Learning Physical Interactions for Molecular Dynamics Simulations

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July 18, 2024
66-110
9:00 - 10:30 AM

From simple clustering techniques to sophisticated neural networks, the use of machine learning has become a valuable tool in many fields of chemistry in the past decades. Here, we describe different ways in which we explore the use of machine learning (ML) to predict physical interactions between particles in molecular dynamics (MD) simulations in order to improve their accuracy. In classical MD simulations, the physical interactions between atoms are described with an empirical force field. This involves a large number of parameters for each molecule, which are fitted to quantum-mechanical (QM) or available experimental data. There is a need for more accurate and general force fields. In this context, we demonstrate how ML approaches can aid in force-field development, from multipole prediction to generalized parametrization. In addition, we explore the use of ML for increasing the speed and accuracy of QM/MM MD simulations, and for improving implicit solvent models to reproduce local effects of explicit solvent molecules.

Sereina Riniker is currently Associate Professor of Computational Chemistry at the Department of Chemistry and Applied Biosciences in ETH Zurich. She received her Master's degree in chemistry and PhD in molecular dynamics simulations from ETH Zurich. From 2012 to 2014, she held a postdoctoral position in cheminformatics at the Novartis Institutes for BioMedical Research in Basel and Cambridge, Massachusetts. In 2014 she returned to ETH Zurich as Assistant Professor with Tenure Track , and was promoted to her current position in April 2020.