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2. CASUS Annual Workshop

Fusing Artificial Intelligence & Simulation

A Path to the Exascale for Atomistic Simulations with Improved Accuracy, Length and Time Scales

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Date: 6 October 2020

Time: 5 p.m. CEST

Location: livestream link follows

Abstract:

"With exascale super computers arriving in the near future, it is timely to ask whether our simulation software is capable of matching this unprecedented computing capability. While many research challenges in material physics, chemistry and biology lie just out of reach on peta-scale machines due to length and time restrictions inherent to Molecular Dynamics(MD), questions of the accuracy of our simulations will continue to linger. Simply running the same peta-scale simulations with more atoms on a larger computer (weak scaling) does not advance the accessible timescales, nor does it avoid the pitfalls of empirically developed constitutive models. This talk will overview the U.S. Department of Energy* EXAALT (EXascale Atomistics for Accuracy, Length and Time) project and our efforts to provide software tools for MD that not only scale efficiently to huge atom counts, but also enable efficient MD simulations for smaller systems too. New parallel time-acceleration methods such as sublattice-ParSplice and local hyperdynamics have been developed along with quantum accurate machine learned interatomic potentials to study damage accumulation in plasma facing materials.

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Biography:

Mitchell Wood is currently a Senior Member of the Technical Staff in the Center for Computing Research at Sandia National Labs. He earned a Ph.D. In material science and engineering from Purdue University in 2016 and a B.S. in physics from Michigan State University in 2011. His research efforts focus on the application of high performance computing for the study of material at extremes such as shock compression and radiation damage. Parallel efforts to this research topic include employing machine learning tools to provide a link between ab initio and classical atomistic simulations. He is also an active developer on the LAMMPS molecular dynamics (lammps.sandia.gov) and FitSNAP (github.com/FitSNAP/FitSNAP) open source software projects