Molecular Dynamics Simulation (ME 850Z), Fall 2015

Department of Mechanical Engineering, Wichita State University

Instructor:	Dr. Gisuk Hwang
Office location/hours:	EB 101C, M/W 5:30pm – 7pm or by appointment
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Class schedule	M/W 7:00-8:35 pm, EB102
Prerequisites:	MATH 555 (Diff. Eqs. I), and ME 360C or AE 373 (Dynamics) or by instructor permission Basic knowledge of Matlab, Fortran, or C/C++ programming is preferred

Textbook: *Understanding Molecular Simulation: From Algorithms to Applications*, Academic Press, San Diego, by D. Frenkel and B. Smit, 1996

Course Description:

The aim of this course is to introduce the molecular simulation methods (classical molecular dynamics simulations and Monte-Carlo simulation) aiming at understanding fundamentals of the nanoscale mechanical, thermal, materials, energy, and bio systems and their engineering for desired functionalities. This course also includes the basics of the statistical thermodynamics (mechanics) and various key computer programing/simulation techniques.

Objectives:

a) To understand the fundamental knowledge of atomic-scale mechanical, material, and energy systems;

b) To make sound judgments on the quality of molecular simulation studies in the literature;

c) To decide whether molecular simulation is suited for application to the student research;

d) To know how to begin developing a simulation program applicable to the student research;

e) To understand the workings and limitations of commercial molecular simulation software.

Grading:

Homework	50%
Project Proposal Presentation	10%
Project Proposal Writing	10%
Final Oral Presentation	10%
Final Project Report	20%

Reading assignments & homework:

Students are strongly encouraged to go through the reading assignments and other course notes/websites before the class. Totally, 6-8 homework both on analytical problems and computer simulations will be assigned. Students are strongly encouraged to come to office hours for homework/projects, and to form study groups with your peers.

Extra credit and make-up assignments:

No extra credit work will be assigned/accepted. Make-up exams will be administered only upon the submission of the relevant documents, explaining the reasons for the missing ones.

Project:

Students can work on the project by themselves or in a team of two students. **If the students work as a team, the instructor will decide the team members.** Student/team could decide the project with the instructor's guidance. A project proposal writing, final oral presentation, and final project report contributes to the final credit (see schedule for the deadlines). Student/team must meet the instructor **at least three times** during the semester to discuss about the project goal, scope, progress, final presentation and report. The report, oral presentation evaluation criteria are provided in BlackBoard. Evaluation temples, the final grade will be made based on your peer review & instructions review.

Disciplinary Infractions and Ethical Behavior:

The use of laptops is allowed during the lesson but only for work related to the course activities. Discussions related to the grade will take place ONLY in in-person meetings scheduled by appointment via e-mail or during office hours. Students are expected to behave courteously and professionally. Disciplinary infractions will be reported to the university authorities.

Cheating/plagiarism policy:

Cheating/plagiarism is considered as a crime in this class, and will be reported to the police. The first time caught will result in the zero point with a verbal warning, and the second time caught will result in "F" grade with a police report.

Other course notes

http://www.courses.physics.helsinki.fi/fys/moldyn/

Molecular Simulations and Advanced Molecular Simulations (by Wei Cai, Stanford University)

A molecular dynamics primer (by Furio Ercolessi, University of Udine)

Molecular Dynamics I (video, .pdf), II (video, .pdf), III (video, .pdf by Nicola Marzari, MIT)

The lectures do not follow any particular book, but it is strongly encouraged to read the following books

- Allen and Tildeslay, Computer Simulation of Liquids, Oxford University Press (1989)
- Leach, Molecular Modelling: Principles and Applications, Prentice Hall (2001)
- Haile, Molecular Dynamics Simulation: Elementary Methods, Wiley Professional (1997)
- Tuckerman, Statistical Mechanics: Theory and Molecular Simulation, Oxford University Press (2010)
- Marx and Hutter, Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods, Cambridge University Press (2009)

The course is still under development, and the class schedule is subject to changes during the term. The tentative course schedule is given below.

Tentative Class Schedule (subject to changes)

Week	Date	Subject	Remark
1	8/17	Introductions and Overview	
	8/19	Review: thermodynamics	
2	8/24	Statistical thermodynamics: equilibrium and thermodynamic properties	
	8/26	Statistical thermodynamics: ensemble average	
3	8/31	Statistical thermodynamics: ideal gas and equation of state	
	9/2	Statistical thermodynamics: applications	Project
4	9/7	No class (labor day)	
	9/9	Basics of molecular dynamics algorithm and programming methods	
5	9/14	Introduction to molecular dynamics simulation (commercial) codes	
	9/16	Interatomic potentials: hard sphere, LJ, SW potentials	
6	9/21	Intraatomic potentials: harmonic potential, bond, angle, and torsion	
	9/23	Rigid molecules and orientation moves	
7	9/28	Force calculation and Integration: Verlet algorithm and others	
	9/30	Boundary conditions: periodic, open, and fix boundaries	
8	10/5	Midterm project presentation	
	10/7	Midterm project presentation	
9	10/12	No class (fall break)	
	10/14	Initial velocity distributions and handling neighbors	
10	10/19	Minimization (optimization)	
	10/21	Minimization (optimization)	
11	10/26	Constant energy: NVE	
	10/28	Constant temperature: NVT	
12	11/2	Constant temperature-pressure: NPT	
	11/4	Post-processing: kinetic and potential energies	
13	11/9	Post-processing: specific heat, diffusivity, viscosity	
	11/11	Monte-Carlo simulation: Introduction	
14	11/16	Monte-Carlo simulation: NVT and NPT ensemble	
	11/18	Monte-Carlo simulation: μVT	
15	11/23	Introductions to other atomic scale simulation methods: ab initio and coarse grain	
	11/25	No class (Thanksgiving)	
16	11/30	Final Project Presentation	
	12/3	Final Project Presentation	