Syllabus for MTSE 4040/MTSE5710 Computational Materials Science

Course Number: MTSE4040 MTSE5710 Computational Materials Science
Time: Monday 2:30PM - 5:20pm
Classroom: Discovery Park D202
Semester: Spring’2019
Instructors: Dr. Jincheng Du

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, and increased computer capability. As a consequence, modeling and simulation are emerging as powerful complementary approaches to experiment and traditional theory in materials research. Computational material science has become an integral part of material science curriculum. The aims of this course are to: (i) introduce students to materials modeling and simulation techniques that cover a wide time and length scales; (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 learn the basis for the simulation techniques, how to use computational modeling with accompanied hands on sessions for each type of methodology introduced, and how to present and interpret the results of simulations.

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

Grading
Class participation & discussions (20%)
Class projects (50%)
Course project (30%)

Class projects: The class projects are assigned after each modeling technique is introduced. Students are expected to have a laptop to run their simulations or to connect to the UNT High Performance Computing (HPC) facility. We will use a combination of open-source and commercial codes for simulations and visualization of results.

After the class projects are completed, the students are required to write project reports summarizing the procedure and results. The report will follow the style of a scientific paper 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 below; pace your effort and don’t wait until the deadline.
Course project: The course project includes a final report and a presentation on a selected area of computational material science. The course project assignment will be given before the Spring break. The student is expected to discuss with the instructor to decide on the course project topic and write a one page summary before deadline (below). The UG course project can be based on literature study on simulation methodologies reported in the class or summary of his or her own simulations from the methods introduced in the class. The Graduate course project has to be, at least partially, based on the student’s simulations with extensive literature study. The topic is picked in consultation with the instructor and more details can be found in the project assignment.

Graduate versus Undergraduate assignments: As this is a mixed Undergraduate and Graduate class, there will be additional assignments for graduate students. Students taking the graduate level credits must complete the additional graduate level assignments.

Deadlines
- February 25 – first class project report due for Module one
- March 18 – second class project report due for Module one
- April 1 – topic choice of Course project due
- April 15 – first project report due for Module two
- April 22 – second project report due for Module two
- May 1 – Course project report due

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)
- Avogadro as visualization software (download: https://avogadro.cc/)
- The following codes will be used in course project:
  - VASP code for DFT simulations
  - LAMMPS code for MD simulations
  - ABAQUS code for FEA simulations

Lecture schedule:

1. General introduction and overview
   Week 1: Introduction of computational material science (1/14)

2. Atomistic Modeling Module
   Week 2: Introduction to atomistic simulations (1/21)
   Week 3: Basics of quantum mechanical methods (1/28)
   Week 4: Density function theory and application to solid materials (2/4)
   Week 5: Interatomic Potentials for atomistic simulations (2/11)
   Week 6: Molecular mechanics simulations (2/18)
   Week 7: Molecular dynamics simulations (2/25)
   Week 8: Finish atomistic modeling projects (3/4)
   Week 9: No Class (Spring break) (3/11)
3. Continuum Modeling Module
   - **Week 9**: Introduction to continuum mechanics (3/18)
   - **Week 10**: Introduction to computational methods (3/25)
   - **Week 11**: Introduction to finite element method (ABAQUS) (4/1)
   - **Week 12**: Finite element modeling of materials deformation (4/8)
   - **Week 13**: Finite element modeling of materials failure (4/15)

4. Course projects
   - **Week 14**: Course project presentation 1 (4/22)
   - **Week 15**: Course project presentation 2 (4/29)