MEEG 5343 – Computational Materials Science
Spring 2014

Dr. Douglas Spearot, NANO 213, 575-3040, dspearot@uark.edu

Lecture
Monday / Wednesday / Friday, 3:05 – 3:55 pm, MEEG 217

Office Hours
Monday / Wednesday / Friday, 4:00 – 5:00 pm, NANO 213

Text
Required: *Introduction to Computational Materials Science*, LeSar, 2013.
Required: Relevant journal papers will be distributed via Blackboard.
Optional: *Computer Simulation of Liquids*, Allen and Tildesley, 1989.
Optional: *The Art of Molecular Dynamics Simulation*, Second Edition, Rapaport, 2004.
Optional: *Understanding Molecular Simulation*, Second Edition, Frenkel and Smit, 2002.

Course Objective
The objective of this course is to provide students with an overview of different modeling techniques in materials science. Applications will be presented that utilize computational tools to study the structural, mechanical, chemical and electrical properties of materials. A broad range of modeling techniques will be covered that span from atomistic to mesoscale domains. Particular focus will be given to atomistic simulation methods, including Monte Carlo, molecular mechanics and molecular dynamics.

Course Topics
1) Introduction
   a) What is computational materials science?
   b) Length and time scale considerations
2) Atomistic Simulations
   a) Basic principles – Thermodynamic properties / Ensembles
   b) Interatomic potentials
3) Molecular Dynamics
   a) Force calculation
   b) Extended boundary conditions (temperature and pressure control)
   c) Integration methods
4) Monte Carlo Simulations
   a) Use of random number generators
   b) Isobaric/isothermal applications
5) Molecular Mechanics
   a) Energy minimization techniques
   b) Minimum energy path between states (nudged elastic band method)
6) Brief Introduction to Multiscale Modeling
   a) Length scale coupling
   b) Time scale extensions

Homework
Homework will be assigned over the course of the semester. The collective goal of the homework assignments will be to write a set of simple atomistic simulation programs using a two-body potential for a 1D chain of atoms. No late homework assignments will be accepted without prior approval.

Project

Students will be required to complete a course project. The course project will involve a literature review of a specific topic that has significant relevance to atomistic simulation. The student will also use the open-source atomistic simulation package LAMMPS to perform simulations relevant to their chosen project. Project results will be disseminated via a written report and an oral presentation (during the regular class period at the end of the semester). Example project topics include:

- Mechanical behavior of carbon nanotubes
- Efficiency of different thermostats for molecular dynamics simulations
- Application of MD to model thermal conductivity in transition metals

It is the responsibility of each student to generate a topic for their project. Topics that relate to the student's area of research are acceptable and encouraged. Students are encouraged to speak with Professor Spearot prior to submitting a project topic.

- **Approval:** All project topics must be approved by Professor Spearot. Please submit a project title, abstract (~200 words) and initial reference list electronically by **February 28**.

- **Report:** 10-12 pages (1 inch margins, 12 point font, 1.5 line spacing). Reports are due electronically to Professor Spearot by **April 14**.

- **Presentation:** ~20 minutes to be given in class between **April 21 and April 25**. Order of student presentations will be determined later in the semester.

- **Grading:** Project grades will be a composite of both oral and written reports.

Course Grading

Final Project 50%, Homework 50%

Course grades will be "curved" if necessary for appropriate grade distribution for a graduate level course.