MEEG 591V – Computational Materials Science
Spring 2012

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

Lecture
Monday / Wednesday / Friday, 8:30 – 9:20 am, MEEG 216

Office Hours
Monday / Wednesday / Friday, 9:30 – 10:30 am, NANO 213

Text
None required. Journal papers will be distributed electronically 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
7) Student Project Presentations

Homework
Homework assignments will be assigned over the course of the semester. The ultimate goal of the homework assignments will be to write a very simple molecular dynamics program using a two-body potential for a system 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 is a critical literature review of a specific topic that has significant relevance to atomistic simulation or multiscale modeling. Project results will be disseminated via a written report and an oral presentation (during the regular class period at the end of the semester). **It is very important in a critical literature review not only to present an overview of the latest work in the literature but to identify opportunities for advancement or improvement.** Example project topics include:

- Interatomic potentials for carbon: Development, accuracy and applications
- Efficiency of different integration algorithms for MD
- Application of MD to model thermal conductivity in transition metals

It is the responsibility of each student to generate a topic for their critical literature review. 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 and abstract (~200 words) electronically by **February 10**.

- **Report:** 10-15 pages (with sufficient references). Reports are due electronically to Professor Spearot by **April 20**.

- **Presentation:** ~25 minutes to be given in class between **April 23 and May 2**. A sign-up sheet will be distributed later in the semester.

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

Course Grading

Final Project 60%, Homework 40%
Course grades will be "curved" if necessary for appropriate grade distribution for a graduate level course.

Contacting Professor Spearot

If you use another email address, it is your responsibility to set up your UARK account to forward incoming mail and to make sure that your UARK email is not full.