

# LDDS: Python package for computing and visualizing Lagrangian Descriptors for Dynamical Systems

## Statement of Need

Nonlinear dynamical systems are ubiquitous in natural and engineering sciences, such as, fluid mechanics, theoretical chemistry, ship dynamics, rigid body dynamics, atomic physics, solid mechanics, condensed matter physics, mathematical biology, oceanography, meteorology and celestial mechanics (Wiggins 1994 and references therein). There have been many advances in understanding phenomena across these disciplines using the geometric viewpoint of the solutions and the underlying structures in the phase space. Chief among these phase space structures are the invariant manifolds that form a barrier between dynamically distinct solutions (Ozorio de Almeida et al. 1990), (Rom-Kedar and Wiggins 1990), (Wiggins 2016). In most nonlinear systems, the invariant manifolds are computed using numerical techniques that rely on some form of linearization around equilibrium points followed by continuation and globalization. However, these methods become computationally expensive and challenging when applied to the high-dimensional phase space of vector fields defined analytically, from numerical simulations or experimental data. This points to the need for techniques that can be paired with trajectory calculations, without excessive computational overhead and at the same time can allow visualization along with trajectory data. The Python package, LDDS, serves this need for analyzing deterministic and stochastic, continuous and discrete high-dimensional nonlinear dynamical systems described either by an analytical vector field or from data obtained from numerical simulations or experiments.

To the best of our knowledge, no other software for calculating Lagrangian descriptors exists. A variety of computational tools is available for competing approaches popular in fluid mechanics, such as the identification of Lagrangian coherent structures via finite-time Lyapunov exponents (Briol and d’Ovidio 2011), (“High-Order Visualization of Three-Dimensional Lagrangian Coherent Structures with DG-FTLE” 2016), (“LCS Tool: A Computational Platform for Lagrangian Coherent Structures” 2015), (Finn and Apte 2013), (Dabiri Lab, n.d.), (Haller et al. 2020) and finite-size Lyapunov exponents (Briol and d’Ovidio 2011) or Eulerian coherent structures (Katsanoulis and Haller 2018).

## Summary and Functionalities

The LDDS software is a Python-based module that provides the user with the capability of analyzing the phase space structures of both continuous and discrete nonlinear dynamical systems in the deterministic and stochastic settings through the method of Lagrangian descriptors (LDs) (Jiménez Madrid and Mancho 2009), (Mancho et al. 2013). The main idea behind this methodology is to define a scalar function, a Lagrangian descriptor, that accumulates the values taken by a positive function of the phase space variables of the system along the trajectory starting from a given initial condition. This operation is carried out in forward and backward time for all initial conditions on a predefined grid, and the output obtained from the method provides an indicator of the underlying geometry of the phase space of the dynamical system under study. One of the main goals we pursue with this software is to give the tools for reproducible scientific research.

Given a continuous-time dynamical system:

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}(t), t) \quad (1)$$

where  $\mathbf{x} \in \mathbb{R}^n$  and  $\mathbf{f}$  represents the vector field. To compute Lagrangian descriptors, select any initial condition  $\mathbf{x}_0 = \mathbf{x}(t_0)$  at time  $t = t_0$  and accumulate a positive function of the phase space coordinates,  $g(\mathbf{x}(t); \mathbf{x}_0)$ , along its trajectory in forward and backward time over the interval  $[t_0 - \tau, t_0 + \tau]$ . This gives the following definition:

$$\mathcal{L}(\mathbf{x}_0, t_0, \tau) = \int_{t_0-\tau}^{t_0+\tau} g(\mathbf{x}(t); \mathbf{x}_0) dt \quad (2)$$

Different formulations of the Lagrangian descriptor exist in the literature where the positive function  $g$  is: the arc length of a trajectory in phase space, the arc length of a trajectory projected on the configuration space, and the sum of the  $p$ -norm of the vector field components, the Maupertuis' action of Hamiltonian mechanics. The approach provided by Lagrangian descriptors for revealing phase space structure has also been adapted to address discrete-time systems (maps) and stochastic systems.

