Physics-based data-driven modeling and uncertainty quantification in computational science and engineering
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STATE-DEPENDENT UNCERTAINTY IN FLOW-INDUCED POLYMER UNFOLDING DYNAMICS

Saugat Upreti[*1], Sruthi Chengalrayan[1] and Mustafa Usta[1]*

[1]Cleveland State University

ABSTRACT

Dilute polymer suspensions interacting with hydrodynamic shear flow exhibit complex, highly nonlinear conformational dynamics arising from the interplay between flow-induced forces, internal structural constraints governing advection and reeling, and stochastic perturbations. Under shear flow, long-chain polymers undergo repeated folding, rolling, and unfolding events, giving rise to a rich spectrum of conformational states. These conformations play a critical role in determining polymer function, as folding and unfolding behavior directly influence biomechanical and biochemical activity. However, conventional scalar descriptors such as instantaneous extension length and radius of gyration are often insufficient to distinguish these states or to predict subsequent dynamical outcomes, particularly in regimes where similar global measures correspond to qualitatively different behaviors.

In this work, we leverage large-scale, physics-based direct numerical simulations of polymer–fluid interactions to generate extensive ensembles of high-dimensional, time-resolved polymer configurations. To systematically organize this complex data, polymer conformations are represented as graphs and analyzed using unsupervised, data-driven representation learning with autoencoder–decoder architectures and attention-based pooling. This approach yields low-dimensional latent embeddings that preserve essential structural and topological features, enabling consistent identification of physically meaningful conformational states, including coiled, partially extended, protruded, and extended configurations. Uncertainty is characterized by conditioning polymer extension outcomes on learned conformational states, revealing intrinsic uncertainty in the dynamical evolution of polymers under shear flow. In particular, minimum-extension (globular) configurations are identified as metastable decision states from which polymers may evolve toward distinct macroscopic outcomes. By analyzing probability distributions of extension outcomes conditioned on state, we characterize the likelihood and range of possible extensions. This enables us to distinguish conformational states that deterministically suppress large extension and exhibit low intrinsic uncertainty from states that admit multiple competing outcomes and therefore exhibit high intrinsic uncertainty. These results illustrate how physics-based simulation ensembles can be mined to distinguish deterministic and stochastic regimes in complex flow-driven polymer dynamics.