Proceedings of the 1st international Symposium on AI and Fluid Mechanics
Abstract No S18 A2

Reliable Collision Predictions in Chaotic Flows with Sequence-to-Sequence Models

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Abstract

Predicting particle collisions in turbulence remains a challenging task due to the highly non-linear and unpredictable nature of turbulent flows. However, generating turbulence data for such predictions is computationally expensive. In this work, we address this challenge by using H. Aref's chaotic advection model as a surrogate for turbulence. Chaotic advection exhibits similar non-linear and sensitive behavior to initial conditions, where small differences lead to completely different particle trajectories, making it a suitable alternative for testing predictive models.

To capture the spatial and temporal relationships inherent in particle movements, we employ a sequence-to-sequence (seq2seq) machine learning model. This model is particularly well-suited for learning sequential dependencies, enabling it to predict particle collisions in complex, non-linear systems. Prior to this, we established a baseline using a simple Multi-Layer Perceptron (MLP) model, which performed poorly due to its inability to capture the temporal dynamics of particle trajectories.

One of the primary challenges in this task is the highly imbalanced nature of the dataset, where collision events are significantly rarer than non-collision events. To address this, we apply the SMOTEENN method, which generates synthetic collision samples to balance the data while removing noisy and redundant points to improve data quality.

The proposed approach aims to demonstrate the feasibility of seq2seq models in predicting particle collisions within chaotic advection flows, serving as a step toward reducing the computational cost of such predictions. By achieving accurate predictions with fewer calculations, this work has the potential to advance applications in industrial mixing, environmental pollutant dispersion, and fluidic device optimization.

Keywords: Seq2Seq, Particle Collision Prediction, Chaotic Advection