MEEG 591V – Multiscale Modeling
Spring 2006

Instructors:
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Lecture: Monday/Wednesday/Friday, 1:30 – 2:20 pm
Classroom: MEEG 101

Course Objectives:
To provide the student 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 quantum to continuum domains. Particular focus will be given to methods that couple simulation techniques across multiple length scales.

Course Topics:

1) Introduction to Numerical Simulation
    a) What is computational materials science?
    b) Length and time scale considerations
2) Atomistic calculations
    a) Basic principles
    b) Interatomic potentials
        i) Classifications
        ii) Potentials for metals, hydrocarbons, ionic materials, etc.
    c) Molecular dynamics
        i) Equations of motion for NVE, NVT and NPT ensembles
        ii) Integration algorithms – Verlet and Gear
        iii) Applications
    d) Molecular mechanics
    e) Monte Carlo methods
3) Overview of finite element methods
4) Coupling methods between atomistic simulation and finite elements
    a) Concurrent coupling versus hierarchical coupling
    b) Hierarchical coupling
    c) Concurrent coupling – Cauchy Born rule, Quasicontinuum, etc.
5) Coupling methods between quantum mechanics and atomistic simulation
    a) Brief overview of Quantum calculations
    b) Method of ‘on the fly’
    c) The Onion method
6) Project Presentations

Homework:
Five 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 1-D chain of atoms. No late homework assignments will be accepted without prior approval.

February 10	Homework 1	calculation of the Lennard-Jones potential
February 24	Homework 2	molecular dynamics for a 1-D chain of LJ atoms
March 10	Homework 3	coupling the 1-D chain of atoms to a thermostat
March 31	Homework 4	1-D atomistic continuum coupling
April 14	Homework 5	the Cauchy-Born rule

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
- Treatment of mobile defects in multiscale coupling methods
- Application of the quasicontinuum method to 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. All topics must be approved by both Profs. Zhang and Spearot.

Grading:
Final Project 50%, Homework 50%