

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

19 May 2021

## 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; for example (MacKay, Meiss, and Percival 1984), (V Rom-Kedar, Leonard, and Wiggins 1990), (Ozorio de Almeida et al. 1990), (V. Rom-Kedar and Wiggins 1990), (Meiss 1992), (Koon et al. 2000), (Waalkens, Burbanks, and Wiggins 2005), (Meiss 2015), (Wiggins 2016), (Zhong, Virgin, and Ross 2018), (Zhong and Ross 2020). Chief among these phase space structures are the invariant manifolds that form a barrier between dynamically distinct solutions. 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 the 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 open-source software exists for computing Lagrangian descriptors. However, a variety of computational tools are available for obtaining phase space structures in fluid mechanics, such as the identification of Lagrangian coherent structures via finite-time Lyapunov exponents (Briol and d’Ovidio 2011), (Nelson and Jacobs 2016), (Onu, Huhn, and Haller 2015), (Finn and Apte 2013), (Dabiri Lab 2009), (Haller et al. 2020) and finite-size Lyapunov exponents (Briol and d’Ovidio 2011), Eulerian coherent structures (Katsanoulis and Haller 2018). Our goal with this software is to make Lagrangian descriptors available to the wider scientific community and enable the use of this method for reproducible and replicable computational dynamical systems.

## 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 using Lagrangian descriptors (LDs). The main idea of this method is to define a scalar valued functional called Lagrangian descriptor as the integral of a non-negative function  $g(\mathbf{x}(t); \mathbf{x}_0)$  which encodes a dynamical property of a trajectory at the initial condition,  $\mathbf{x}_0$ . Different formulations of the Lagrangian descriptor exist in the literature where the non-negative function  $g(\mathbf{x}(t); \mathbf{x}_0)$  is given by: the arclength of a trajectory in phase space (Jiménez Madrid and Mancho 2009), (Mancho et al. 2013), the arclength of a trajectory projected on the configuration space (Craven and Hernandez 2015), the  $p$ -norm or  $p$ -quasinorm (Lopesino et al. 2017), and the Maupertuis’ action of Hamiltonian mechanics (Gonzalez Montoya and Wiggins 2020). The approach provided by Lagrangian descriptors for revealing phase space structure has also been adapted to address discrete-time systems (maps) and stochastic systems.

Briefly, for a continuous-time dynamical system:

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

where  $\mathbf{x} \in \mathbb{R}^n$  and  $\mathbf{f}$  is the vector field, starting from an initial condition  $\mathbf{x}_0 = \mathbf{x}(t_0)$  at time  $t = t_0$ ,  $g(\mathbf{x}(t); \mathbf{x}_0)$  is integrated along with the trajectory in forward and backward time over the interval  $[t_0 - \tau, t_0 + \tau]$ , respectively, to obtain the Lagrangian descriptor,

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

at the initial condition. When this computation is performed for a 2D grid of initial conditions over long enough integration time interval and the corresponding contour map is visualized, one can detect phase space structures at the points with extremum LD values that also have a singularity (non-differentiability) (Lopesino et al. 2017, @naik2019a).

This open-source software incorporates the following features:

- Computation of LDs for two dimensional maps.
- Computation of LDs for two dimensional continuous-time dynamical systems.
- Computation of LDs for two dimensional stochastic differential equations with additive noise.
- Computation of LDs on two-dimensional sections of Hamiltonian systems with 2 or more degrees of freedom (DoF).
- Computation of LDs for 2 DoF Hamiltonian systems where the potential energy surface is known on a grid of points in the configuration space of a chemical reaction.
- Computation of LDs from a spatio-temporal discretization of a two-dimensional time-dependent vector field.
- Numerical gradient based identification of the invariant stable and unstable manifolds from the LD contour map.
- Addition of time-dependent external forcings in two-dimensional continuous dynamical systems.
- Different formulations of the Lagrangian descriptor available in the literature.

