The 689th

MANA & GREEN

The 78th

The 12th Joint Seminar

(*Co-organised by MEXT Fugaku Battery & Fuel Cell Project*)

On-the-fly machine-learned inter-atomic potentials

Chair: Dr. Yoshitaka TATEYAMA (MANA PI / Deputy Director, GREEN)

Dr. Ryosuke Jinnouchi

(Toyota Central R&D Labs., Inc., Japan)

First principles molecular dynamics (FPMD) is a powerful method to predict properties of a wide variety of materials. However, predicting finite-temperature properties of complex systems is still challenging because of its limitations in time- and length-scales. Empirical interatomic potentials can extend the applicability of MD simulations, but their constructions always need a lot of human interventions, and constructed potentials often suffer from significant errors. Machine learned interatomic potential (MLP) is a promising method to solve the problems. Flexible functional forms of MLPs allow to accurately reproduce FP potential energy surfaces, and recently emerging active-learning schemes enable efficient constructions of MLPs. In this presentation, We present an active-learning scheme constructing MLPs on the fly during FPMD simulations [1,2]. Similarly to other MLP schemes [3,4,5], structures that appear during the MD simulations are mapped onto descriptors [6,7] representing atomic distributions, and the potential energy is described as a function of the descriptors. Bayesian inference provides a framework to estimate uncertainty in energies and forces predicted by the MLP. The estimation allows the machine to judge whether the predicted results can be used to update atomic positions in solving equation of motion or not. Only when the machine judges that the MLP is inaccurate, FP calculations are carried out. The obtained FPMD data is incorporated in the training dataset and is used to update the MLP. The MLP scheme has been successfully applied to predicting liquid-solid phase transitions [1], solid-solid phase transitions [8, 9, 10], thermal conductivity [10], and hydration free energies of ions and adsorbates [11,12]. After presenting these application examples, We present remained challenges in present MLP schemes particularly in applications to heterogeneous systems. Required improvements in the MLP scheme will be discussed.

Venue: Auditorium, 1F, WPI-MANA Bldg., Namiki-site / Zoom (Hybrid)

Date: November 26th, Friday Time: 13:30-14:30

Registration for both on-site & on-line: https://forms.gle/W11hP951K59ebHSE8

(*Registration Deadline: Evening on 25th November)

Contact: International Center for Materials Nanoarchitectonics (MANA) & Dr. Y. Tateyama at TATEYAMA.Yoshitaka -at- nims.go.jp