Syllabus for MTSE 4040 and 5710 Computational Materials Science

Course Number: MTSE 4040/5710 Computational Materials Science
Semester: Spring 2024
Classroom: DP B142
Time: Thursdays 2:30 - 5:20 pm
Dates: Jan 17, 2024-May 12, 2024
Instructors: Prof. Jincheng Du
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Office hour: by appointment

Course Summary

Computational materials modeling has emerged as an important branch of materials science due to the rapid growth of the capability of various simulation methodologies and rapid growth of applications in different fields of materials research and engineering. Modeling and simulation now play an important role in materials research and discovery, in addition to traditional experimental methods and theories. This course aims to: (i) introduce students the basics of multiscale materials simulations with a focus on atomistic materials modeling and simulation; (ii) show how these modeling methods can be used to understand the structure, defects and behaviors of materials; and (iii) develop an understanding of the assumptions and approximations that are involved in the modeling frameworks at the various time and length scales. New topics such as machine learning and materials informatics will also be introduced. The class includes mixed sessions of lectures and hands-on modules to provide students opportunities to learn simulation software and run simulation mini projects. Through the course, a student will learn various materials simulation techniques, how to perform simulations with softwares and the usage of the High Performance Computing facilities, and how to present and interpret the simulation results for particular materials problems.

Course Requirements

Introduction to Materials Science (MTSE3000, MTSE3001 or MTSE5000) or an equivalent course. Prior computer programming knowledge is welcome but NOT a prerequisite.

Text and Reference Books

The main materials are the lecture notes and handouts. Two reference books are recommended:

- "Atomistic Simulations of Glasses: Fundamentals and Applications", J. Du and A.N. Cormack, Wiley (2022).
- "Computational Material Science: an Introduction", J. G. Lee, CRC Press (2017).

Grading

Class participation (10%)
Class project report (60% total)

- Report 1 Quantum Mechanical calculations (15%)
- Report 2 Energy minimization and MD simulations (15%)
- Report 3 Mechanical property calculations (15%)
- Report 4 FEM and ML of materials (15%)

Course project report and presentation (30%)

Class projects: The class projects include several modules. We will use the classroom desktop computers or through which to access the HPC to run most of the simulations. We will use various softwares (including both commercial and open-source codes) for simulations visualization of results. 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 is a team project (consisting of two students) based on a research topic the team choose in consultation with the instructor. The student team applies one of the techniques learned in the classroom to a practical materials problem. The project includes a project report and a final presentation. It is expected the student team choose the topic and submit an one page summary of the project plan (background, methodology chosen, planned simulation experiments and expected results) before the mid-term. A project presentation and written report will be due close to the end of the semester. Detailed instruction of the course project will be given in the class.

Project report format requirements: The reports should follow the general format of a scientific paper. It 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. Report length: minimum 7 pages plus references.

Codes to be used in the class:
Class desktops and remote HPC will be mainly used 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
  - Gaussian for QM calculations
  - LAMMPS code for MD simulation
  - Avogadro/VMD for model building & visualization
  - ABAQUS code for FEA simulation
  - Python3.7

Lecture and lab schedule:

1. General introduction and overview

- General introduction of computational material science
- Introduction to HPC, Linux environment and scripting

Hands-on project 1: HPC account creation, log in, and familiar with Linux operations

2. First Principles Calculations

- Introduction to atomistic simulations
- Basics of quantum mechanical (QM) methods
- Cluster based QM calculations
- Density function theory (DFT) and application to solid materials

Hands-on project 2: QM calculation of molecules and clusters (software used: Gaussian)
Hands-on project 3: QM calculation carbon nanotube (software used: Gaussian)
Hands-on project 4: QM calculation of silicon and gallium nitride (software used: VASP)

3. Classical Atomistic Simulations

- Interatomic potentials for atomistic simulations
- Molecular mechanics / energy minimization simulations
- Molecular dynamics simulations
- Monte Carlo simulations

Hands-on project 5: Geometry optimization of molecules (software used: Avogadro)
Hands-on project 6: Defect formation energies of solids (software used: Lammps)
Hands-on project 7: MD simulations of melting of copper (software used: Lammps)
Hands-on project 8: MD simulations of tensile testing of bulk crystal and nanorod (software used: Lammps)

4. Continuum Modeling Methods

- Introduction to finite element method
- Finite element modeling of materials deformation and material failure

Hands-on project 9: FEM analysis of board with hole (software used: ABAQUAS)

5. Machine Learning Methods and Application to Materials Modeling

- Basics of ML methods
- Applications of ML to materials research and discovery

Hands-on project 10: ML of band gap of semiconductor materials (Python)

6. Course Projects

- Course project topic choice and presentation (due mid-term)
- Final course project presentations (I, II)