## Syllabus for MTSE 4040 and 5710 Computational Materials Science

Course Number: MTSE 4040/5710 Computational Materials Science
Semester: Spring 2026
Classroom: DP B142
Time: Mondays 9:00 -11:50 am
Dates: Jan 12, 2025-May 8, 2025
Instructors: Prof. Jincheng Du
Email: jincheng.du@unt.edu
Office hour: by appointment

**Course Summary**
Computational materials modeling has emerged as an important branch of materials science, due to the maturing of various simulation methodologies (including application of AI and ML in simulations) and ever increase of access of computing powers. This leads to rapid growth of applications in different fields from fundamental materials research and engineering fields. This course aims to: (i) introduce students the basics of multiscale materials simulation methods from quantum mechanics, atomistic to continuum level (e.g. finite element analysis), with a focus on atomistic materials level simulation; (ii) show how these modeling methods can be used to understand material structure, defects, mechanical and other behaviors; and (iii) develop an understanding and appreciation of the strength and limitation 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 several materials simulation techniques and associated common software, how to access and use the High Performance Computing (HPC) facilities, and how to present and interpret the simulation results.

**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 (20%)
- Report 2 Energy minimization and MD simulations (20%)
- Report 3 FEM and ML of materials (20%)

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 software (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 based on a research topic a student choose in consultation with the instructor. The student applies one of the simulation techniques learned in the classroom to a practical materials problem. It is expected the student 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.

**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)

**3. Classical Atomistic Simulations**

- Interatomic potentials for atomistic simulations

- Molecular mechanics / energy minimization simulations
- Molecular dynamics simulations
- Monte Carlo simulations

Hands-on project 4: Geometry optimization of molecules (software used: Avogadro)
Hands-on project 5: Defect formation energies of solids (software used: Lammps)
Hands-on project 6: MD simulations of melting of copper (software used: Lammps)
Hands-on project 7: 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 8: Design and FEM analysis (software used: ABAQUAS)
Hands-on project 9: 3D printing of designed object

**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)