This open-source package incorporates the following features:

- Computation of LDs for two-dimensional maps.
- Study of the phase space structure of two-dimensional continuous dynamical systems with LDs.
- Computation of LDs for a system of two stochastic differential equations with additive noise.
- Computation of LDs on two-dimensional phase space planes for Hamiltonian systems with 2 or more degrees of freedom (DoF).
- Application of LDs to Hamiltonian systems with 2 DoF where the potential energy surface is known on a discrete spatial grid.
- Computation of LDs from a Spatio-temporal discretization of a two-dimensional time-dependent vector field.
- Visual extraction of the invariant stable and unstable manifolds from the LD scalar field values.
- Addition to time-dependent external forcings for two-dimensional continuous dynamical systems.
- Different definitions for the Lagrangian descriptor function found in the literature.

All the different features of the module, and their usage across different settings, are illustrated through Jupyter-notebook tutorials. These tutorials would help users better understand how to set up a model dynamical system to which LDs is applied, and present them with different options for visualizing the results obtained from the analysis. We believe that these resources provide useful material for the development of an effective learning process that could motivate the integration of this tool into users' research/academic projects. Moreover, this will surely encourage future contributions from the scientific community to extend the features and applicability of this software package to other areas.

## Example systems

The following dynamical systems are included in this software package as examples to illustrate the application of Lagrangian descriptors:

### Maps:

- Standard map

The standard map (kicked rotator) is a two-dimensional map used in dynamical systems to study a periodically kicked pendulum. The equations of the discrete system are given by the expressions:

$$\begin{cases} x_{n+1} = x_n + y_n - \frac{K}{2\pi} \sin(2\pi x_n) \\ y_{n+1} = y_n - \frac{K}{2\pi} \sin(2\pi x_n) \end{cases} \quad (3)$$

where  $K$  is the parameter that controls the forcing strength of the perturbation. The inverse map is described by:

$$\begin{cases} x_n = x_{n+1} - y_{n+1} \\ y_n = y_{n+1} + \frac{K}{2\pi} \sin(2\pi(x_{n+1} - y_{n+1})) \end{cases} \quad (4)$$

In the following figure, we show the output produced by the LDDS software package for the standard map using the model parameter value  $K = 1.2$ .

