24-623: Molecular Simulation of Materials

Spring 2010, 12 units

Scaife Hall 219, Monday & Wednesday, 9:30 AM–11:20 AM

Instructor: Professor Alan McGaughey
Scaife Hall 310
412-268-9605
mcgaughey@cmu.edu
Office hours: Monday, 11:30 AM - 12:30 PM

I. Description and Objectives

At length scales on the order of atomic spacings and time scales on the order of atomic vibrations, continuum descriptions of material behavior (e.g., the Fourier law of conduction, the beam equations) are no longer valid. To understand material behavior at these extreme scales, theories based on quantum mechanics and condensed matter physics are required. The resulting theoretical formulations can be very complex for even the simplest of systems. At the same time, designing and performing experiments to look at the phenomena of interest in these systems is very difficult. Numerical techniques for solving the governing equations and making observations at the atomic level are thus of critical importance for understanding the behavior of materials at the micro- and nano-scales. This area of research is of great interest in many technological applications, including the design and fabrication of electronic, optoelectronic, and chemical-sensing devices.

The purpose of this course is to expose students to the theory and implementation of numerical techniques for modeling atomic level behavior. The main focus will be on classical molecular dynamics (MD) and Monte Carlo (MC) simulations. Consideration will be given to heat transfer, mass transfer, fluid mechanics, mechanics, and materials science applications. The interests of the class will play a role in choosing the applications to be discussed. In the course, you will

- Write MD and MC codes and use them to perform computer experiments.
- Apply thermodynamics to understand the theoretical basis behind MD and MC calculation techniques (e.g., specific heat, thermal conductivity, elastic constants, etc.).
- Critically assess information from MD or MC calculations in the scientific literature in terms of technical correctness and physical relevance.

Students are expected to have taken an undergraduate thermodynamics course. Background knowledge in quantum mechanics, solid state physics, and statistical thermodynamics will be helpful but is not required. Computer programming is an integral part of the course but extensive previous experience is not required. Students are free to program in a language of their choice, but should note that the instructor will be of the most help with C++ (recommended) and Fortran. The use of math programs such as Matlab and Mathematica is strongly discouraged, as they will perform miserably for some of the required tasks. If you need extra material on any of these topics, please speak to the instructor.

II. Logistics

A. Class Time

There are two 2-hour meetings per week (the first class is January 11th). The time will include formal lecturing, computer demonstrations, and work in groups. You are responsible for all material discussed in class, whether you attended or not. Class will not be held on February 15.

Use of electronic devices (laptop computers, cell phones, mp3 players, dvd players, etc.) is not permitted in lecture. No student may record or tape any classroom activity without the express written consent of the instructor. If a student believes that he/she is disabled and needs to record or tape classroom activities, the student should contact the Office of Disability Resources to request an appropriate accommodation. In the event that such an accommodation has been arranged, the material may not be further copied, distributed, published, or otherwise used for any other purpose without the express written consent of the instructor.

B. Website

Course materials are available on Blackboard.

C. Reading Material

The textbook is: *Understanding Molecular Simulation*, 2nd Edition, D. Frenkel and B. Smit, Academic Press, 2002, ISBN 0122673514.

D. Grades

A: 90-100, A-: 85-89, B+: 80-84, B: 70-79, B-: 60-69, R: <60

Any grading disputes will be handled by the instructor. Any request for a grade change should be made to the instructor, in writing, within one week after the graded work is returned. Your entire submission will be subject to regrading. Cheating and plagiarism is unethical behavior and is not tolerated in this course or at Carnegie Mellon University. The Carnegie Mellon University policy on cheating and plagiarism will be strictly followed. Students are advised to read and adhere to the policy, which can be found at http://www.cmu.edu/policies/documents/Cheating.html.

(a) Homework assignments: 75%
There will be 6 homework assignments that will lead you through the development of your own MD and MC codes. There will be occasional pencil and paper problems in addition to the programming requirements. Students are encouraged to work together but must submit their own work for grading. If applicable, on your submission you must indicate who you worked with. The number of points for a homework will give its relative weight. Discussion about the homework will take place on Blackboard discussion boards. Do not email the instructor with questions. He will check the board at the end of most days. Homework must be handed in at the beginning of class on the day it is due. Homework handed in by the end of the day it is due will be penalized 25%. Homework handed in by the end of the day after it is due will be penalized 50%. Homework not submitted within one day of the due date will result in a grade of zero.

(b) Case study presentation and report: 25%
Each student will give a fifteen minute talk and prepare a report evaluating and critiquing at least two papers from the literature. More details will be provided later in the term.

E. Teaching Philosophy

Students are welcome to ask questions at all times. Don't be afraid to interrupt if a point is not clear. A statement of the instructor's teaching philosophy is on the Blackboard website.

III. Schedule

Week	Monday	Wednesday
1 Jan 11, 13	1. Course logistics, introduction to molecular simulation.	2. Physical origins of empirical potentials.
2 Jan 18, 20	3. Continuous vs. discrete systems, equations of motion.	4. LJ potential, framework of a MD code. **HW#1**
3 Jan 25, 27	5. Temperature and pressure, equilibration, averaging.	6. Periodic boundary conditions and cutoffs. Averaging.
4 Feb 1, 3	7. Temperature control in MD (NVT ensemble).	8. Ensemble vs. time averaging, structure of matter, radial distribution function. **HW#2**
5 Feb 8, 10	9. Pressure control in MD (NPT ensemble). Summary of MD methods.	10. Application: Diffusion and droplet evaporation.
6 Feb 15, 17	No class.	11. Application: Polyatomic fluids, water inside and outside carbon nanotubes. **HW#3**
7 Feb 22, 24	12. Introduction to statistical mechanics.	13. NVT Monte Carlo (Metropolis method).
8 March 1, 3	14. More on Metropolis method.	15. NPT Monte Carlo, Grand Canonical Monte Carlo. **HW#4**
9 March 15, 17	16. Measuring chemical potentials.	17. Review of Monte Carlo methods.
10 Mar 22, 24	18. Activated processes, transition state theory.	19. Transition state theory with MD and MC. **HW#5**
11 Mar 29, 31	20. Wissam Al-Saidi guest lecture: Quantum mechanics-based methods.	21. Mesoscale methods.
12 April 5, 7	22. Craig Maloney guest lecture: Parinello-Rhaman technique for full stress tensor control	23. John Thomas guest lecture: Fluid flow and heat transfer in carbon nanotubes. **HW#6**
13 April 12, 14	24. Application: Thermal transport in semiconductors.	25. Case study presentations.
14 April 19, 21	26. Application: TBA.	27. Case study presentations.
15 April 26, 28	28: Case study presentations.	29: Case study presentations. **Case study report due May 7.**

All information is subject to change