MSE 614 Course Syllabus

A. Course Details

MSE 614 Modeling & Simulation in Materials Science & Engineering: Classical Mechanics

Meeting Place: Room TBD, Ferris Hall
Meeting Time: Tuesday & Thursday at 3:40-4:55

Instructor: Prof. David Keffer, room 301 Ferris Hall, dkeffer@utk.edu
Teaching Assistant: None

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

Required Text: None.

Reference Texts: http://utkstair.org/clausius/docs/mse614/text/references.html

Catalog Description:

- 3 credit hours
- Introduction to and applications of classical modeling and simulation of advanced materials at atomic and mesoscale levels of description. Development of structure/property relationships for functional, structural, and energy materials.

Registration Restriction(s): Minimum student level – graduate.
Registration Permission: Consent of instructor.

Prerequisites: None.
Note: This course is entirely different from MSE 613: Modeling and Simulation in MSE: Quantum Mechanics, which focuses on first principles techniques and which has been taught by Prof. Haixuan Xu. MSE 613 is not a prerequisite for MSE 614. The courses are complementary and both can be taken for credit in any order.

B. Course Philosophy:

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 105 and 109 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.

C. Course Objective:

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).

D. Grading Policy

D.1. Grade Breakdown

The course grade is based on four homeworks and two projects. The first project is chosen in consultation with the instructor and is designed to use MD to reproduce a result in the literature. The project includes a formal, written report, including a review of the relevant literature and an oral or poster presentation, depending upon the number of students enrolled. The second project is chosen by the student on a topic of research interest. This project also includes a formal, written report and a presentation of results. Both projects are worth 40% of the grade. The homeworks are each worth 5% of the grade.

D.2. Course Grades

Course grades will be assigned on the following basis.

A: A grade of "A" signifies that the student attended class, participated in discussion and successfully completed the technical, written and presentation requirements of both projects and the homework assignments.

B: A grade of "B" signifies that the student participated significantly and had some partial degree of success in completion of the projects and the homework assignments.

C: A grade of "C" signifies that the student failed to put forth the effort to participate in class and had minimal success in one or both projects and the homework assignments.

E. Getting Help

When you do not understand something in class or have difficulty with a concept, you are encouraged to seek out the instructor. Extra-effort will be made to meet with students who regularly attend lecture.

E.1. Email

The best way to contact the instructor is via email.

- Questions regarding the course should be sent via email to the Instructor.

- To guarantee that the email is read promptly, make the subject of the email "MSE 614" Emails with the subject "Help Me!" or similar subjects are identified as spam and deleted without being opened.

E.2. Office Hours

- The office hours for this course will be determined.

F. Course Schedule:

The schedule for this course is provided in a separate document located at

http://utkstair.org/clausius/docs/mse614/pdf/schedule.pdf