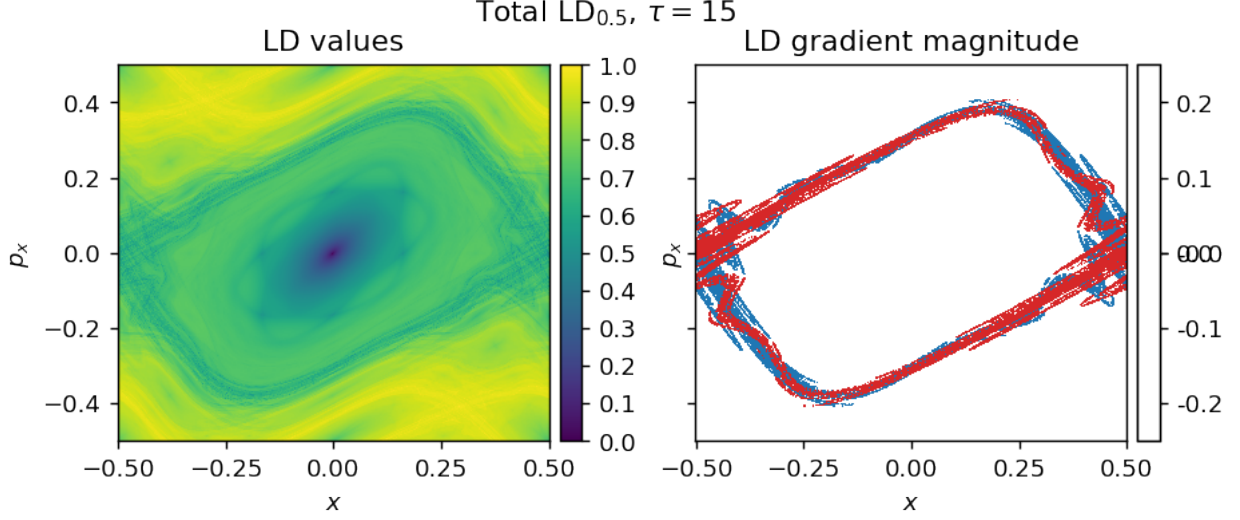


Figure 1: Lagrangian descriptor for the standard map

#### Flows:

- Forced undamped Duffing oscillator

The time-dependent Hamiltonian that describes the forced Duffing oscillator is:

$$H(x, p_x, t) = \frac{1}{2}p_x^2 - \frac{\alpha}{2}x^2 + \frac{\beta}{4}x^4 - f(t)x \quad (5)$$

where  $\alpha$  and  $\beta$  are the model parameters and  $f(t)$  is the time-dependent forcing added to the system. The non-autonomous vector field that defines the dynamical system is given by:

$$\begin{cases} \dot{x} = \frac{\partial H}{\partial p_x} = f_1(x, p_x) = p_x \\ \dot{p}_x = -\frac{\partial H}{\partial x} = f_2(x, p_x) = \alpha x - \beta x^3 + f(t) \end{cases} \quad (6)$$

In the following figure we show the output produced by the LDDS software package for the forced Duffing oscillator using the model parameter value  $\alpha = \beta = 1$ . The initial time is  $t_0 = 0$  and the perturbation used is of the form  $f(t) = A \sin(\omega t)$  where  $A = 0.25$  and  $\omega = \pi$ .

- Double-gyre flow with stochastic forcing

The stochastic dynamical system for the double gyre flow with additive noise is described by the following stochastic differential equation:

$$\begin{cases} dX_t = \left( -\pi A \sin\left(\frac{\pi f(X_t, t)}{s}\right) \cos\left(\frac{\pi Y_t}{s}\right) - \mu X_t \right) dt + \sigma_1 dW_t^1 \\ dY_t = \left( \pi A \cos\left(\frac{\pi f(X_t, t)}{s}\right) \sin\left(\frac{\pi Y_t}{s}\right) \frac{\partial f}{\partial x}(X_t, t) - \mu Y_t \right) dt + \sigma_2 dW_t^2 \end{cases} \quad (7)$$

where  $W^1$  and  $W^2$  are Wiener processes and we have that:

$$f(X_t, t) = \varepsilon \sin(\omega t + \phi) X_t^2 + (1 - 2\varepsilon \sin(\omega t + \phi)) X_t \quad (8)$$

