数学与系统科学研究院

计算数学所学术报告

报告人：　　王涵 副研究员

（ 北京计算数学与应用物理研究所 ）

报告题目：

Modeling the interatomic potential by deep learning

邀请人：张硕 副研究员

报告时间：**2020** 年 **12** 月 **16** 日（周三）

上午 **10:00-11:00**

报告地点：科技综合楼

311 教室

摘要：

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 principle PES by a symmetry-preserving deep neural network. In terms of data generation we present a new 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. By contrast to the empirical PESs the DP-GEN opens the opportunity of continuously improving the quality of DP by exploring the chemical and configurational space of the system. We briefly introduce the open-source implementations of DP and DP-GEN and then debut the DP library that provides the platform for openly sharing DP models and data in the community. In the last part of the talk we briefly introduce the optimization of DeePMD-kit on Summit supercomputer which wins the 2020 ACM Gordon Bell prize for its unprecedented power of simulating 100M atoms with the first-principle accuracy in one day.

欢迎大家参加！