Course Announcement for Spring 2016

Modeling and Simulation in Materials Science and Engineering: Classical Mechanics

MSE 614

Instructor: David J. Keffer
T&Th 3:40 - 4:55 pm in Ferris Hall

Simulation & Modeling has become the third pillar of modern research, able to provide unique and complementary insights when used in tandem with theory and experiment. One particularly pervasive type of simulation is "molecular dynamics" (MD), in which classical mechanics is used to describe the distribution and evolution of atomic coordinates in space and time. Classical simulation is the investigative tool of choice for resolving hypotheses regarding atomic-level mechanisms in complex materials in which the simulation of between 10^5 and 10^9 atoms is required to capture the phenomena of interest. These systems are too large to be explored with quantum mechanics but too small to be described by continuum models. The results of MD simulations are typically a fundamental, physics-based understanding of structure/property relationships in materials.

The goal of this course is to introduce and to apply classical modeling and simulation of advanced materials at atomic and mesoscale levels of description. The first part of the course is lecture-based, providing a fundamental understanding of the theory underlying MD and its relationship to finer and coarser simulation techniques. The remainder of the course is project based, in which students bring a system of interest from their research to be studied. The software to be used is LAMMPS, the current industry standard for MD simulation. Students will be given accounts on Newton and/or Titan (through NICS) for the class. Specific topics to be covered include (i) basic execution of LAMMPS, (ii) initial model building, and (iii) post-processing analysis of LAMMPS output files to obtain thermodynamic (e.g. heat capacities) and transport properties (e.g. diffusivities).

This course will satisfy a "domain science" requirement of the Interdisciplinary Graduate Minor in Computational Science. This course is entirely different from MSE 613: Modeling and Simulation in MSE: Quantum Mechanics, which focuses on first principles techniques. MSE 613 is not a prerequisite for MSE 614.

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Course website: http://utkstair.org/clausius/docs/mse614/index.html