Syllabus for MTSE 5710 Computational Materials Science

Course Number: MTSE 5070 Computational Materials Science
Time: Monday 2:30PM - 5:20pm
Classroom: Discovery Park D209B
Dates: Jan. 16, 2018-May 11, 2018
Instructors: Dr. Jincheng Du, Dr. Zhenhai Xia

Course Summary

Computational materials modeling has emerged as an increasingly important branch of materials science due to the evolution of multiscale modeling frameworks, maturing of numerical algorithms, and ever increasing computer capability. As a consequence, modeling and simulation has become highly valuable material research methods that supplement experiments and traditional theory in new material discovery. The aims of this course are to: (i) introduce students to materials modeling and simulation techniques that cover a wide time and length scales with a focus on the microscopy scale (first principles and atomistic levels simulations) and continuum level simulations (finite element analysis); (ii) show how these modeling methods can be used to understand fundamental material structure, material defects and the relationships between material structure and material behavior; and (iii) develop an understanding of the assumptions and approximations that are involved in the modeling frameworks at the various time and length scales. Students will be introduced to the basis for the simulation techniques, learn how to use computational modeling, and how to present and interpret the results of simulations. The students will work with simulation modules to reinforce concepts learned in the lectures.

Course Requirements

Introduction to Materials Science or an equivalent course. Prior computer programming knowledge is NOT a prerequisite.

Grading

Class participation	(20%)
Class projects	(40%)
Course project	(40%)

Class project: The class projects include two modules, which will be assigned in each of two sections of the class. Students are expected to have a laptop to run their simulations. We will use open-source codes for simulations visualization of results. Please download the executable for two codes from sources provided in the classes on your laptops.

After the projects are completed, the students are required to write project reports summarizing his or her work on their class project modeling. This report must be typed, single spaced, 12 point Symbol and/or Times New Roman fonts, and with 1-inch margins around. The report will follow the style of a standard laboratory report and must include the following sections: Title, Author and affiliation, Abstract, Introduction (of the method used and properties calculated), Results, Discussions (comparing the results from simulations with corresponding experimental values, or theory), Conclusions, and References. You must include appropriate visual figures from the simulations (including charts and graphs, and material structures). All the legends and labels in the charts and graphs must be at least a 12-point font when scaled to fit to the report. ***CAUTION***: follow the timeline above; pace your effort and don't wait until the deadline.

Course project: it includes a literature review (minimum seven pages, double space) and a final presentation on a selected area of computational material science. The topic is picked in consultation with one of the instructors and can be related to current research work you are carrying out. Detailed instruction of the course project will be given in the class.

Deadlines

- March 19 – turn in the first project report in Module one
- April 23 – turn in the second project report in Module two
- April 2 – choose the topic of Course project after consultation with instructors
- April 23 – turn in the review report

Codes to be provided

Each student is required to bring his/her laptop to install the codes needed for class projects

- PUTTY and SSH file exchange (for remote computing cluster access)
- The following codes will be used in course project:
  - VASP code for DFT simulations
  - LAMMPS code for MD simulation
  - ABAQUS code for FEA simulation

Lecture schedule:

1. General introduction and overview; (Instructor: Drs. Xia & Jincheng Du)
Week 1: Introduction (1/22)
2. Atomistic Modeling Module (Instructor: Dr. Jincheng Du)
Week 2: Introduction to atomistic simulations (1/29)
Week 3: Basics of quantum mechanical methods (2/5)
Week 4: Density function theory and application to solid materials (2/12)
Week 5: Interatomic Potentials for atomistic simulations (2/19)
Week 6: Molecular mechanics simulations (2/26)
Week 7: Molecular dynamics simulations (3/5)
3. Continuum Modeling Module (Instructor: Dr. Zhenhai Xia)
Week 8: Introduction to continuum mechanics (3/19)
Week 9: No Class (Spring break) (3/26)
Week 10: Introduction to computational methods (4/2)
Week 11: Introduction to finite element method (ABAQUS) (4/9)
Week 12: Finite element modeling of materials deformation (4/16)
Week 13: Finite element modeling of materials failure (4/23)
4. Course project (Instructors: Dr. Jincheng Du, Dr. Zhenhai Xia)
Week 14: Course project presentations **(4/30)**