SHOCK19-2019-000346
Abstract for an Invited Paper
for the SHOCK19 Meeting of
the American Physical Society

Molecular Dynamics Simulation: Engine of Discovery or Bridge to Nowhere?[1]

AIDAN THOMPSON, Sandia National Laboratories

Molecular dynamics (MD) is a powerful atomistic simulation tool for exploring the microscopic behavior of a wide variety of condensed matter systems by tracking the motion of large collections of atoms over millions of timesteps. It can be viewed as a bridge connecting macroscopic models based on continuum mechanics to rigorous quantum electronic structure calculations. Continuum mechanics simulations can describe complex phenomena and behaviors using macroscopic material models for things like viscosity, strength, and rates of reaction. They do not have the ability to explain the atomic-scale origins of these phenomena or to make predictions about new materials or physical conditions. Quantum methods can make very accurate predictions, but only for collections of atoms (100's) and spans of time (picoseconds) that are too small to be broadly useful. In MD, we simply replace the quantum mechanics with a classical interatomic potential (IAP) that expresses the total energy of the quantum system as a sum of contributions from atoms, bonds, etc. This greatly reduces the computational cost of classical MD relative to quantum methods. It also scales efficiently on parallel computers, so that large MD simulations can be distributed over thousands or millions of processors. This enables unique opportunities to validate and improve continuum models by direct comparison with atomistic simulation. However, the accuracy of these simulations is still limited by the quality of the IAP. This has lead to the development of increasingly more complex and computationally expensive IAPs that provide accurate descriptions of real materials. Moreover, because of the vast difference between the atomic and macroscopic scales there is an insatiable demand for bigger and longer simulations. So MD is constantly being pushed in three directions at once: accuracy, length, and time. In this talk, I will provide an overview of the molecular dynamics method, highlighting some recent developments in Sandia's LAMMPS code. I will then describe ongoing work in two areas (i) large-scale molecular dynamics simulation of chemical energy release in explosive crystals under shock loading (ReaxFF) (ii) automated generation of high-accuracy machine-learning IAPs using very large data sets of quantum calculations (SNAP). We have applied SNAP to a variety of complex material systems, including plasticity in tantalum, plasma-surface interactions in tungsten/beryllium bimetallic materials, and radiation damage in III-V semiconductors.

[1]Supported by the Laboratory Directed Research and Development program at Sandia National Laboratories, a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.