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The Hong Kong University of Science and Technology

Department of Mathematics

Seminar on Applied Mathematics and Machine Learning

Learning assisted modeling of molecules and materials

by

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Abstract

In recent years, machine learning (ML) has emerged as a promising tool for dealing with the difficulty of representing high dimensional functions. This gives us an unprecedented opportunity to revisit theoretical foundations of various scientific fields and solve problems that were too complicated for conventional approaches to address. Here we identify a list of such problems in the context of multi-scale molecular and materials modeling and review ML-based strategies that boost simulations with *ab initio* accuracy to much larger scales than conventional approaches. Using examples at scales of many-electron Schrödinger equation, density functional theory, and molecular dynamics, we present two equally important principles: 1) ML-based models should respect important physical constraints in a faithful and adaptive way; 2) to build truly reliable models, efficient algorithms are needed to explore relevant physical space and construct optimal training data sets. Finally, we present our efforts on developing related software packages and high-performance computing schemes, which have now been widely used worldwide by experts and practitioners in the molecular and materials simulation community.

Biography:

Linfeng Zhang is temporarily working as a research scientist at the Beijing Institute of Big Data Research. In the May of 2020, he graduated from the Program in Applied and Computational Mathematics (PACM), Princeton University, working with Profs. Roberto Car and Weinan E. Linfeng has been focusing on developing machine learning based physical models for electronic structures, molecular dynamics, as well as enhanced sampling. He is one of the main developers of DeePMD-kit, a very popular deep learning based open-source software for molecular simulation in physics, chemistry, and materials science. He is a recipient of the 2020 ACM Gordon Bell Prize for their project, "Pushing the limit of molecular dynamics with *ab initio* accuracy to 100 million atoms with machine learning."

Date : 2 December 2020 (Wednesday)

Time : 3:00pm – 4:30pm

Zoom Meeting : https://hkust.zoom.us/j/98248767613 **(Passcode: math6380p)**

All are Welcome!