Building a New Generation of Multiscale Materials Models with Machine-Learned Interatomic Potentials

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ABSTRACT

Applying the techniques of machine learning to multiscale simulation has led to a revolution in atomistic materials modeling. Machine-learned interatomic potentials (MLIAPs) connect highly accurate but computationally expensive quantum modeling techniques with lower fidelity but fast classical molecular dynamics (MD) models. In other words, MLIAPs allow MD simulations to achieve quantum accuracy at unprecedented system sizes and time scales. These developments, coupled with advances in high-performance computing, open exiting new opportunities to incorporate accurate atomistic insights into higher length scale methods.

In addition to providing accuracy, MLIAPs also offer enormous flexibility in the choice of model form, descriptor type, and training set construction, enabling the modeling of new classes of materials and their behavior. However, traditional problems in machine learning regarding retaining accuracy while extrapolating remain. This talk will overview our working group's strategies in addressing those problems in developing MLIAPs for large-scale simulations of complex materials systems, where model performance cannot always be measured using traditional metrics.