All the features of the package and their usage across different settings are illustrated using Jupyter notebooks as hands-on tutorials. These tutorials are meant to be worked through to understand how to set up a model dynamical system to which LDs is applied and use different options for visualizing the computational results. We believe that these notebooks are effective in integrating this method into classroom courses, independent study, and research projects. Moreover, the tutorials will encourage future contributions from the scientific community to expand the features and application of the Lagrangian descriptor method in other areas of computational science and engineering.

## Example systems

To illustrate the use of this software, we have applied the method to some of the benchmark dynamical systems. These are included as examples:

### Maps:

- Standard map

The standard map is a two-dimensional map used in dynamical systems to study a number of physical systems such as the cyclotron particle accelerator or a kicked rotor (Chirikov 1971),(Meiss 1992),(Meiss 2008). The equations of the discrete system are given by the expressions:

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

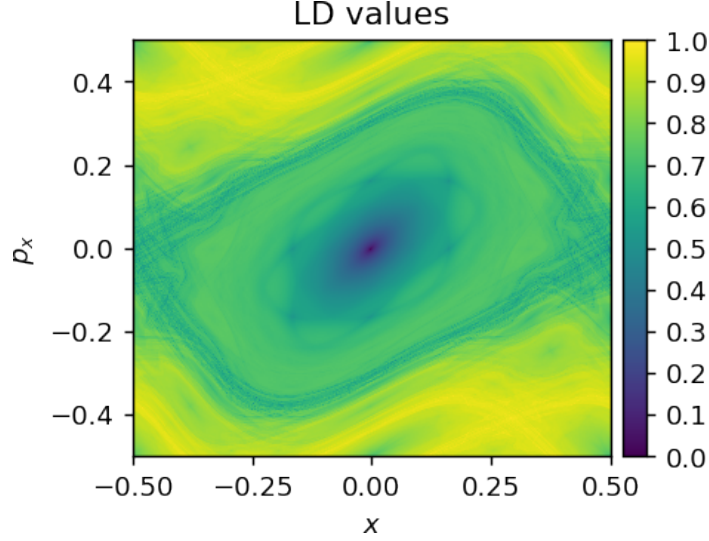


Figure 1: Lagrangian descriptor contour plot for the standard map, using  $p = 0.5$ -quasinorm and integration time  $\tau = 15$ .

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  $K = 1.2$ .

#### Flows:

- Forced undamped Duffing oscillator

The Duffing oscillator is an example of a periodically driven oscillator with nonlinear elasticity (Duffing 1918), (Kovacic and Brennan 2011). This can model the oscillations of a pendulum whose stiffness does not obey Hooke's law or the motion of a particle in a double-well potential. It is also known as a simple system that can exhibit chaos.

As a special case, the forced undamped Duffing oscillator is described by a time-dependent Hamiltonian given by:

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

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:

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

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  $\omega = \pi$ .

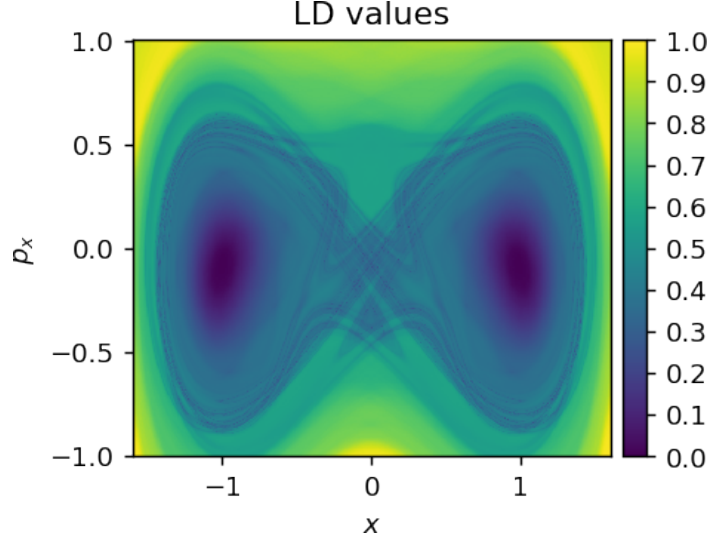


Figure 2: Lagrangian descriptor contour plot for the Duffing oscillator, using  $p = 0.5$ -quasinorm and integration time  $\tau = 15$ .

