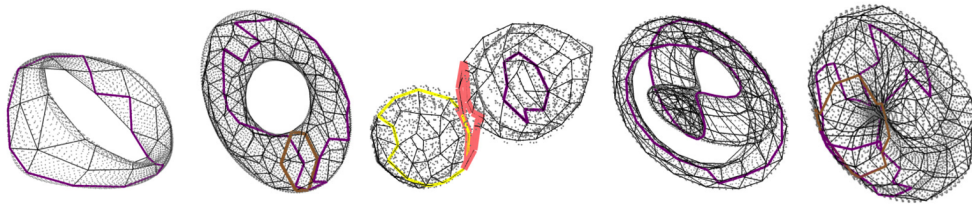


Fig. 2: Five types of topological structures that are represented by five cell complexes. The 1-cells, i.e., the lines that are highlighted in color, indicate the generators of the homology group H_1 of holes in each cell complex. Source: [Charó et al., 2021]

Integrating this equation system for different initial conditions yields particle trajectories in the DDG domain. Instead of working in the state space spanned by the four state variables x , y , u , and v , we choose to work using time-delay embeddings of the horizontal particle position x , which carries information concerning both gyres. This choice is made because we expect to be able to apply the method even when the governing equations are unknown. The embedding dimension m is determined using a False Nearest Neighbors algorithm, and is found to be $m = 4$, even if the fraction of false neighbors is already quite low in 3 dimensions. These dynamical reconstructions are not expected to match, neither the actual state space of the autonomous version of the DDG system nor the long-term behavior of the particles. The time-delay that is adopted is $\tau = T_p/5$ with $T_p = 10$. The delay parameter can vary slightly without altering the topological results: m and τ are thus kept fixed for the full set of 8528 time series (particles) considered in this study. The properties of the BraMAH cell complexes approximating these embeddings are of five classes. Results are shown in Figure 2 and 3. The properties of the cell complexes identify the LCSs in the DDG. Notice that the frontiers between colours remain considerably well defined, even if the LCSs deform in shape as they move. For further details, the reader is referred to the source paper [Charó et al., 2021].

Using algebraic topology, a fluid particle can thus be related to a set of properties obtained from a cell complex that encodes its finite-time topological structure. The strategy was called ‘topological colouring of fluid particles’ because of the use of colours to tag particles according to the topological class that emerges from the analysis. Of course, the robustness of the result depends on the quality of the dynamical reconstruction, related to the length, level of noise, or observability of the scalar variable of the time series under analysis. The existence of a Klein bottle among the five cell complexes in Fig. 2 underlines the importance of working in a phase space of sufficiently high dimension that guarantees an autonomous framework: let us recall that the Klein bottle cannot be immersed in three dimensions without self-intersections. In terms of LCSs detection, the BraMAH method differs from previous ones because it describes transport by how particles behave without looking at where they go.

The topological characterization of a flow structure in the state space can be improved. Templates or knot-holders developed in the eighties [Birman and Williams, 1983] and nineties [Mindlin and Gilmore, 1992, Ghrist et al., 1997] or [Gilmore, 1998] can distinguish, for instance, the spiral and the funnel Rössler attractor in terms of strips, while

