24-623/12-623: Molecular Simulation of Materials

Fall 2016, 12 units

Wean 5302, Monday & Wednesday, 9:30 AM–11:20 AM

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Office hours: Monday & Wednesday, 11:30 AM - 12:30 PM or by appointment.

I. Description, Objective, and Outcomes

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vibrations, continuum descriptions of material behavior (e.g., the Fourier law of conduction, the beam equations) are no longer valid.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, condensed matter physics, and statistical mechanics are required. The resulting theoretical formulations can be complex for even the simplest of systems. At the same time, designing and performing laboratory experiments to look at the phenomena of interest in these systems can be 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, energy conversion, and chemical-sensing devices.

The objective 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

- Compare and contrast atomistic and continuum-level modeling tools.
- Apply thermodynamics and statistical mechanics to understand the theoretical basis behind the MD and MC techniques.
- Write MD and MC computer codes and apply them to perform and interpret computer experiments.
- Critically assess results from MD and MC simulations presented 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, condensed matter physics, and statistical mechanics 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 or C++. 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 August 29th). The time will include formal lecturing, computer demonstrations, and group work. You are responsible for all material discussed in class, whether you attended or not. There will be a set of online videos that you will be required to watch. Class will not be held on November 21st.

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. Communication

The subject of any email sent to the instructor should start with "24-623:" Do not send the instructor emails regarding homework (see below).

D. Reading Material

There is no required textbook. You will be provided with notes and papers from the literature during the semester. The following books may be useful for reference:

- *Computer Simulation of Liquids*, M. P. Allen and D. J. Tildesly, Oxford, 1989, ISBN 0198556454.
- *Understanding Molecular Simulation*, 2nd Edition, D. Frenkel and B. Smit, Academic Press, 2002, ISBN 0122673514.
- *The Art of Molecular Dynamics Simulation*, D. C. Rapaport, Cambridge, 2004, ISBN 0521825687.

E. 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/student-and-student-life/academic-integrity.html.

(a) Homework assignments: 75%
There will be seven homework assignments that will lead you through the development of your own MD and MC codes. There will be occasional short writing exercises and 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 will be due on Thursdays at midnight and should be submitted to Blackboard. Please put all files (codes and one document that contains all your text and figures) into one zip file with the naming scheme (lastname)_HW(homework number).zip. For example, mcgaughey_HW3.zip. Homework submitted by noon of the day after it is due will be penalized 25%. Homework submitted by midnight of the day after it is due will be penalized 50%. Homework submitted after that time 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 papers from the literature. More details will be provided later in the semester.

F. 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 Blackboard.

G. Take Care of Yourself

Do your best to maintain a healthy lifestyle by eating well, exercising, getting enough sleep, and taking some time to relax. These steps will help you to achieve your goals and to cope with stress.

All of us benefit from support during times of struggle. There are resources available on campus and an important part of the college experience is learning how to ask for help. Asking sooner rather than later is often better. If you or anyone you know experiences academic stress, difficult life events, or feelings like anxiety or depression, I strongly encourage you to seek support. CMU Counseling and Psychological Services (CaPS) is available to help. Call 412-268-2922 and visit their website at http://www.cmu.edu/counseling/. Consider reaching out to a friend, faculty, or family member you trust to assist in getting connected to the support that can help.

III. Schedule

Homework is due on Thursday at midnight to Blackboard. All information is subject to change

Week/Days	Monday	Wednesday
1 08/29 08/31	1. Course logistics, introduction to molecular simulation	2. Continuous vs. discrete systems, coding workshop
2 09/07	Labor Day (no class)	3. Physical origins of empirical potentials VIDEO: Dimensionless LJ potential
3 (HW#1) 09/12 09/14	4. Equations of motion, energy calculation	5. Force calculation, initialization VIDEO: Visualization
4 09/19 09/21	6. Temperature and pressure VIDEO: Temperature VIDEO: Pressure	7. Averaging
5 (HW#2) 09/26 09/28	8. Cutoffs	9. Periodic boundary conditions
6 10/03 10/05	10. Temperature control in MD (*NVT* ensemble).	11. Pressure control in MD (*NPT* ensemble). VIDEO: *NPT* Ensemble
7 (HW#3) 10/10 10/12	12. Guest Lectures	13. LAMMPS workshop
8 10/17 10/19	14. Introduction to statistical mechanics	15. Integration, Metropolis algorithm
9 (HW#4) 10/24 10/26	16. *NVT* Monte Carlo I: Harmonic oscillator VIDEO: Harmonic Oscillator	17. *NVT* Monte Carlo II: Two-state system VIDEO: Two-state system
10 10/31 11/02	18. *NVT* Monte Carlo III: LJ Fluid	19. *NPT* Monte Carlo, grand canonical Monte Carlo
11 (HW#5) 11/07 11/09	20. Activated processes, transition state theory VIDEO: Transition State Theory	21. Transition state theory with Monte Carlo
12 11/14 11/16	22. Guest Lectures	23. Guest Lectures
13 (HW#6) 11/21	No class	Thanksgiving (no class)
14 11/28 11/30	24. Case study presentations	25. Case study presentations
15 (HW#7) 12/05 12/07	26. Case study presentations	27. Case study presentations