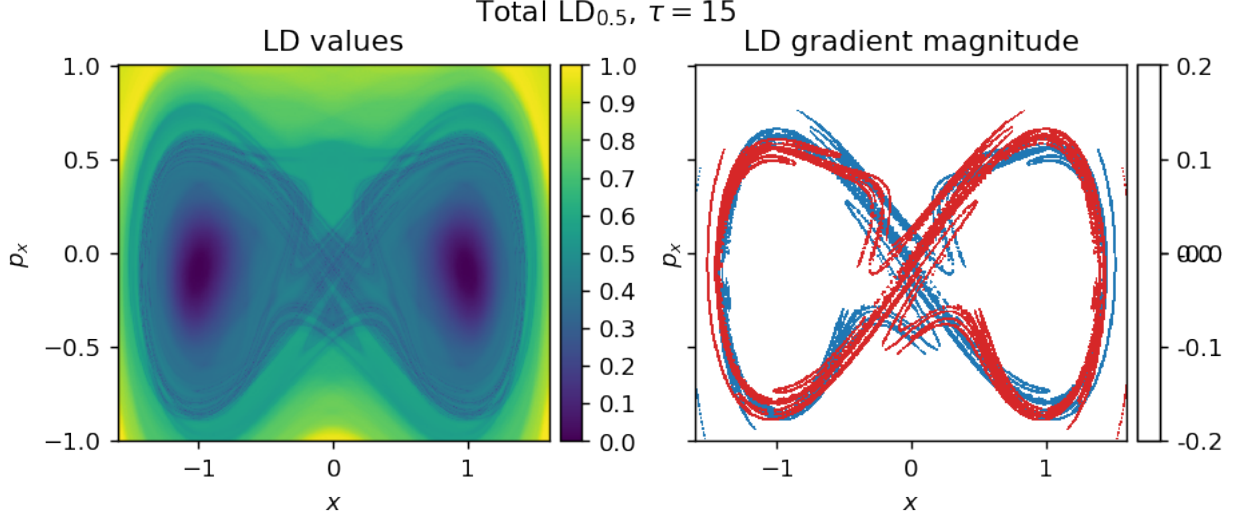


Figure 2: Lagrangian descriptor for the Duffing oscillator

In the following figure we show the output produced by the LDDS software package for the stochastically forced double gyre using a noise amplitude of  $\sigma_1 = \sigma_2 = 0.1$ . The double gyre model parameters are  $A = 0.25$ ,  $\phi = 2\pi$ ,  $\psi = \mu = 0$ ,  $s = 1$ ,  $\varepsilon = 0.25$ , and the initial time is  $t_0 = 0$ .

Four-dimensional phase space:

- Hénon-Heiles Hamiltonian.

The Hénon-Heiles Hamiltonian is given by the function:

$$H(x, y, p_x, p_y) = \frac{1}{2}(p_x^2 + p_y^2) + x^2y - \frac{1}{3}y^3 \quad (9)$$

where the vector field is:

$$\begin{aligned} \dot{x} &= \frac{\partial H}{\partial p_x} = p_x \\ \dot{y} &= \frac{\partial H}{\partial p_y} = p_y \\ \dot{p}_x &= -\frac{\partial H}{\partial x} = -x - 2xy \\ \dot{p}_y &= -\frac{\partial H}{\partial y} = -x^2 - y + y^2 \end{aligned} \quad (10)$$

IN the next figure we show the computation of Lagrangian descriptors with the LDDS software package on the phase space slice described by the condition  $x = 0$ ,  $p_x > 0$  for the energy of the system  $H_0 = 1/5$ .

## Relation to ongoing research projects

Lagrangian descriptors form the basis of several past and present research projects (Cámara et al. 2012), (Cámara et al. 2013), (Lopesino et al. 2015), (Craven and Hernandez 2015), (Craven and Hernandez 2016), (García-Garrido et al. 2016), (Balibrea-Iniesta et al. 2016), (Demian and Wiggins 2017), (Craven, Junginger, and Hernandez 2017), (Feldmaier et al. 2017), (Junginger et al. 2017), (García-Garrido et al. 2018), (Patra and Keshavamurthy 2018), (Naik, García-Garrido, and Wiggins 2019), (Naik and Wiggins 2019), (Curbelo et al. 2019b), (Curbelo et al. 2019a), (Revuelta, Benito, and Borondo 2019), (García-Garrido, Naik, and Wiggins 2020), (García-Garrido, Agaoglou, and Wiggins 2020), (Krajňák, Ezra, and Wiggins 2020), (Naik and Wiggins 2020), (Gonzalez Montoya and Wiggins 2020), (Katsanikas, García-Garrido, and Wiggins 2020).

