MTE 591- Introduction to Computational Materials Science
Fall Semester 2015

Class Schedule:
Lecturer: Lin Li, office hours Tuesdays at 11am at NERC 2007
Lecture: Tuesdays, and Thursdays 9:30am-10:45am, Morgan Hall 203

Prerequisites:
Graduate standing in MTE or permission of instructor.

Textbook/References:
- Syllabus, lecture notes, homework assignments, supplementary materials will be distributed via the blackboard

Course Objectives:
The course objective is to create familiarity with state-of-the-art methods to model and simulate materials and provide hands-on experience with using these methods. A broad range of modeling techniques will be covered that span from atomistic to continuum domains. Applications will be presented that utilize computational tools to study the structural, mechanical, chemical and electrical properties of materials.

Course Topics:
1) Introduction
   a) What is computational materials science?
   b) Length and time scale considerations
2) Meso-scale and Continuum Modeling
   a) Cellular automation
   b) Dislocation dynamics
   c) Phase field modeling
   d) Finite element method
   e) Crystal plasticity
3) Atomistic Modeling
   a) Basic principles – Thermodynamic properties / Ensembles
   b) Interatomic potentials
   c) Molecular statics
   d) Molecular dynamics
   e) Monte Carlo methods
4) Multiscale Modeling Techniques
a) Concurrent coupling versus hierarchical coupling
b) Length scale coupling
c) Time scale extensions
5) Student Project Presentations

Homework:
Homework will be assigned over the course of the semester. 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 computational materials. The students will also use the modeling techniques discussed in class 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 bismuth telluride nanosheet
- Texture evolution of nanocrystalline Ni subjected to uniaxial compression
- Application of molecular dynamics to model thermal conductivity in transition metals

It is the responsibility of students 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 discuss with Dr. Lin Li prior to submitting a project topic.

- Approval: All project topics must be approved by Dr. Lin Li. Please submit a project title, abstract (~150 words) and initial reference list electronically by October 23.
- Report: 10-12 pages (1 inch margins, 12 point font, 1.5 line spacing). Reports are due electronically to Dr. Lin Li by December 4.
- Presentation: ~20 minutes to be given in class between December 1 and December 3. 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:
- Homework 50% (including in class assignment)
- Final Project 40%
- Class preparation/knowledge 10%
Course grades will be normalized if necessary for appropriate grade distribution for a graduate level course.

Class Policies:
Attendance is required for class assessment and lab work. If you must miss a scheduled laboratory or quiz due to serious illness, family death, accident, etc., notify Dr. Lin Li as soon as possible. Excuses of a non-urgent nature will not be accepted.
**Academic Integrity and Misconduct**

Academic misconduct is viewed as any action that tends to distort the accurate assessment of your individual accomplishments or knowledge. Discussion of course concepts with other students (and instructors) is encouraged, but you must *independently* solve and write up solutions to specific homework and in-class assignments.

**Disabilities:**

Students with disabilities who may require more time than is allotted for the exams/quizzes must contact the UA Office of Disability Services (ODS) to obtain PRIOR APPROVAL and THE PROPER PAPERWORK in accordance with the rules and regulations of The University of Alabama. Alternate exams/quizzes must be scheduled through the ODS (348-4285).