LDDS: A python package for computing and visualizing Lagrangian Descriptors for Dynamical Systems

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Statement of Need

Nonlinear dynamical systems are ubiquitous in natural and engineering sciences, for example, fluid mechanics, theoretical chemistry, ship dynamics, rigid body dynamics, atomic physics, solid mechanics, condensed matter physics, mathematical biology, oceanography, meteorology, celestial mechanics (see Wiggins 1994 for a list of collated references). There has 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. 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 chemical reactions [rephrase the introduction from the CNSNS paper] or vector field defined using numerical simulation 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 be visualized along with trajectory data. The Python package, `LDDS`, serves this need for analyzing deterministic, stochastic, high-dimensional nonlinear dynamical systems described either by an analytical vector field or a trajectory data obtained from numerical simulations or experiments.

Summary

`LDDS` has the following features:

Example systems

Visualization of Lagrangian Descriptors

Relation to ongoing research projects

We are developing geometric methods of phase space transport in the context of chemical reaction dynamics that rely on identifying and computing the UPOs.

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References

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