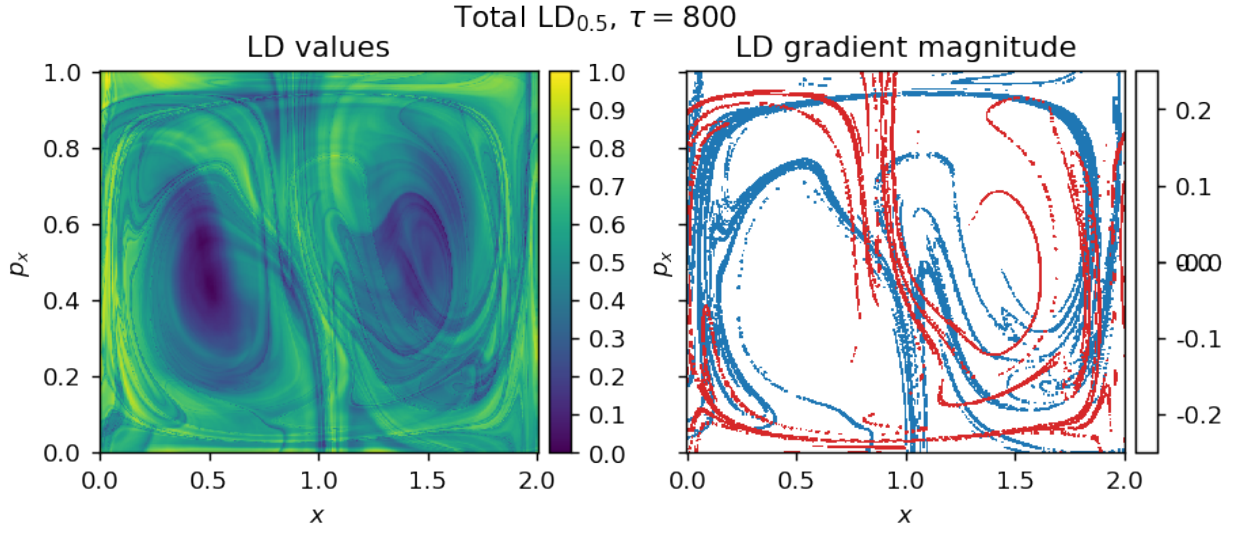


Figure 3: Lagrangian descriptor for the Double-gyre with stochastic forcing

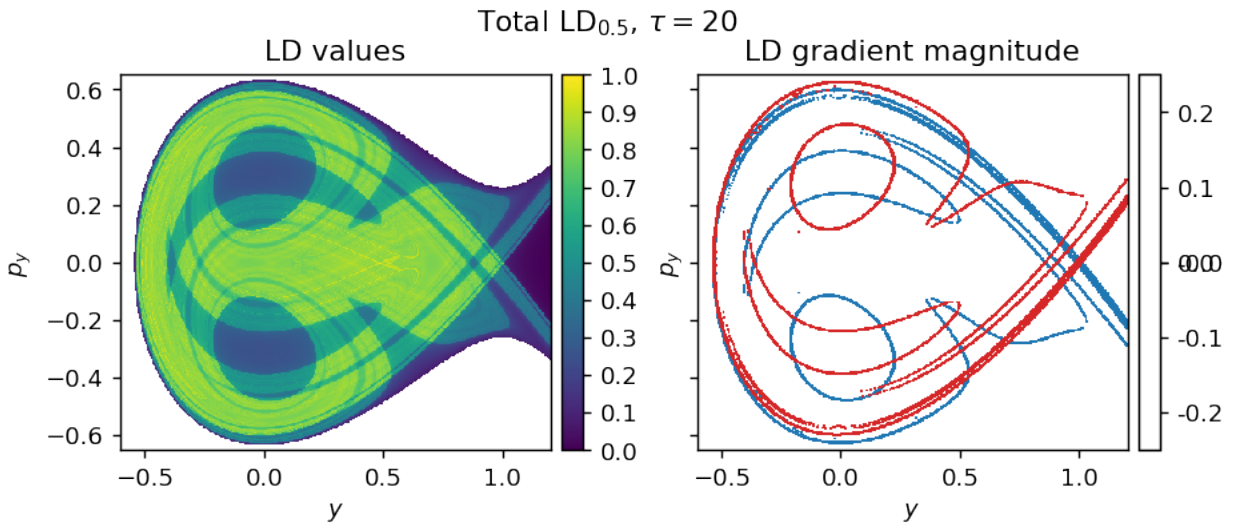


Figure 4: Lagrangian descriptor for the Hénon-Heiles Hamiltonian

The common theme of all these projects is the investigation of phase space structures that govern phase space transport in nonlinear dynamical systems. We have also co-authored an open-source book project using Jupyter book (Community 2020) on the theory and applications of Lagrangian descriptors (Agaoglou et al. 2020). This open-source package is the computational companion to that book.

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## References

- Agaoglou, M., B. Aguilar-Sanjuan, V. J. García-Garrido, F. González-Montoya, M. Katsanikas, V. Krajnak, S. Naik, and S. Wiggins. 2020. *Lagrangian Descriptors: Discovery and Quantification of Phase Space Structure and Transport*. zenodo: 10.5281/zenodo.3958985. <https://doi.org/10.5281/zenodo.3958985>.
- Balibrea-Iniesta, F., C. Lopesino, S. Wiggins, and A. M. Mancho. 2016. “Lagrangian Descriptors for Stochastic Differential Equations: A Tool for Revealing the Phase Portrait of Stochastic Dynamical Systems.” *International Journal of Bifurcation and Chaos* 26 (13). World Scientific: 1630036.
- Briol, F., and F. d’Ovidio. 2011. “Lagrangian.” [https://bitbucket.org/cnes\\_aviso/lagrangian/src/master/](https://bitbucket.org/cnes_aviso/lagrangian/src/master/).
- Cámara, A. de la, A. M. Mancho, K. Ide, E. Serrano, and C. R. Mechoso. 2012. “Routes of transport across the Antarctic polar vortex in the southern spring.” *J. Atmos. Sci.* 69 (2): 753–67. <https://doi.org/10.1175/JAS-D-11-0142.1>.
