LAMMPS and Classical Molecular Dynamics for Materials Modeling

Steve Plimpton, Sandia National Labs

Abstract

LAMMPS is molecular dynamics (MD) code primarily used for modeling materials. In this talk I'll discuss areas of active research where many MD codes, including LAMMPS, are working to improve and extend. I'll illustrate with some recent successes we have had in developing quantum-accurate potentials and coarse-graining to extend the length and time scales accessible to classical MD. I'll also discuss the end-of-Moore's Law challenge all HPC simulation codes are facing, and how we are adapting LAMMPS for the changing HPC hardware landscape.