Generative Networks for Re-inserting Atomic detail in Coarse-grained Multi-component Macromolecules

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Abstract

Despite the modern advances of the available computational resources, the length and time scales of the physical systems that can be studied in full atomic detail, via molecular simulations, are still limited. To overcome such limitations mathematical methods to reduce the dimensionality of the physical system under study are necessary. The most common technique to tackle this task is by developing systematic coarse-grained (CG) models for chemically-specific systems [1-2]. CG models have found practical applications in simulations of long entangled macromolecular systems. Restoring the atomistic detail from the CG description requires us to produce information from the physics and statistics of the system at the two representations considered. The methods proposed so far balance among accuracy, efficiency and general applicability [3-5]. Here, we introduce an efficient and versatile method for backmapping multi-component CG macro-molecules. By utilizing deep learning algorithms, we train a convolutional neural network to learn structural correlations (probability distribution functions) between polymer configurations at the atomistic and corresponding CG scales, obtained from atomistic simulations. The trained model was then utilized to get predictions of atomistic structures from input CG configurations. As an illustrative example we apply the new generative networks to polybutadiene copolymers of various microstructures, in which each monomer microstructure (i.e, *cis*-1,4, *trans*-1,4, and *vinyl*-1,2) is represented as a different CG particle type. Moreover, to examine the chemical transferability of the proposed method we modify the chemistry (CG particle types) of the input CG configurations, thus creating a set of well equilibrated polymer configurations of different microstructures (chemistry) than the one of the original CG configuration.

Keywords: Machine learning, Multi-scale modeling, Backmapping, Polybutadiene, Structural correlations

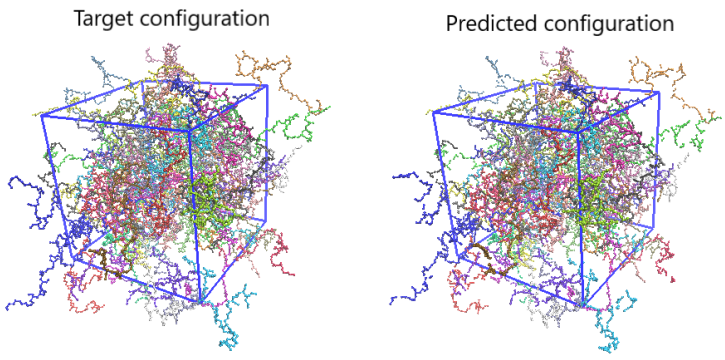

Figure 1: Target and predicted configurations of the UA model (polymer chains are unwrapped in the periodic simulation box and colored differently for visualization)

Acknowledgments

This work was supported by European Union's Horizon 2020 research and innovation program under grant agreement No810660.

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