- Cámara, A. de la, C. R. Mechoso, A. M. Mancho, E. Serrano, and K. Ide. 2013. “Isentropic transport within the Antarctic polar night vortex: Rossby wave breaking evidence and Lagrangian structures.” *J. Atmos. Sci.* 70: 2982–3001.
- Community, Executable Books. 2020. *Jupyter Book* (version v0.10). Zenodo. <https://doi.org/10.5281/zenodo.4539666>.
- Craven, G. T., and R. Hernandez. 2015. “Lagrangian Descriptors of Thermalized Transition States on Time-Varying Energy Surfaces.” *Physical Review Letters* 115 (14). APS: 148301.
- . 2016. “Deconstructing Field-Induced Ketene Isomerization Through Lagrangian Descriptors.” *Physical Chemistry Chemical Physics* 18 (5). Royal Society of Chemistry: 4008–18.
- Craven, G. T., A. Junginger, and R. Hernandez. 2017. “Lagrangian Descriptors of Driven Chemical Reaction Manifolds.” *Physical Review E* 96 (2). APS: 022222.
- Curbelo, J., C. R. Mechoso, A. M. Mancho, and S. Wiggins. 2019a. “Lagrangian Study of the Final Warming in the Southern Stratosphere During 2002: Part II. 3D Structure.” *Climate Dynamics* 53 (3): 1277–86. <https://doi.org/10.1007/s00382-019-04833-x>.
- . 2019b. “Lagrangian Study of the Final Warming in the Southern Stratosphere During 2002: Part I. The Vortex Splitting at Upper Levels.” *Climate Dynamics* 53 (5): 2779–92. <https://doi.org/10.1007/s00382-019-04832-y>.
- Dabiri Lab. n.d. “LCS Matlab Kit.” <http://dabirilab.com/software>.
- Demian, A. S., and S. Wiggins. 2017. “Detection of Periodic Orbits in Hamiltonian Systems Using Lagrangian Descriptors.” *International Journal of Bifurcation and Chaos* 27 (14): 1750225. <https://doi.org/10.1142/S021812741750225X>.
- Feldmaier, M., A. Junginger, G. Main J. and Wunner, and R. Hernandez. 2017. “Obtaining Time-Dependent Multi-Dimensional Dividing Surfaces Using Lagrangian Descriptors.” *Chemical Physics Letters* 687. Elsevier: 194–99.

