Poster Session

Modeling and Simulation in Materials Science and Engineering: Classical Mechanics

MSE 614

Instructor: David J. Keffer

Thursday 3:45 pm in Ferris Hall Rooms 510 & 501

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.

In Spring semester, 2016, twenty-eight graduate students from seven departments and programs (CBE, CEE, Chem, CIRE, MABE, MSE, and NE) at UT enrolled in this class. Each student is presenting the results of their final project for the course as a poster during this poster session. The session is open to the public. In fact, there will be two "Best Poster" competitions—the first based on a tally of votes of the enrolled students and the second based on votes of the members of the public in attendance. Poster winners receive an "A" on the poster component of the final project grade for MSE 614.

At the poster sessions for the midterm project, the breadth of work done and the depth of the analysis displayed in the posters was incredible. Come and support the work of these industrious students. See how, in the course of a semester, students can learn a modern simulation tools (LAMMPS) and use it to investigate structure-property relationships at the atomic level. Prepare to be impressed!

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