Molecular Modeling & Interface to Micromechanics (ME 317) Fall Quarter 2010 9:30-11am M120

Instructors: Wing Kam Liu, w-liu@northwestern.edu

Reference Material

- Liu, Wing Kam, Eduard G. Karpov and Harold S. Park. 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 Ted Belytschko. A First Course in Finite Elements. John Wiley & Sons, Ltd, 2007.
- Belytschko, Ted, Wing Kam Liu and Brian Moran. Nonlinear Finite Elements for Continua and Structures. John Wiley & Sons, Ltd, 2000.

Topics

Multi-scale Analysis Motivation and Techniques, Molecular Dynamics, Thermodynamics, Finite Elements, Applications

Course Objectives:

1) Understand the principles behind molecular dynamics (atom equations of motion and atom interactions)
2) Be able to implement a molecular dynamics simulation using available software (LAMMPS)
3) Understand the connection between information available on small (atomistic) and large (continuum) scales
4) Be able to use molecular dynamic simulation data in a finite element simulation (ANSYS) , and be able to explain the results

Grading

Class Participation (10%), Homework (30%), Midterm (30%),
Molecular Dynamics Presentation (10%), Final Project (20%)

Molecular Dynamics Presentation

Individuals present a molecular dynamics simulation in class. This simulation will be part of the final project. Presentations should include formulations, strengths and weaknesses.

Project

Individuals will choose a multi-scale topic to explore further and present to the class. Topic choice and summary (with preliminary references) are due on Tuesday 10/6/09. Midterm presentation will be 10 minutes long, and the final presentation will be 20 minutes.

Lab session will be held on Wed (if needed) or mutually agreeable time.

Date	Topic	Reading Assignment	Important Events
Week #1 T:	Why multiscale methods?	Liu – Chapter 1	*HW #1 given*
Week #1 W:	LAMMPS Setup	LAMMPS Tutorial	
Week #1 Th:	Molecular Dynamics I	Liu – Chapter 2	
Week #2 T:	Molecular Dynamics II	Liu – Chapter 3	
Week #2 W:	LAMMPS Files & Commands		**HW #1 due** *HW #2 given*
Week #2 Th:	Lattice Mechanics	Liu – Chapter 4	
Week #3 T:	Thermodynamics and Statistical Mechanics	Schroeder –	
Week #3 W:	LAMMPS Post-Processing & Questions		
Week #3 Th:	Thermodynamics and Statistical Mechanics		
Week #4 T:	Thermodynamics and Statistical Mechanics		
Week #4 W:	LAMMPS Questions		
Week #4 Th:	Thermostats		**HW #2 due**
Week #5 T:	Finite Element Intro		
Week #5 W:	ANSYS	U. Alberta Online ANSYS Tutorial	
Week #5 Th:	Comp Lab – ANSYS II		
Week #6 T:	**Midterm 1**		
Week #6 W:	**No Computer Lab**		
Week #6 Th:	**MD Presentation**		
Week #7 T:	Polymers		*HW #3 given*
Week #7 W:	Project/Homework Questions		
Week #7 Th:	Application: Nanocomposites		
Week #8 T:	Bridging Scale Method	Wagner, Liu, *J Comp Phys*, 190 (2003)	
Week #8 W:	Project/Homework Questions		
Week #8 Th:	Bridging Scale Method		
Week #9 T:	Bridging Domain Method	Xiao, Belytschko, *Comp Meth Appl Engrg*, 193 (2004)	
Week #9 W:	Project/Homework Questions		
Week #9 Th:	Bridging Domain Method		
Week #10 T:	Course Wrap-up		
Week #8 W:	Project/Homework Questions		
Week #10 Th:	No Class – Thanksgiving		
Week #11 T:	Review	Liu – Chapter 4	
Week #11 W:	Project/Homework Questions		
Week #11 Th:12/3	Course Wrap-up		**HW #3 due**