- Finn, J., and S. V. Apte. 2013. “Integrated Computation of Finite Time Lyapunov Exponent Fields During Direct Numerical Simulation of Unsteady Flows.” *Chaos* 23: 013145. <https://doi.org/10.1063/1.4795749>.
- García-Garrido, V. J., M. Agaoglou, and S. Wiggins. 2020. “Exploring Isomerization Dynamics on a Potential Energy Surface with an Index-2 Saddle Using Lagrangian Descriptors.” *Communications in Nonlinear Science and Numerical Simulation* 89: 105331. <https://doi.org/https://doi.org/10.1016/j.cnsns.2020.105331>.
- García-Garrido, V. J., J. Curbelo, A. M. Mancho, S. Wiggins, and C. R. Mechoso. 2018. “The Application of Lagrangian Descriptors to 3D Vector Fields.” *Regular and Chaotic Dynamics* 23 (5): 551–68. <https://doi.org/10.1134/S1560354718050052>.
- García-Garrido, V. J., S. Naik, and S. Wiggins. 2020. “Tilting and Squeezing: Phase Space Geometry of Hamiltonian Saddle-Node Bifurcation and Its Influence on Chemical Reaction Dynamics.” *International Journal of Bifurcation and Chaos* 30 (04): 2030008. <https://doi.org/10.1142/S0218127420300086>.
- García-Garrido, V. J., A. Ramos, A. M. Mancho, J. Coca, and S. Wiggins. 2016. “A dynamical systems perspective for a real-time response to a marine oil spill.” *Marine Pollution Bulletin.*, 1–10. <https://doi.org/10.1016/j.marpolbul.2016.08.018>.
- Gonzalez Montoya, F., and S. Wiggins. 2020. “Revealing Roaming on the Double Morse Potential Energy Surface with Lagrangian Descriptors.” *Journal of Physics A: Mathematical and Theoretical* 53 (23). IOP Publishing: 235702. <https://doi.org/10.1088/1751-8121/ab8b75>.
- Haller, G., S. Katsanoulis, M. Holzner, B. Frohnapfel, and D. Gatti. 2020. “Objective Barriers to the Transport of Dynamically Active Vector Fields.” *J. Fluid Mech.* 905: A17. <https://doi.org/10.1017/jfm.2020.737>.
- “High-Order Visualization of Three-Dimensional Lagrangian Coherent Structures with DG-FTLE.” 2016. *Computers & Fluids* 139: 197. <https://doi.org/10.1016/j.compfluid.2016.07.007>.
- Jiménez Madrid, J. A., and A. M. Mancho. 2009. “Distinguished Trajectories in Time Dependent Vector Fields.” *Chaos* 19. AIP. <http://dx.doi.org/10.1063/1.3056050>.
- Junginger, A., L. Duvenbeck, M. Feldmaier, G. Main J.and Wunner, and R. Hernandez. 2017. “Chemical Dynamics Between Wells Across a Time-Dependent Barrier: Self-Similarity in the Lagrangian Descriptor and Reactive Basins.” *The Journal of Chemical Physics* 147 (6). AIP Publishing: 064101.
- Katsanikas, M., V. J. García-Garrido, and S. Wiggins. 2020. “The Dynamical Matching Mechanism in Phase Space for Caldera-Type Potential Energy Surfaces.” *Chemical Physics Letters* 743: 137199. <https://doi.org/https://doi.org/10.1016/j.cplett.2020.137199>.
- Katsanoulis, S., and G. Haller. 2018. “BarrierTool.” <https://github.com/haller-group/BarrierTool>.
- Krajňák, V., G. S. Ezra, and S. Wiggins. 2020. “Using Lagrangian Descriptors to Uncover Invariant Structures in Chesnavich’s Isokinetic Model with Application to Roaming.” *International Journal of Bifurcation and Chaos* 30 (5): 2050076. <https://doi.org/10.1142/S0218127420500765>.
- “LCS Tool: A Computational Platform for Lagrangian Coherent Structures.” 2015. *J. Comput. Sci.* 7: 26. <https://doi.org/10.1016/j.jocs.2014.12.002>.
- Lopesino, C., F. Balibrea-Iniesta, S. Wiggins, and A. M. Mancho. 2015. “Lagrangian Descriptors for Two Dimensional, Area Preserving Autonomous and Nonautonomous Maps.” *Communications in Nonlinear Science and Numerical Simulation* 27 (1-3): 40–51. <https://doi.org/10.1016/j.cnsns.2015.02.022>.
- Mancho, A. M., S. Wiggins, J. Curbelo, and C. Mendoza. 2013. “Lagrangian Descriptors: A Method for Revealing Phase Space Structures of General Time Dependent Dynamical Systems.” *Communications in Nonlinear Science and Numerical Simulation* 18 (12): 3530–57.
- Naik, S., V. J. García-Garrido, and S. Wiggins. 2019. “Finding NHIM: Identifying High Dimensional Phase Space Structures in Reaction Dynamics Using Lagrangian Descriptors.” *Communications in Nonlinear Science and Numerical Simulation* 79: 104907. <https://doi.org/10.1016/j.cnsns.2019.104907>.