- A double gyre flow with stochastic forcing

The double gyre is a recurrent pattern occurring in geophysical flows (Coulliette and Wiggins 2001). The stochastic dynamical system for a simplified model of this flow (Shadden, Lekien, and Marsden 2005) with additive noise is described by the following stochastic differential equations (Balibrea-Iniesta et al. 2016):

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

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

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

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  $A = 0.25$ ,  $\omega = 2\pi$ ,  $\psi = \mu = 0$ ,  $s = 1$ ,  $\varepsilon = 0.25$ , and the initial time is  $t_0 = 0$ .

Four-dimensional phase space:

- Hénon-Heiles Hamiltonian.

The Hénon-Heiles system is a simplified model describing the restricted motion of a star around the center of a galaxy (Henon and Heiles 1964). This system is a paradigmatic example of a time-independent Hamiltonian with two degrees of freedom, given by the function:

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

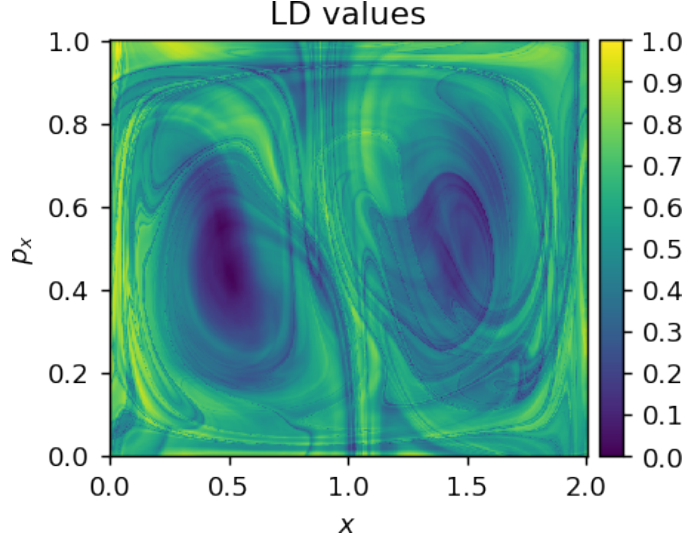


Figure 3: Lagrangian descriptor contour plot for the Double-gyre with stochastic forcing, using  $p = 0.5$ -quasinorm and integration time  $\tau = 15$ .

where the vector field is:

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

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 on-going 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), (Ramos 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). 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 published an open-source book using Jupyter Book (Executable Books Community 2020) on the theory and applications of Lagrangian descriptors (Agaoglou et al. 2020). This open-source package is the computational companion to the book.

## Acknowledgements

We acknowledge the support of EPSRC Grant No. EP/P021123/1 (CHAMPS project) and Office of Naval Research (Grant No. N00014-01-1-0769).

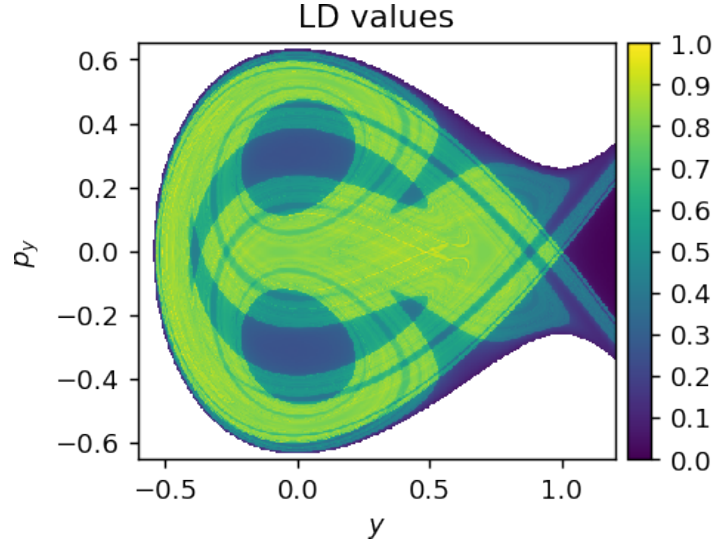


Figure 4: Lagrangian descriptor contour plot for the Hénon-Heiles Hamiltonian, using  $p = 0.5$ -quasinorm and integration time  $\tau = 15$ .

