Multi-scale Modeling and Simulation in Solid Mechanics:
Introduction to Data-Driven Integrated Computational Materials Engineering (ICME)
ME417
Instructor: Prof. Wing Kam Liu
Graders: Satyajit Mojumder, Sourav Saha
Class Time: Tu, Th 9:30am-10:50am, Tech LG52
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) through multiscale modeling approach.
4) Applications
   a. Nanostructure materials: Nanowires (single crystal Si); Nanotube, Nanopillar, 2D-materials (Graphene) etc.
   b. Polymer nano-composite: polymer mechanics, polymer and polymer-fillers modeling, Multi-scale modeling (MD, Continuum)
   c. Data-driven multiscale simulation for advanced materials system (polymer nano-composite, alloys etc.)

Homework
There will be three 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. The following book will be followed along with other resources:
• Liu, Wing Kam, Karpov, Eduard G., and Park. Harold S., Nano Mechanics and Materials: Theory, Multiscale Methods and Applications. John Wiley & Sons, Ltd, 2006.

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 high performance computer system QUEST for Midterm and Final projects.

Class Schedule

Date		Topic	Detail description
Week #1 Sept 24 T:	Molecular dynamics and multiscale modeling	Introduction to Multiscale Simulations	(HW#1 Assigned)
Week #1 Sept 26 Th:		Introduction to MD I	Atomic structure and interatomic bonding
Week #2 Oct 1 T:		Introduction to MD II	Hamiltonian, Lagrangian mechanics (HW#1 Due, HW#2a Assigned)
Week #2 Oct 3 Th:		Project Tutorial I (LAMMPS introduction)	
Week #3 Oct 8 T:		Thermodynamics-I	(HW#2a Due, HW#2b Assigned)
Week #3 Oct 10 Th:		Project Tutorial II	VMD and post-processing
Week #4 Oct 15 T:		Lattice Mechanics-I	Midterm Project Assigned
Week #4 Oct 17 Th:		Lattice Mechanics-II	
Week #5 Oct 22 T:		Nanostructure	
Week #5 Oct 24 Th:	Nano-Polymer composite	Introduction to Polymer	(HW#2b Due)
Week #6 Oct 29 T:		Polymer mechanics	
Week #6 Oct 31 Th:		Polymer coarse grain MD	
Week #7 Nov 5T:		Midterm Presentation	(Final Project Assigned)
Week #7 Nov 7 Th:		Meso-scale viscoelastic model	(Midterm Report Due)
Week #8 Nov 12 T:	**Data-driven Multiscale Modeling**	**Basics of data science for multiscale modeling**	**Introduce basic terminology and different machine learning methods (supervised and unsupervised method: Principal Component Analysis (PCA), K-means clustering, Self-Organizing Map (SOM), Neural networks for regression and classification)**
Week #8 Nov 14 Th:		**Data Science Tutorial (Basics of NN and their implementation in mechanics problem)**	**HW #3 (assigned) (Use MD data to train NN)**
Week #9 Nov 19 T:		Discuss student projects	(Final Project Proposal Due. Sign up for a time during class to meet with TA's about project)
Week #9 Nov 21 Th:		**Data-driven methods in multiscale modeling**	**Application of surrogate model, genetic programming, FFNN, CNN in mechanics of materials problem**
Week #10 Nov 26 T:	Special Topics	Special Topics: Bridging atomistic to continuum model-I	**(HW #3 Due)**
Week #10 Nov 28 Th:		No class (Thanksgiving)	
Week #11 Dec 3 T:		Special Topics: Bridging atomistic to continuum model-	1D concurrent bridging scale

		II	
Week #11 Dec 5 Th:		Final project discussion	
Week #12 Dec 11 T:	Final Week	Final project Presentation	
Week #12 Dec 13 Th:			(Final Report Due)

Module 1: Introduction (5 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. Thermodynamics (0.5wk)

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

D. 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

E. Midterm Project (0.5 wk)

1. Students present their midterm project

Module 2: Polymer Nanocomposite (2.5 wks)

1. Introduction to Integrated Computational Material Engineering (ICME)
2. Introduction to Polymer
3. Molecular modeling and simulation of polymer
4. Force field for polymer
5. Mechanics of polymer and composite
    - Viscoelasticity, Creep, Stress relaxation, DMA test, Time-temperature superposition
6. Coarse graining molecular dynamics of polymer composite

Module 3: Data-driven Multiscale Modeling (1.5 wks)

1. Introduce basic terminology used in Data Science

2. Introduce different machine learning methods (supervised and unsupervised method: Principal Component Analysis (PCA), K-means clustering, Self-Organizing Map (SOM), Neural networks for regression and classification)
3. Data-driven methods in Multiscale Modeling (surrogate model, genetic programming, FFNN, CNN mechanics of materials problem)

Module 4: Special Topics (1.0 Wk)

A. Bridging atomistic to continuum model (1D Concurrent problem)