Learning physical interactions for molecular dynamics simulations

Sereina Riniker

ETH Zürich, Department of Chemistry and Applied Biosciences,
HCI G225, Vladimir-Prelog-Weg 2, 8093 Zürich
sriniker@ethz.ch

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) for 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.