Modeling the interatomic potential by deep learning

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In silico design of materials requires an accurate description of the interatomic potential energy surface (PES). However, in the context of molecular simulation, one usually faces the dilemma that the first principle PESs are accurate but computationally expensive, while the empirical PESs (force fields) are efficient but of limited accuracy. We discuss the solution in two aspects: PES construction and data generation. In terms of PES construction, we introduce the Deep Potential (DP) method, which faithfully represents the first principles PESs by a symmetry-preserving deep neural network. In terms of data generation, we present a concurrent learning scheme named Deep Potential Generator (DP-GEN). This approach automatically generates the most compact training dataset that enables the training of DP with uniform accuracy. In the last part of the talk, we present the attempt of implementation and optimization of DP on a heterogeneous high-performance supercomputer Summit, by which one can simulate more than 1 nanosecond-long molecular dynamics trajectory of over 100 million atoms per day.