Atomistic Scale Simulations

Course Summary

This class covers computer simulations on atomistic length and time scales for (structural or thermodynamic) properties of materials, numerical algorithms, and systematic and statistical error estimations. Concepts of statistical mechanics such as phase space and averages are critically important for this class. For a detailed list of topics see Course Coverage.

Objectives

The objective is to learn and apply fundamental techniques used in (primarily classical) simulations in order to help understand and predict properties of microscopic systems in materials science, physics, chemistry, and biology. Students will work towards a final project, where they will define, model, implement, and study a particular problem using atomic-scale simulation techniques. Use of the Python programming language, writing of proper reports, and presentation of results are important components of this class.

Prerequisites

MSE401 (or equivalent) and its prerequisites. One of Python, C, C++, or Fortran programming experience. **If you have not passed a prerequisite course, please see the instructor before continuing. Also, if you have no prior coding experience, please talk to the instructor.**

Class

- **Location**: 144 Loomis Laboratory
- **Time**:   9:30 – 10:50 am onTuesdays and Thursdays, for a detailed schedule and due dates, see Class Schedule.
- **Sections**: CRN-64701 to CRN-64706

Enrolled students will receive an email with links to Campuswire, PrairieLearn and Gradescope in the first week of class.

This class utilizes **Campuswire** for communications, **Gradescope** and **PrairieLearn** for assignments. The course is divided by week and there are assignments and activities to be completed each week, including in-person lectures, homework, and quizzes. All class communications and interactions with other students, TAs, Graders, and me should follow common social standards for respect and courtesy; rude, abusive, or discriminatory language will not be tolerated. I will communicate with students using Campuswire and your Illinois email account; please check both regularly. Students can expect graded work to be returned within 10 days and questions will be answered as quickly as possible. Campuswire is preferred way to

communicate with me and the TAs, but I am also available via email in emergency situations, and Zoom (for office hours or a 1:1 meeting scheduled in advance).

Covid-19 policies

Following University policy, all students are required to engage in appropriate behavior to protect the health and safety of the community. Students are also required to follow the campus COVID-19 protocols.

Students who feel ill must not come to class. In addition, students who test positive for COVID-19 or have had an exposure that requires testing and/or quarantine **must not attend class**.

All students, faculty, staff, and visitors **are required to wear face coverings in classrooms and university spaces at all times**. This means **no eating and drinking** in the classroom. To account for that, we will take a 10 min break halfway through the lecture, so that everyone can leave the building for a few minutes. The mask policy is in accordance with CDC guidance and University policy and expected in this class. Please refer to the University of Illinois Urbana-Champaign's COVID-19 website for [further information on face coverings](#). Thank you for respecting all of our well-being so we can learn and interact together productively.

In order to implement COVID-19-related guidelines and policies affecting university operations, we will **ask students when entering the classroom to show their Building Access Status in the Safer Illinois app or the Boarding Pass**.

Students who fail to abide by these rules will first be asked to comply; if they refuse, they will be required to leave the classroom immediately. If a student is asked to leave the classroom, the non-compliant student will be judged to have an unexcused absence and reported to the Office for Student Conflict Resolution for disciplinary action. Accumulation of non-compliance complaints against a student may result in dismissal from the University.

Recommended Textbooks

- Understanding Molecular Simulation, *D. Frenkel and B. Smit*, Second Edition (Academic Press, 2001).
- Computational Materials Science, *Richard LeS*ar, Cambridge University Press, 2013.
- A Guide to Monte Carlo Simulations in Statistical Physics, David P. *Landau*, Kurt *Binder*, Cambridge University Press
- Computer Simulation of Liquids 2nd Edition, Michael Allen, Dominic Tildesley, Oxford Science Publications

Course Coverage

- **Molecular Dynamics:** integration algorithms, static and dynamic correlations functions and their connection to order and transport.

- **Monte Carlo and Random Walks:** variance reduction, Metropolis algorithms, Kinetic Monte Carlo, heat diffusion, Brownian motion, etc.
- **Phase Transitions:** melting-freezing, calculating free energies.
- **Polymers:** growth and equilibrium structure.
- **Quantum Simulation:** zero temperature and finite temperature methods.
- **Optimization techniques** such as simulated annealing.

Homework

Homework assignments for this class will be issued via Gradescope (see Class Schedule). Students need to complete the assignment and reports are to be submitted on Gradescope, usually **every second week, Thursdays 6pm CT**. Students are strongly encouraged to complete all assignments to assess their own understanding of the course material. It is acceptable to work with fellow students on homework problems, and to ask as well as answer questions pertaining homework online on Campuswire. Plagiarism will not be tolerated, each student must submit their own solutions.

Late submissions will be penalized by 50 % for each day late, unless excused in advance. You need to contact me directly if you are late. Your homework reports must be submitted electronically via Gradescope. The only format for the report that will be accepted for submission is a single, properly-ordered PDF, in portrait format; your name must be printed legibly on the top of the first page. These homework assignments require you to write code that is **bug free and actually works**. This code will be automatically graded and checked using the PrairieLearn web site, which will provide you with immediate feedback, allowing you to fix buggy code before using it to prepare the data needed to write your reports. The TAs grade only your report.