## References

- Agaoglou, M., B. Aguilar-Sanjuan, V. J. García-Garrido, F. González-Montoya, M. Katsanikas, V. Krajňák, 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. <https://doi.org/10.1142/S0218127416300366>.
- 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. <https://doi.org/10.1175/JAS-D-12-0274.1>.
- Chirikov, B. V. 1971. “Research Concerning the Theory of Non-Linear Resonance and Stochasticity [Translated at CERN by A. T. Sanders].” *CERN Trans.* 71 (40). CERN. <https://cds.cern.ch/record/325497>.
- Coulliette, C., and S. Wiggins. 2001. “Nonlinear Processes in Geophysics Intergyre transport in a wind-driven, quasigeostrophic double gyre: An application of lobe dynamics.” *Nonlinear Processes in Geophysics* 8: 69–94.
- 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. <https://doi.org/10.1103/physrevlett.115.148301>.
- . 2016. “Deconstructing Field-Induced Ketene Isomerization Through Lagrangian Descriptors.” *Physical Chemistry Chemical Physics* 18 (5). Royal Society of Chemistry: 4008–18. <https://doi.org/10.1039/C5CP06624G>.
- Craven, G. T., A. Junginger, and R. Hernandez. 2017. “Lagrangian Descriptors of Driven Chemical Reaction Manifolds.” *Physical Review E* 96 (2). APS: 022222. <https://doi.org/10.1103/PhysRevE.96.022222>.

- 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. 2009. “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>.
- Duffing, G. 1918. *Erzwungene Schwingungen Bei Veränderlicher Eigenfrequenz Und Ihre Technische Bedeutung*. Sammlung Vieweg, No 41/42. Vieweg & Sohn, Braunschweig.
- Executable Books Community. 2020. *Jupyter Book* (version v0.10). Zenodo. <https://doi.org/10.5281/zenodo.4539666>.
- 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. <https://doi.org/10.1016/j.cplett.2017.09.008>.
- 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/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. Frohnepfel, 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>.
- Henon, M., and C. Heiles. 1964. “The Applicability of the Third Integral Of Motion: Some Numerical Experiments.” *THE ASTRONOMICAL JOURNAL* 69 (1). <https://doi.org/10.1086/109234>.
- 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. <https://doi.org/10.1063/1.4997379>.

