Prediction, Analysis, and Learning of Advective Transport in Dynamic Fluid Flows

by

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Abstract

Transport of any material quantity due to background fields, *i.e.* advective transport, in fluid dynamical systems has been a widely studied problem. It is of crucial importance in classical fluid mechanics, geophysical flows, micro and nanofluidics, and biological flows. Even though mathematical models that thoroughly describe such transport exist, the inherent nonlinearities and the high dimensionality of complex fluid systems make it very challenging to develop the capabilities to accurately compute and characterize advective material transport. We systematically study the problems of predicting, uncovering, and learning the principal features of advective material transport in this work. The specific objectives of this thesis are to: (i) develop and apply new numerical methodologies to compute the solutions of advective transport equations with minimal errors and theoretical guarantees, (ii) propose and theoretically investigate novel criteria to detect sets of fluid parcels that remain the most coherent / incoherent throughout an extended time interval to quantify fluid mixing, and (iii) extend and develop new machine learning methods to infer and predict the transport features, given snapshot data about passive and active material transport.

The first part of this work deals with the development of the PDE-based 'method of flow map composition', which is a novel methodology to compute the solutions of the partial differential equation describing classical advective and advective–diffusive–reactive transport. The method of composition yields solutions almost devoid of numerical errors, and is readily parallelizable. It can compute more accurate solutions in less time than traditional numerical methods. We also complete a comprehensive theoretical analysis and analytically obtain the value of the numerical timestep that minimizes the net error. The method of flow map composition is extensively benchmarked and its applications are demonstrated in several analytical flow fields and realistic data-assimilative ocean plume simulations.

We then utilize the method of flow map composition to analyze Lagrangian material coherence in dynamic open domains. We develop new theory and schemes to efficiently predict the sets of fluid parcels that either remain the most or the least coherent over an extended amount of time. We also prove that these material sets are the ones to maximally resist advective stretching and diffusive transport. Thus, they are of significant importance in understanding the dynamics of fluid mixing and form the skeleton of material transport in unsteady fluid systems. The developed theory and numerical methods are utilized to analyze Lagrangian coherence in analytical and realistic scenarios. We emphasize realistic marine flows with multiple time-dependent inlets and outlets, and demonstrate applications in diverse dynamical regimes and several open ocean regions.

The final part of this work investigates the machine inference and prediction of the principal transport features from snapshot data about the transport of some material quantity. Our goals include machine learning the underlying advective transport features, coherent / incoherent sets, and attracting and repelling manifolds, given the snapshots of advective and advective–diffusive material fields. We also infer and predict high resolution transport features by optimally combining coarse resolution snapshot data with localized high resolution trajectory data. To achieve these goals, we use and extend recurrent neural networks, including a combination of long short-term memory networks with hypernetworks. We develop methods that leverage our knowledge of the physical system in the design and architecture of the neural network and enforce the known constraints that the results must satisfy (e.g. mass conservation) in the training loss function. This allows us to train the networks only with partial supervision, without samples of the expected output fields, and still infer and predict physically consistent quantities. The developed theory, methods, and computational software are analyzed, validated, and applied to a variety of analytical and realistic fluid flows, including high-resolution ocean transports in the Western Mediterranean Sea.

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