The written homework reports are assigned to practice the communication of scientific concepts in writing. They will be graded based on presentation, neatness, correct use of symbols, quality of drawings and diagrams, and clarity of explanation. Reports should be typed, neat and organized! Tables and graphical representations of results need to be generated using some software program such as Python, MatLab, etc., rather than being hand-drawn. Correct interpretation and implementation of the problem and correct final answers are important.

Quizzes

S*hort* online multiple-choice quizzes will be issued via Gradescope (see Class Schedule), usually due on **Thursdays 6pm CT**, to gauge elementary understanding and mastery of the course material. Each quiz has a **time limit of 60 minutes and can be attempted only once.** Late submissions will be penalized by 50 % for each day late, unless excused in advance. You need to contact me directly if you are late.

Group Project

The group project consists of a status report, final project presentation, and project report. In the next few weeks, we will form teams that balance interests, programming ability, and experience. Each team will be given (i) a collective grade for a **status report/proposal/abstract** and its **presentation** in class, (ii) a collective grade for the **final report**, and (iii) a collective grade for the **presentation of the final results**. For your status report and final report we will use peer review, which will also be part of your grade. We expect the project itself to take into account:·

- **Scientific Research:** Each project should be research oriented, something concerning new developments in classical or quantum simulations and with a scientific component.
- **Algorithm development:** This could involve an optimization of an existing code or algorithm, a new implementation, some interesting science, the use of new computer architectures, or databases.
- **Presentation:** We expect a written report from each team that explains your project. This should include graphics, literature links, and potentially web references. With your permission, we may use these in future years as examples of class projects. You will also give an **oral presentation** (13 min including questions) of your project at the end of the semester during the time allotted for the final exam.

Prior to the status report/abstract/proposal, 2-4 slides used for this presentation (including references) need to be submitted to GradeScope. It needs to outline a problem ("Scientific Research") and explain what the team will do to solve it ("Algorithm development"), according to the criteria given above. You will give an **oral presentation** (5 min) of your project status report.

The final reports and the final presentations need to be submitted electronically via GradeScope. Late submissions will be penalized by 50 % for each day late, unless excused in advance. You need to contact me directly if you are late. If you have any questions about the suitability of your project please get in touch with me.

Office hours

TA office hours will be held, see Campuswire for location and time. Do not ask TAs to work the homework problems before they are due; it is fine to ask specific questions on the details of your attempted solutions, or to work out problems that are similar to homework problems.

Instructor office hours by appointment only; Please contact me via Campuswire in advance.

Plagiarism

Each student is responsible for submitting their own original quiz responses, homework assignments, and each group is responsible for submitting their own original project. Collaborative interaction is permissible and encouraged via Campuswire and in-person interactions, but each student must perform all coding, writing, and calculations themselves, and submit their own work, except for the group project where group submissions are expected.

Plagiarism will not be tolerated, and verified incidents will result in all parties receiving a zero on their project and formal academic sanctions. Students are responsible for familiarizing themselves with the definition and penalties for plagiarism detailed in [Section I-401 of the UIUC Student Code](). Ignorance of these policies is not an excuse for any academic dishonesty. As a student it is your responsibility to refrain from infractions of academic integrity and from conduct that aids others in such infractions. A short guide to academic integrity issues may be found [here](). Do not hesitate to ask the instructor(s) if you are ever in doubt about what constitutes plagiarism, cheating, or any other breach of academic integrity. Note that the code's definition of plagiarism includes "copying another student's paper or working with another person when both submit similar papers without authorization to satisfy an individual assignment".

Please note that all course materials are protected by copyright and are considered intellectual property. Course materials should only be used for this course and should not be shared with anyone not in the course, including uploading to a study site, social media, or other online sharing mechanisms.

Grading

Homework: 50%

Quizzes: 10%

Project: 40%

Letter grades will be based on final aggregate student scores, with numerical cutoffs specified by the instructor. However, students with aggregate scores >96% are guaranteed *at least* an A, >86% *at least* a B, and >76% *at least* a C (i.e. cutoffs will not be higher than these values).

Tentative Class Schedule

The schedule is preliminary. Check for updates in the first week of class!

Class	Date	Day	Lecture Topic	Due Dates
1	Aug 24	Tu	Course Introduction Motivation, Statistics	
2	Aug 26	T	Statistics, Statistical Mechanics	
3	Aug 31	Tu	Molecular Dynamics	Quiz #1 due
4	Sep 2	T	Potentials and Forces	HW #1 due
5	Sep 7	Tu	TBD	Quiz #2 due
6	Sep 9	T	TBD	
7	Sep 14	Tu	TBD	Quiz #3 due
8	Sep 16	T	TBD	HW #2 due