- 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/10.1016/j.cplett.2020.137199>.
- Katsanoulis, S., and G. Haller. 2018. “BarrierTool.” <https://github.com/haller-group/BarrierTool>.
- Koon, W. S., M. W. Lo, J. E. Marsden, and S. D. Ross. 2000. “Heteroclinic Connections Between Periodic Orbits and Resonance Transitions in Celestial Mechanics.” *Chaos: An Interdisciplinary Journal of Nonlinear Science* 10 (2): 427–69. <https://doi.org/10.1063/1.166509>.
- Kovacic, Ivana, and Michael J. Brennan. 2011. *The Duffing Equation: Nonlinear Oscillators and their Behaviour*. John Wiley; Sons. <https://doi.org/10.1002/9780470977859>.
- 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>.
- Lopesino, C., F. Balibrea-Iniesta, V. J. García-Garrido, S. Wiggins, and A. M. Mancho. 2017. “A Theoretical Framework for Lagrangian Descriptors.” *International Journal of Bifurcation and Chaos* 27 (01): 1730001. <https://doi.org/10.1142/S0218127417300014>.
- 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>.
- MacKay, R. S., J. D. Meiss, and I. C. Percival. 1984. “Transport in Hamiltonian Systems.” *Physica D: Nonlinear Phenomena* 13 (1-2). Elsevier: 55–81. [https://doi.org/10.1016/0167-2789\(84\)90270-7](https://doi.org/10.1016/0167-2789(84)90270-7).
- 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. <https://doi.org/10.1016/j.cnsns.2013.05.002>.
- Meiss, J. D. 1992. “Symplectic Maps, Variational Principles, and Transport.” *Rev. Mod. Phys.* 64 (3): 795–848. <https://doi.org/10.1103/RevModPhys.64.795>.
- . 2015. “Thirty Years of Turnstiles and Transport.” *Chaos* 25 (9). <https://doi.org/10.1063/1.4915831>.
- Meiss, J D. 2008. “Visual explorations of dynamics: The standard map.” 6. Vol. 70. <https://doi.org/10.1007/s12043-008-0103-3>.
- 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>.
- Nelson, D.A., and G. B Jacobs. 2016. “High-Order Visualization of Three-Dimensional Lagrangian Coherent Structures with DG-FTLE.” *Computers & Fluids* 139: 197. <https://doi.org/10.1016/j.compfluid.2016.07.007>.
- Onu, K., F. Huhn, and G. Haller. 2015. “LCS Tool: A Computational Platform for Lagrangian Coherent Structures.” *J. Comput. Sci.* 7: 26. <https://doi.org/10.1016/j.jocs.2014.12.002>.
- 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. [https://doi.org/10.1016/0167-2789\(90\)90040-V](https://doi.org/10.1016/0167-2789(90)90040-V).



- 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. <https://doi.org/10.1039/C7CP05912D>.
- Ramos, A. G., V. J. García-Garrido, A. M. Mancho, S. Wiggins, J. Coca, S. Glenn, O. Schofield, et al. 2018. “Lagrangian Coherent Structure Assisted Path Planning for Transoceanic Autonomous Underwater Vehicle Missions.” *Scientific Reports* 8: 4575. <https://doi.org/10.1038/s41598-018-23028-8>.
- 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. <https://doi.org/10.1103/PhysRevE.99.032221>.
- Rom-Kedar, V, A Leonard, and S Wiggins. 1990. “An Analytical Study of Transport, Mixing and Chaos in an Unsteady Vortical Flow.” *Journal of Fluid Mechanics* 214. Cambridge University Press: 347–94. <https://doi.org/10.1017/S0022112090000167>.
- Rom-Kedar, V., and S. Wiggins. 1990. “Transport in Two-Dimensional Maps.” *Arch. Ration. Mech. A.I.* 109 (3). <https://doi.org/10.1007/BF00375090>.
- Shadden, S. C., F. Lekien, and J. E. Marsden. 2005. “Definition and properties of Lagrangian coherent structures from finite-time Lyapunov exponents in two-dimensional aperiodic flows.” *Physica D: Nonlinear Phenomena* 212 (3-4). Elsevier: 271–304. <https://doi.org/10.1016/j.physd.2005.10.007>.
- Waalkens, H., A. Burbanks, and S. Wiggins. 2005. “Escape from Planetary Neighbourhoods.” *Monthly Notices of the Royal Astronomical Society* 361 (3): 763–75. <https://doi.org/10.1111/j.1365-2966.2005.09237.x>.
- Wiggins, S. 1994. *Normally Hyperbolic Invariant Manifolds in Dynamical Systems*. Vol. 105. Springer Science & Business Media. <https://doi.org/10.1007/978-1-4612-4312-0>.
- . 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>.
- Zhong, J., and S. D. Ross. 2020. “Geometry of Escape and Transition Dynamics in the Presence of Dissipative and Gyroscopic Forces in Two Degree of Freedom Systems.” *Communications in Nonlinear Science and Numerical Simulation* 82: 105033. <https://doi.org/10.1016/j.cnsns.2019.105033>.
- Zhong, J., L. N. Virgin, and S. D. Ross. 2018. “A Tube Dynamics Perspective Governing Stability Transitions: An Example Based on Snap-Through Buckling.” *International Journal of Mechanical Sciences* 149: 413–28. <https://doi.org/10.1016/j.ijmecsci.2017.10.040>.