MEEG 591V – Computational Materials Science
Spring 2010

Instructor: Dr. Douglas Spearot, MEEG 103, 575-3040, dspearot@uark.edu
Lecture: Monday/Wednesday/Friday, 8:30 – 9:20 am
Classroom: MEEG 101

Course Objective:
The course objective 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 continuum domains. Particular focus will be given to atomistic simulation methods, including Monte Carlo, molecular mechanics and molecular dynamics.

Course Topics:
1) Introduction to Numerical Simulation
   a) What is computational materials science?
   b) Length and time scale considerations
2) Atomistic Simulations
   a) Basic principles – Thermodynamic properties / Ensembles
   b) Interatomic potentials
   c) Molecular mechanics
   d) Molecular dynamics
   e) Monte Carlo methods
3) Multiscale Modeling Techniques
   a) Concurrent coupling versus hierarchical coupling
   b) Quasicontinuum method
   c) Bridging domain method
   d) Time scale extensions
4) 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 for a Lennard-Jones or Morse (two-body potential) 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 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.** Examples of project topics include:

- Interatomic potentials for XXX material – development, accuracy and application
- Efficiency of different integration algorithms for MD
- Application of MD to model YYY process or ZZZ phenomenon
- etc.

It is the responsibility of each student to generate a topic for the critical literature review. Topics that relate to the student's area of research are acceptable and encouraged. All topics must be approved by Professor Spearot.

- **Approval:** All project topics must be approved by Professor Spearot. Please submit a project title and abstract (~200 words) electronically by February 12.

- **Report:** 10-15 pages (with sufficient references). Reports are due electronically to Professor Spearot by April 30.

- **Presentation:** ~15 minutes to be given in class between April 21 and April 28. 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.

Sickness Policy:
The following will serve as the illness and academic continuity policy for this course.

- In the event that you become sick, go directly to the University Health Center and do not come to class unless cleared by the University Health Center. As you are aware, flu season this year has been and is expected to continue to be severe. The other students and I will appreciate it greatly if you went to the doctor instead of attending class. The University Health Center will write a note documenting your visit and the number of days that you are to miss class. You will be given the opportunity to make-up all assignments with no penalty once you return.

- In the event that I become sick, I will cancel class for at most one week (three lectures). If my illness continues beyond this duration, I will organize guest lecturers (faculty and graduate students) to teach the lecture topics and will continue with the course material and assignments. I will make use of Blackboard to post copies of my lecture notes, slides and homework solutions.

- In the event that the University of Arkansas suspends classes campus-wide due to a mass outbreak of the flu, or for any other weather-related reason (tornado, ice-storm, etc.). University of Arkansas policy is that a maximum of 13% of the class can be eliminated (this translates to two weeks in a 15 week semester). Thus, if an extended campus-wide cancellation is necessary, we will continue the course electronically through Blackboard with electronic lecture delivery and electronic homework submission.