Recent Application of Machine Learning Force Field: Beyond Simple Molecular Dynamics Simulation

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Molecular Dynamics (MD) is a computational scientific tool that tracks the movement of atoms. The underlying physical interactions are obtained from force fields, which are sets of functional forms and parameters representing physical interactions between atoms. However, as evidenced by the existence of multiple force fields, determining the appropriate functional forms and parameters is non-trivial. Machine learning force fields (MLFFs) are an approach that delegates this task to neural networks. Since the early development of MLFFs in the late 2000s, there has been explosive growth in their development and use across physics, chemistry, and engineering. As demonstrated in extensive validation studies ranging from simple liquids and molecules to high-entropy alloys and biomolecules, MLFFs can serve as excellent substitutes for highly sophisticated first-principle calculations, such as density functional theory (DFT), at greatly reduced computational cost.

Recent interest has shifted towards exploring the discoveries and value MLFFs bring to atomic and molecular science beyond simple proof of concept. In this talk, I will start by briefly introducing popular MLFFs and some of the recent discoveries enabled by their use. Next, I will discuss the current limitations of MLFFs and how they can be circumvented through advanced molecular dynamics technique.