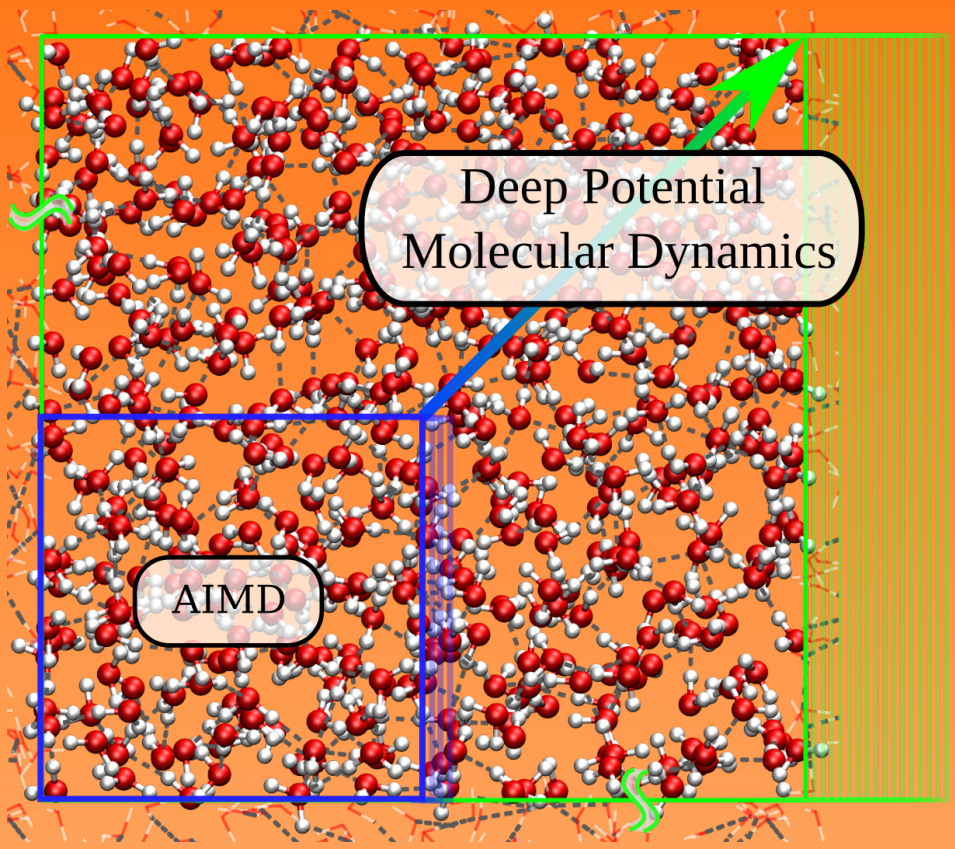
Molecular Simulation with Machine Learning

Online Workshop, July 13-14, 2020



Speakers (tentative)

S. Baroni (SiSSA)
M. Bokdam (U. Vienna)
M. Ceriotti (EPFL)
R. DiStasio (Cornell)
W. E (Princeton)
M. Fernandez-Serra (SUNY)
G. Grest (Sandia)
J. M. Martirez (UCLA)
T. Kuhne (U. Paderborn)
P. Piaggi (Princeton)

Schedule

Invited talks: 9 am – 12 pm
Hands-on: 2 pm – 5:30 pm

A two-day **virtual** workshop covering theory and hands-on tutorials on the software package for molecular simulation with machine learning (ML) tools developed at the Computational Chemical Science Center "Chemistry in Solution and at Interfaces"(http://chemlabs.princeton.edu/ccsc/). The package includes codes to construct and use deep neural network models of the potential energy surface and electronic properties of multi-atomic systems that reproduce the results of electronic density functional theory.

ML codes need interfacing with community codes for electronic structure and *ab-initio* simulation, classical molecular dynamics, path-integral molecular dynamics, and enhanced sampling of rare events. The workshop will promote discussions on how to better achieve code integration within the molecular simulation community across disciplines ranging from physical chemistry to condensed matter physics and materials science. The workshop will include general presentations, panel discussions, and tutorial sessions.

Registration is free. A registration form, available on the workshop webpage at http://chemlabs.princeton.edu/csi2020/ should be completed by the **deadline of June 26, 2020**. Only a maximum of 50 registered participants will be admitted to the tutorial sessions. Information on admissions and use of cloud computer resources will be provided by July 5, 2020.

Contact information:

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