Syllabus for MTSE 4040 and 5710 Computational Materials Science

Course Number: MTSE 4040/5710 Computational Materials Science
Semester: Spring 2021
Time: Monday 2:30PM - 5:20pm
Classroom: Remote
Dates: Jan 11, 2021-May 1, 2021
Instructors: Dr. Jincheng Du, Dr. Zhenhai Xia
Zoom link: https://unt.zoom.us/j/87952105957 (code: 2021)

Course Summary

Computational materials modeling has emerged as an increasingly important branch of materials science due to the evolution of modeling frameworks, invention of novel numerical algorithms, applications in wide range of material systems and problems, and ever increasing computer capability. As a consequence, modeling and simulation are emerging as powerful complementary approaches to experiments and traditional theory. The aims of this course are to: (i) introduce students to materials modeling and simulation techniques that cover a wide time and length scales from quantum mechanics, atomistic to continuum methods; (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. The class includes mixed sessions of lectures and handson modules to provide students opportunities to learn simulation software and run simulation mini projects. Through the course, 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 project report (40%)

- Module 1 report (20%)
- Module 2 report (20%)

Course project/Presentation (40%)

Class projects: The class projects include two modules, in which of which class projects are signed. 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. Additional questions and assignments will be given to students taken the graduate level (MTSE5710).

Course project and presentation: The course project can be a literature review of a selected topic of computational materials, which can focus on a methodology and its application or applications of a series of methodologies on a material problem. The student can also choose to do the project as a literature review or to use one of the learned simulation techniques on a practical materials problem. In either case, the student should consult with one of the instructors. It also includes a project report and a final presentation. The topic is picked in consultation with the instructor and can be related to current research work you are carrying out. Detailed instruction of the course project will be given in the class.

Project report format requirements: The 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.

<u>Class project due dates:</u>
Report of project 1 of Module 1: 2/15
Report of project 2 of Module 1: 3/8
Report of project 1 of Module 2: 3/19
Report of project 2 of Module 2: 4/12

<u>Course project due date:</u>
Report of course project: 4/19
Final project presentation: 4/19

CAUTION: follow the timeline above; pace your effort and don't wait until the deadline.

Codes to be used in the class:
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
    - Avogadro2 for model building & visualization
    - ABAQUS code for FEA simulation

Lecture schedule:

1. General introduction and overview (Dr. Zhenhai Xia, Dr. Jincheng Du)
Week 1: General Introduction of computational material science (1/11)
Introduction to HPC and softwares (1/11)

2. Atomistic Modeling Module (Dr. Du)

Week 2: No Class (MLK Jr Day) (1/18)
Week 3: Introduction to atomistic simulations (1/25)
Week 4: Basics of quantum mechanical methods (2/1)
Week 5: Density function theory (DFT) and application to solid materials (2/8)
Week 6: Interatomic Potentials for atomistic simulations (2/15)
Week 7: Molecular mechanics simulations (2/22)
Week 8: Molecular dynamics simulations (3/1)

3. Continuum Modeling Module (Dr. Xia)

Week 9: Introduction to continuum mechanics (3/8)
Week 10: Introduction to computational methods (3/15)
Week 11: Introduction to finite element method (ABAQUS) (3/22)
Week 12: Finite element modeling of materials deformation (3/29)
Week 13: Finite element modeling of materials failure (4/5)
Week 14: Finite element modeling of materials impact (4/12)

4. Final project (Drs. Du and Xia)

Week 15: Final project presentations (I) **(**4/19**)**