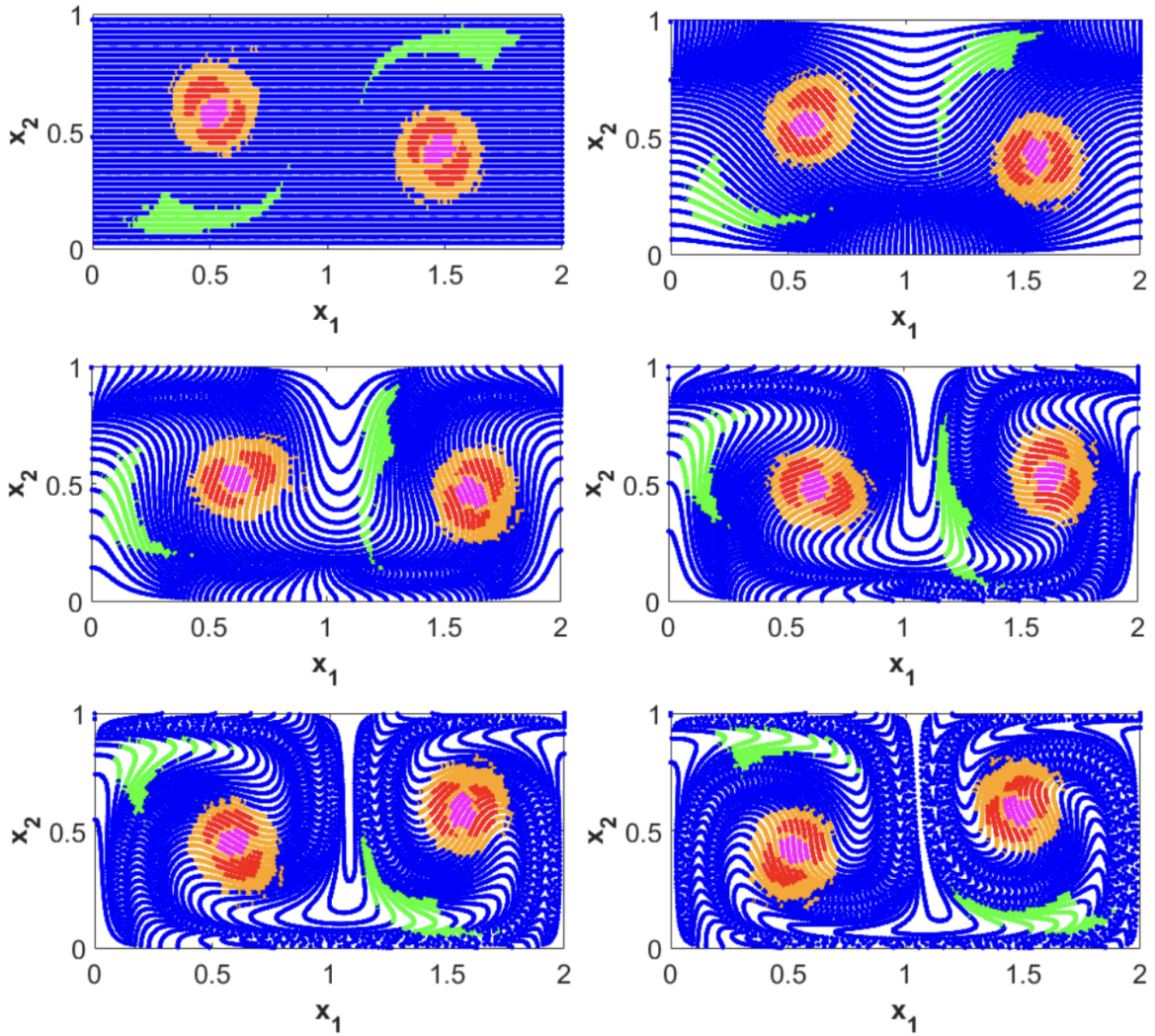


Fig. 3: One colour is assigned to each topological class (to the properties of each of the cell complexes in Fig. 13). The colours are used to tag the 8528 particles in motion in the DDG field. The LCSs in green, orange, red or magenta cut out from the chaotic sea in blue. Source: [Charó et al., 2021]

homologies cannot. Both, spiral and funnel Rössler attractors are associated to single-holed, homologically equivalent, cell complexes. The main hindrance with templates is their dependence on knot-theory which nails them to three dimensional state spaces. The next section discusses how the templex approach provides a mathematical framework bearing the possibility of generalizing templates to higher dimensions, without relying on orbits or knots.

3 Templexes for the LCSs

For over twenty years, homology theory was expected to offer an extension to the topological program for higher-dimensional systems. However, homologies provide only a partial solution to the problem, as they do not take the flow into account. The templex is a cell complex endowed with a directed graph. Cell complex and digraph work as two companion objects, since the nodes of the digraph are the highest dimensional cells of the complex, and the edges of the graph are the cell connections permitted by the flow. The term templex was born from the contraction of

two previously existing terms: template and complex. The new mathematical object brings a long-sought formalism for describing the topology of a flow along a spatial structure. In the particular context of deterministic dynamical systems, the properties of a templex enable determining whether two dynamics are equivalent, or whether a particular model is an adequate representation of the dynamics underlying an observed or numerically simulated time series.

But, can we build a templex for the five topological classes identified in the DDG flow? The answer is yes, and not only for the particles flowing the chaotic sea, where the elements needed to construct a template are present. A template is conceived to represent the strip-structure between a splitting and a joining chart. Quasi-periodic flows do not have splitting or joining loci, but they still can be represented with a templex, as we shall see.