Naik, S., and S. Wiggins. 2019. “Finding Normally Hyperbolic Invariant Manifolds in Two and Three Degrees of Freedom with Hénon-Heiles Type Potential.” *Phys. Rev. E* 100 (2): 022204. <https://doi.org/10.1103/PhysRevE.100.022204>.

———. 2020. “Detecting Reactive Islands in a System-Bath Model of Isomerization.” *Phys. Chem. Chem. Phys.* The Royal Society of Chemistry. <https://doi.org/10.1039/D0CP01362E>.

Ozorio de Almeida, A. M., N. De Leon, M. A. Mehta, and C. C. Marston. 1990. “Geometry and Dynamics of Stable and Unstable Cylinders in Hamiltonian Systems.” *Physica D: Nonlinear Phenomena* 46 (2): 265–85.

Patra, S., and S. Keshavamurthy. 2018. “Detecting Reactive Islands Using Lagrangian Descriptors and the Relevance to Transition Path Sampling.” *Physical Chemistry Chemical Physics* 20 (7). Royal Society of Chemistry: 4970–81.

Revuelta, F., R. M. Benito, and F. Borondo. 2019. “Unveiling the Chaotic Structure in Phase Space of Molecular Systems Using Lagrangian Descriptors.” *Physical Review E* 99 (3). APS: 032221.

Rom-Kedar, V., and S. Wiggins. 1990. “Transport in Two-Dimensional Maps.” *Arch. Ration. Mech. A.l.* 109 (3). <https://doi.org/10.1007/BF00375090>.

Wiggins, S. 1994. *Normally Hyperbolic Invariant Manifolds in Dynamical Systems*. Vol. 105. Springer Science & Business Media.

———. 2016. “The Role of Normally Hyperbolic Invariant Manifolds (NHIMs) in the Context of the Phase Space Setting for Chemical Reaction Dynamics.” *Regular and Chaotic Dynamics* 21 (6): 621–38. <https://doi.org/10.1134/S1560354716060034>.