9	Sep 21	Tu	TBD	Quiz #4 due
10	Sep 23	T	TBD	Teams formed
11	Sep 28	Tu	TBD	Quiz #5 due
12	Sep 30	T	TBD	HW #3 due
13	Oct 5	Tu	TBD	Quiz #6 due
14	Oct 7	T	TBD	
15	Oct 12	Tu	TBD	Quiz #7 due
16	Oct 14	T	TBD	HW #4 due
17	Oct 19	Tu	**STATUS REPORT PRESENTATIONS**	Status Report due
18	Oct 21	T	TBD	
19	Oct 26	Tu	TBD	Quiz #8 due
20	Oct 28	T	TBD	HW #5 due
21	Nov 2	Tu	TBD	Quiz #9 due
22	Nov 4	T	TBD	
23	Nov 9	Tu	TBD	Quiz #10 due
24	Nov 11	T	TBD	HW #6 due
25	Nov 16	Tu	TBD	Quiz #11 due
26	Nov 18	T	TBD	
	Nov 20-28		**FALL BREAK**	
27	Nov 30	Tu	TBD	Quiz #12 due, Final presentation slides are due
28	Dec 2	T	**FINAL PRESENTATIONS**	
29	Dec 7	Tu	**FINAL PRESENTATIONS**	Final reports are due

Changes to syllabus

Changes to the syllabus or schedule may occur as deemed necessary by the instructor; they will be announced.

Anti-Racism and Inclusivity Statement

The Grainger College of Engineering is committed to the creation of an anti-racist, inclusive community that welcomes diversity along a number of dimensions, including, but not limited to,

race, ethnicity and national origins, gender and gender identity, sexuality, disability status, class, age, or religious beliefs. The College recognizes that we are learning together in the midst of the Black Lives Matter movement, that Black, Hispanic, and Indigenous voices and contributions have largely either been excluded from, or not recognized in, science and engineering, and that both overt racism and micro-aggressions threaten the well-being of our students and our university community.

The effectiveness of this course is dependent upon each of us to create a safe and encouraging learning environment that allows for the open exchange of ideas while also ensuring equitable opportunities and respect for all of us. Everyone is expected to help establish and maintain an environment where students, staff, and faculty can contribute without fear of personal ridicule, or intolerant or offensive language. If you witness or experience racism, discrimination, micro-aggressions, or other offensive behavior, you are encouraged to bring this to the attention of the course director if you feel comfortable. You can also report these behaviors to the Bias Assessment and Response Team (BART) (https://bart.illinois.edu/)**.** Based on your report, BART members will follow up and reach out to students to make sure they have the support they need to be healthy and safe. If the reported behavior also violates university policy, staff in the Office for Student Conflict Resolution may respond as well and will take appropriate action.

Mental Health

Diminished mental health, including significant stress, isolation, mood changes, excessive worry, substance/alcohol abuse, or problems with eating and/or sleeping can interfere with optimal academic performance, social development, and emotional wellbeing. The University of Illinois offers a variety of confidential services including individual and group counseling, crisis intervention, psychiatric services, and specialized screenings at no additional cost. If you or someone you know experiences any of the above mental health concerns, it is strongly encouraged to contact or visit any of the University's resources provided below. Getting help is a smart and courageous thing to do -- for yourself and for those who care about you.

Counseling Center: 217-333-3704, 610 East John Street Champaign, IL 61820

McKinley Health Center: 217-333-2700, 1109 South Lincoln Avenue, Urbana, Illinois 61801

Disability-Related Accommodations

To obtain disability-related academic adjustments and/or auxiliary aids, students with disabilities must contact the course instructor and the Disability Resources and Educational Services (DRES) as soon as possible. To contact DRES, you may visit 1207 S. Oak St., Champaign, call 333-4603, e-mail disability@illinois.edu or go to https://www.disability.illinois.edu. If you are concerned you have a disability-related condition that is impacting your academic progress, there are academic screening appointments available that can help diagnosis a previously undiagnosed disability. You may access these by visiting the DRES website and selecting "Request an Academic Screening" at the bottom of the page.

Family Educational Rights and Privacy Act (FERPA)

Any student who has suppressed their directory information pursuant to Family Educational Rights and Privacy Act (FERPA) should self-identify to the instructor to ensure protection of the privacy of their attendance in this course. See https://registrar.illinois.edu/academic-records/ferpa/ for more information on FERPA.

Religious Observances

Illinois law requires the University to reasonably accommodate its students' religious beliefs, observances, and practices in regard to admissions, class attendance, and the scheduling of examinations and work requirements. You should examine this syllabus at the beginning of the semester for potential conflicts between course deadlines and any of your religious observances. If a conflict exists, you should notify your instructor of the conflict and follow the procedure at https://odos.illinois.edu/community-of-care/resources/students/religious-observances/ to request appropriate accommodations. This should be done in the first two weeks of classes.

Sexual Misconduct Reporting Obligation

The University of Illinois is committed to combating sexual misconduct. Faculty and staff members are required to report any instances of sexual misconduct to the University's Title IX Office. In turn, an individual with the Title IX Office will provide information about rights and options, including accommodations, support services, the campus disciplinary process, and law enforcement options.

A list of the designated University employees who, as counselors, confidential advisors, and medical professionals, do not have this reporting responsibility and can maintain confidentiality, can be found here: wecare.illinois.edu/resources/students/#confidential.

Other information about resources and reporting is available here: wecare.illinois.edu.