The methodology implies the generation of a cell complex from a point cloud gathering subsets of points in cells. This objective can be achieved as done in the BraMAH approach. Alternative algorithmic procedures are being studied. A directed graph must then be generated from the data. This is done by collecting the information of how the flow visits the cells in the complex. Neighboring cells that are glued to each other but that are not connected by the flow, will not bring an edge to the digraph. Edges will represent cell connections allowed by the flow. This is how the flow information is integrated to the already constructed complex.

An algorithm in Wolfram Mathematica (<https://git.cima.fcen.uba.ar/sciamarella/templex-properties>) can be used to compute all the topological properties that are necessary to identify the topology of a system's branched 2-manifold represented by the cell complex (homologies, torsion groups, orientability). If a digraph associated with the complex is provided, too, then the algorithm also computes the generatex set and its properties, fully describing the templex. The algorithm will look for joining loci. A joining locus in a templex is formed by the group of cells neighboring the location where the state space flow splits into non-equivalent paths. If the dynamics being studied has no such location, the templex will not have joining lines and only one non-redundant path along the structure will be found. This does not mean that the structure will be topologically simple: as we have seen in the previous section, there is a Klein bottle among the topological classes encountered for the DDG. This makes the templex a more general tool than the template, not only because of dimensional issues, but also because it provides a distinct description of the spatial structure (through the cell complex) and of the flow paths along that structure (through the digraph).

Let us give an example of how the templex approach works, using the Lorenz attractor – see Figure 4. The cell complex provides a sort of kirigami or paper model of the butterfly shape in three-dimensional phase space. Non-equivalent paths (chains of cells) in the cell complex can be expressed as digraph cycles. Such cycles – strong or weak, with or without twists – can be calculated from the combined algebraic handling of the cell complex and the associated digraph. The result of this computation is the so-called 'generatex set'. These sub-templexes indicate the dynamical paths that are compatible with the underlying branched manifold. The three coloured lanes in the digraph correspond to the generatexes of the Lorenz attractor, structured as the cell complex.

The figure showing the five DDG templexes corresponding to the cell complexes in Fig.3 will be shown in the talk. We must remark that, for the DDG flow discussed here, the templexes are as good as the complexes in discriminating the different LCSs: the number of topological classes (and therefore of Lagrangian regions) remains five. Of course, the templex unveils a more detailed description of the topological structure of the particle dynamics in each Lagrangian region. Notice that the templex properties confirm that the particles of the blue LCS have a chaotic behavior, evidenced by the existence of a joining locus and a generatex set, while the regions where particles exhibit quasi-periodic motions are free of joining lines. Discriminating between topologically different quasi-periodic behaviors is possible because the cell complexes are not equivalent in terms of homology and torsion groups.

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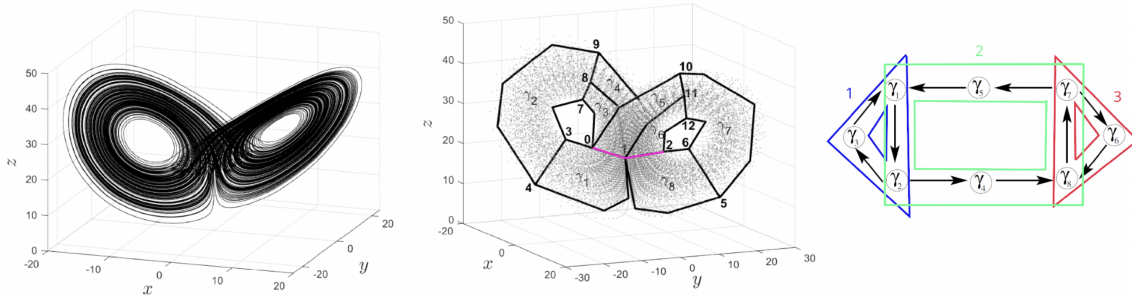


Fig. 4: Templex for the Lorenz 63 attractor (a), the cell complex juxtaposed on the point cloud (b), and the joining locus formed by: the joining 1-cell in magenta, and the joining 2-cells $\gamma_1, \gamma_2, \gamma_3, \gamma_4, \gamma_8$. The directed graph (digraph) (c) shows the connections between the 2-cells allowed by the flow.

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