Research highlights

Data-driven methods

[S. Naik, V. Krajnák, and S. Wiggins. Support vector machines for learning reactive islands. Chaos: An Interdisciplinary Journal of Nonlinear Science, 31(10):103101, October 2021](https://doi.org/10.1063/5.0062437)

We developed a machine learning approach based on trajectory data to discover structures in the phase space of a chemical reaction. We also verified the predictions of the learned model by comparing it with the results from dynamical systems analysis for a classical Hamiltonian. These structures, reactive islands, are pertinent for computing and understanding the structure of reactive and non-reactive trajectories and can be used to improve transition path sampling methods. Thus, this work presents a machine learning approach that leverages the phase space viewpoint of chemical reactions.

Chemical reaction dynamics

[S. Naik and S. Wiggins. Detecting reactive islands in a system-bath model of isomerization. Physical Chemistry Chemical Physics, 22(32):17890–17912, 2020](https://doi.org/10.1039/ D0CP01362E)

We discovered a significant structure in the phase space, reactive islands, of a high dimensional ($N \geq 2$ degrees of freedom) model representative of a solution-phase chemical reaction. We presented the computational method based on the Lagrangian descriptor for discovering reactive islands using a Hamiltonian model. This work also established the Hamiltonian model, derived by Robert Zwanzig (1973), as a high-dimensional deterministic model for dynamical systems analysis of solution-phase reactions. Thus, the method developed for this model lends itself to analysing the effects of a solution (or bath) on a solute using a large number of anharmonic coupling terms.

Geometric theory of escape and transition

S. Naik and S. Wiggins. Finding normally hyperbolic invariant manifolds in two and three degrees of freedom with Hénon-Heiles-type potential. Physical Review E, 100(2):022204, August 2019

We developed a computational method for finding normally hyperbolic invariant manifolds in two and three degrees of freedom Hamiltonian systems. These invariant manifolds are fundamental structures in the phase space view of a system that exhibits transition across a saddle. Instead of complete geometric construction of the structure, our method discovers pieces of this manifold which can then be used for training a machine learning or deep learning model or as a starting point for a numerical continuation algorithm. Thus, the method applies to a wide range of systems in physical sciences and engineering with dissipative and stochastic forcing.

S. D. Ross, A. E. BozorgMagham, S. Naik, and L. N. Virgin. Experimental validation of phase space conduits of transition between potential wells. Physical Review E, 98(5):052214, 2018

This work validated the theory of flux over a saddle which is relevant for computing transition or escape rate in many physical sciences and engineering systems such as chemical reaction rates, buckling failure characteristics of columns, capsize criteria for ships, asteroid capture by planets, to name but a few. We developed the physical experiment and numerical method for computing the global phase space structures, cylindrical invariant manifolds, and reactive islands associated with the index-1 saddles on a multiwell

potential energy surface. Our numerical and experimental results also showed agreement for high values of the energy above the saddle.