

We introduce a few deep learning based methods that allow us to boost ab-initio molecular dynamics simulations without loss of accuracy. We discuss this topic in two aspects: model construction and data exploration. In terms of model construction, we introduce the Deep Potential Molecular Dynamics (DPMD) scheme based on a potential energy surface (PES) and interatomic forces generated by a carefully crafted deep neural network trained with ab-initio data. In terms of data exploration, we show an active learning procedure called Deep Potential Generator (DP-GEN), which has three major components: exploration, labeling, and training. We show that the proposed schemes provides an efficient and accurate protocol for a variety of systems. As an important application, we generate an ab-initio trained reactive force field for water that describes both the molecular and the dissociated water and ice phases in a wide range of thermodynamic conditions.