COARSE GRAINED MOLECULAR SIMULATIONS FACILITATED BY MACHINE LEARNING

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ABSTRACT

Molecular simulation is a powerful tool to investigate at the microscopic level the properties of complex chemical systems and understand the mechanistic aspects that underly materials properties at different operating conditions. In particular, coarse-grained (CG) molecular simulations allow to surpass the limitations of classical molecular dynamics in terms of length and time scales, enabling the exploration of a wider range of physical properties and phenomena.

Polymeric systems are one important category of complex materials of great technological importance and are particularly challenging to simulate. Due to the wide range of timescales that are present in these systems hierarchical multiscale strategies are required, that are usually elaborate and system-specific [1-3]. These schemes could be generalized and streamlined by the application of Machine Learning (ML) methods. Machine learning is having increasing impact in the physical sciences, engineering and technology, addressing research problems that range from molecular reaction mechanisms to high-throughput screening of functional materials.

A main advantage of ML models in the context of molecular simulations is that they are not constrained to a predefined mathematical function, therefore they are endowed with higher flexibility and expressive character compared to traditional CG models. Recently, neural networks have shown great promise in the development of improved atomistic force fields, trained on quantum mechanical calculations [4]. On the other hand, the implementation of ML for the generation of CG mapping models [5] or force fields [2,3] on the basis of atomistic simulations is a less explored topic.

In this work, we investigate the use of ML schemes in the construction of CG mapping models and the utilization of neural networks to create optimized CG force fields, using suitable descriptors for the local environment. The structural and thermodynamic properties of the CG systems simulated with a Neural Network potential were systematically compared with the underlying atomistic gold standard. The artificial intelligence aided multi-scale approach proposed constitutes a generalized methodology for the efficient computational study of complex systems, bringing this challenging problem within computational reach. This is a stepping stone towards the rational design of advanced processes from the molecular level all the way up to industrial applications.

KEYWORDS: Multiscale Modelling, Molecular Simulations, Machine Learning, Neural Networks

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