Subramanian Sankaranarayanan
Center for Nanoscale Materials, Nanoscale Science and Technology Division
Argonne National Lab
Institute of Molecular Engineering, University of Chicago.

"Accelerating Materials Discovery and Design using AI and Machine Learning."

Abstract: The ever-increasing power of modern supercomputers, along with the availability of highly scalable atomistic simulation codes, has begun to revolutionize predictive modeling of materials. Molecular dynamics (MD), in particular, has led to breakthrough advances in diverse fields, including tribology, energy storage, catalysis, sensing. Furthermore, recent integration of MD simulations with X-ray characterization has demonstrated promise in real-time 3-D atomistic characterization of materials. The popularity of MD is driven by its applicability at disparate length/time-scales, ranging from *ab initio*MD (hundreds of atoms and tens of picoseconds) to all-atom classical MD (millions of atoms and tens of nanoseconds), and coarse-grained (CG) models (microns and tens of micro-seconds). Nevertheless, a substantial gap persists between AIMD, which is highly accurate but restricted to extremely small sizes, and those based on classical force fields (atomistic and CG) with limited accuracy but access to larger length/time scales. The accuracy and predictive power of classical MD is dictated by the empirical force fields, and their capability to capture the relevant physics.

In this talk, I will present some of our recent work on the use of machine learning (ML) to seamlessly bridge the electronic, atomistic and mesoscopic scales for materials modeling. Our automated ML framework aims to bridge the significant gulf that exists between the handful of research groups that develop new interatomic potential models (often requiring several years of effort) and the increasingly large user community from academia and industry that applies these models. Our ML approach showed marked success in developing force fields for a wide range of materials from metals, oxides, nitrides, hetero-interfaces to two-dimensional (2-D) materials and even water (arguably the most difficult system to capture from a molecular perspective). This talk will also briefly discuss our ongoing efforts to integrate such cheap yet accurate atomistic models with (a) AI techniques to perform inverse design and construct metastable phase diagrams of materials (b) Deep learning to improve spatiotemporal resolutions of ultrafast X-ray imaging.