Learning Non-Equilibrium Dynamics of Polymer Chains: A Data-Driven Approach

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1. Introduction

We present a data-driven approach for the study of dynamical systems away from equilibrium. Using the stretching of individual polymer chains as a case study, we demonstrate the capability of this approach in learning and predicting the stochastic, non-equilibrium dynamics. Furthermore, it enables the construction of a set of reduced coordinates which are found to be physically interpretable, i.e. they are related to measurable physical variables. For a fixed temperature and flow strength, we can construct an energy landscape on the reduced coordinates, and find the stationary points of the system. We extend this approach to learn dynamics under varied flow strengths and temperatures, and use this to construct an evolving free energy landscape and phase transitions.

2. Methodology and Results

Understanding the non-equilibrium dynamics of complex systems is an active area of research within a range of fields – from nanotechnology [1] to weather prediction [2]. Differential equations and microscopic simulations are commonly used to describe the behavior of such systems, but solving them numerically becomes computationally intractable as the number of variables increases. Data-driven approaches have been proposed as a means of addressing this challenge, based on their ability to learn from large sets of variables. However, most models developed are black-box, trading short term predictive accuracy for stability and interpretability [3]. Since our aim is to provide meaningful insights into the dynamics of systems away from equilibrium, we chose to follow the data-driven approaches that leverage physical insights to design model architectures which have been shown to provide better interpretability and long-term predictive accuracy [3,4].

Our data-driven approach leverages the generalized Onsager principle [5] to learn macroscopic dynamical descriptions of complex stochastic dissipative systems influenced by varying external parameters. The approach simultaneously constructs reduced thermodynamic coordinates and interprets dynamics on these coordinates, addressing challenges of complexity and size that arise when constructing equations of state. The approach is applied to the problem of polymer stretching under elongational flow. We are interested specifically in the unfolding of DNA molecules because of the growing use of DNA in nanotechnology, including in the field of soft programmable materials, yet, understanding and controlling the deformation of DNA under external forces remains a challenge. Our results show that the approach is capable of identifying stable states and meta-stable states, as well as predicting statistics of unfolding accurately for a specific temperature and flow rate. The logical progression involves assessing the ability of the approach to generalize to varying conditions, such as different temperatures and flow strengths, in order to define a more comprehensive equation of state.

To achieve this, we extended the model to incorporate elongational flow strength and temperature, and generated a series of stretching trajectories for varied forces and temperatures. The objective is to ensure that the thermodynamic coordinates remain interpretable and that the energy landscape accurately reflects the stable and meta-stable states associated with each condition.

In conclusion, we were able to demonstrate that the approach can be extended to incorporate varying forces with minimal loss of predictive accuracy, and capture the energy landscape evolution, including changes in stable states and meta-stable states. Integrating the approach into the control feedback system of a high-throughput single molecule platform could enable both a better understanding of such systems and enhanced control capabilities of the platform.

References

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