Multi-scale Modeling and Simulation in Solid Mechanics: Introduction to Data-Driven Integrated Computational Materials Engineering (ICME)

ME417

Instructor: Prof. Wing Kam Liu
Graders: Jiaying Gao, Hengyang Li, Puikei Cheng, Mahsa Tajdari
Class Time: Tu, Th 9:30am-10:50am, Tech L160
Office Hours: 11:15AM-12:15PM Tu, Th, 9-10AM F when available, by appointment; Tech A326

Course Objectives:

1) Understand the underlying principles of molecular dynamics (equations of motion for atoms, atomic interactions).
2) Understand the connection between information available on small (atomistic) and large (continuum) scales.
3) Understand the concept of Integrated Computational Material Engineering (ICME) though multiscale modeling approach. Gain exposure the role of data-science in multiscale modeling and ICME process.
4) Applications
    - **a.** Polymer nano-composite: polymer mechanics, polymer and polymer-fillers modeling, Multi-scale modeling (MD, Continuum)
    - **b.** Nanostructure materials: Nanowires: single crystal Si; Nano Carbons: nanotube
    - **c.** Data driven multiscale simulation: Self-consistent clustering analysis (SCA), deep learning in Materials Genome Initiative, design of microstructural materials system.

Homework

There will be two homework assignments during the term. The purpose of the homework is to provide the students with an opportunity to apply theoretical and computational concepts to multi-scale problems.

Projects

Projects typically include an ICME aspect and some preliminary theoretical concepts on the expected observations. There will be one midterm project and one final project. Topic of midterm project: An ICME study on Carbon Fiber Reinforced Polymer material system. Topic for the final project: students will have the opportunity to apply the concepts that they have learned in class to a research problem of their own interest.

Grading

Homework (30%), Midterm project (30%), Final project (30%), Participation (10%)

Textbook

There is no required textbook. Some resources relevant to this class are provided below:

• Liu, Wing Kam, Karpov, Eduard G., and Park. Harold S., Nano Mechanics and Materials: Theory, Multiscale Methods and Applications. John Wiley & Sons, Ltd, 2006.
• Schroeder, Daniel V. An Introduction to Thermal Physics. Addison Wesley Longman, 1999.

• Fish, Jacob and Belytschko, Ted. A First Course in Finite Elements. John Wiley & Sons, Ltd, 2007.
• Belytschko, Ted, Liu, Wing Kam, and Moran, Brian, Nonlinear Finite Elements for Continua and Structures. John Wiley & Sons, Ltd, 2000.
• LAMMPS Documentation (for reference): http://lammps.sandia.gov/doc/Manual.html
•Müller, Andreas C., and Sarah Guido. *Introduction to machine learning with Python: a guide for data scientists*. " O'Reilly Media, Inc.", 2016.
Friedman, Jerome, Trevor Hastie, and Robert Tibshirani. *The elements of statistical learning*. Vol. 1. No. 10. New York, NY, USA:: Springer series in statistics, 2001.

Software: LAMMPS, ABAQUS, and MATLAB will be used for the simulations. Lab session may be held on Wed (if needed) or mutually agreeable time. We will be using Northwestern's super computer system QUEST for Midterm and Final projects.

Class Schedule

Date		Topic	Detail description
Week #1 Sept 27 Th:	Molecular dynamics and multiscale modeling	Introduction to Multiscale Simulations	(HW#1 Assigned)
Week #2 Oct 2 T:		Introduction to MD I	Atomic structure and interatomic bonding
Week #2 Oct 4 Th:		Introduction to MD II	Hamiltonian, Lagrangian mechanics (HW#1 Due, HW#2a Assigned)
Week #3 **Oct 9 T:**		Introduction to ICME process	
Week #3 **Oct 11 Th:**		Midterm Tutorial I LAMMPS introduction	(HW#2a Due, HW#2b Assigned)
Week #4 **Oct 16 T:**		Midterm Tutorial II	VMD and post-processing
Week #4 **Oct 18 Th:**	Polymer composite	Introduction to Polymer	(Midterm Assigned)
Week #5 **Oct 23 T:**		Polymer mechanics	
Week #5 **Oct 25 Th:**		Polymer coarse grain MD	
Week #6 Oct 30 T:		Midterm Presentation	
Week #6 Nov 1 Th:		Meso-scale viscoelastic model	(Midterm Report Due)
Week #7 Nov 6 T:	Thermodynamics and Lattice Mechanics	Nanostructure	
Week #7 Nov 8 Th:		Thermodynamics I	(Final Project Assigned)
Week #8 **Nov 13 T:**		Thermodynamics II	
Week #8 **Nov 15 Th:**		Lattice Mechanics I	(HW#2b Due)
Week #9 Nov 20 T:			(Final Project Proposal Due. Sign up for a time during class to meet with TA's about project)
Week #9 Nov 22 Th:		No class (Thanksgiving) Discuss student projects	
Week #10 Nov 27 T:		Lattice Mechanics II	
Week #10 Nov 29 Th:	Data-driven Multiscale Modeling	Introduction of Mechanistic Data-driven Method I	
Week #11 Dec 4 T:		Introduction of Mechanistic Data-driven Method II	
Week #11 Dec 6 Th:		TBD	
Week #12 Dec 11 T:	Final Week	Final project Presentation	
Week #12 Dec 13 Th:			(Final Report Due)

Module 1: Introduction (3 wks)

A. Introduction_MD (1.5wk)

1. Why multi-scale modeling?
2. Lagrangian and Hamiltonian equations of motion
3. Interatomic potentials
   a. Particle dynamics (Multi-body interaction) using interatomic potential
4. Algorithms, Periodic Boundary Condition

B. Introduction to Integrated Computational Material Engineering (ICME) Processing (0.5wk)

1. What is ICME?
2. How are scales connected together?

B. Midterm tutorial (1 wk)

1. What is LAMMPS and the basics how it works
2. Quest HPC login and job submission
3. VMD and post-processing of your MD results
3. Details of Midterm explained

G. Midterm Project (0.5 wk)

1. Students present their midterm project

Module 2: Polymer Nanocomposite (2.0 wks)

1. Introduction to Polymer
2. Molecular modeling and simulation of polymer
3. Force field for polymer
4. Mechanics of polymer and composite
   - Viscoelasticity, Creep, Stress relaxation, DMA test, Time-temperature superposition
5. Coarse graining molecular dynamics of polymer composite
6. Tube model for viscoelasticity

Module 3: Thermodynamics and Lattice Mechanics (2.5 wks)

A. Nanostructure (0.5 wk)

1. Single crystal silicon nanowire and carbon nanotubes

B. Thermodynamics (1 wk)

1. First and second law of thermodynamics, Entropy
2. Statistical ensembles: NVE, NVT, NPT
3. Free energy, Enthalpy,

C. Lattice Mechanics(1 wk)

1. Regular lattice structure
2. Equation of motion

Module 4: Data-driven Multiscale Modeling (1.0 ~ 1.5 wk)

A. Introduction of Mechanistic Data-driven Method
   1. What is data-science
   2. Mechanistic Machine Learning approach
   3. Data-driven Multiscale Modeling