Fall 2025-MSE 485-Atomic Scale Simulations-

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**: 4101 MSEB
- **Time**: 9:30 – 10:50 am on Tuesdays and Thursdays
- **Sections**: CRN-64701 to CRN-64706

This class utilizes **Canvas** for communications/assignments 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/surveys. 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 Canvas and 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. Canvas is the 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).

Students who are ill must not come to class. There is no penalty for not attending class.

Recommended Textbooks

- Understanding Molecular Simulation, *D. Frenkel and B. Smit*, Second Edition (Academic Press, 2001).
- Computational Materials Science, *Richard LeSar*, 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 Models:** intramolecular and pair interactions, force fields, periodic boundary conditions
- **Statistical Mechanics and Thermodynamics:** ensembles, measurements, phase space, averages
- **Molecular Dynamics:** integration algorithms, static and dynamic correlations functions and their connection to order and transport.
- **Monte Carlo:** Metropolis algorithms, Kinetic Monte Carlo,

Homework

Homework assignments for this class will be issued via Canvas. Students need to complete the assignment and reports are to be submitted on Canvas, usually **every second week, Fridays**. 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 Canvas. 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 prepared using Overleaf and submitted electronically via Canvas.

Quizzes/Pre-lecture surveys

Short online quizzes will be issued via Canvas usually due on **Mondays**, to gauge elementary understanding and mastery of the course material. These quizzes/surveys

will be ***graded on completion and effort*** and serve the purpose to encourage you to familiarize yourself with the next weeks content before lecture.

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 **proposal/abstract**, and a **first draft** , (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** (~15 min including questions) of your project at the end of the semester during the time allotted for the final exam.

A abstract/proposal must be submitted. 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 halfway through the semester.

The final reports and the final presentations need to be submitted electronically via Canvas. 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.

All project code and its development history must be in GitHub. All reports must be prepared in Overleaf.

Office hours

TA office hours will be held, TBD. 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 TBD

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 Canvas 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".

All assignments should be fully prepared by the students. Developing strong competencies in the skills associated with this course, from student-based coding, writing, to project development, will prepare you for success in your degree pathway and, ultimately, a competitive career. Therefore, the use of generative AI tools to complete any aspect of assignments for this course are not permitted and will be treated as plagiarism.

Please note that all course materials are protected by copyright and are considered intellectual property. Uploading course materials to a (cheating) study site or a large language model is considered a violation of copyright.

Grading

Homework: 40%

Quizzes: 10%

Project: 50%

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).

Schedule

1. Overview
2. Molecular Models
    1. Periodic Boundary Conditions
    2. Intramolecular Potentials
    3. Short-ranged Potentials
    4. Electrostatics / Ewald Summation
3. Statmech & Thermo
    1. Statistics / Python
    2. Statistical Mechanics
    3. Thermodynamics, Properties
    4. Structural Correlations
    5. Transport Coefficients
4. Molecular Dynamics
    1. Classical Mechanics
    2. Verlet Integration
    3. Thermostats
    4. Langevin Dynamics
    5. Constraints for MD
    6. MD Packages
    7. Initialization / Neighbor search
    8. HPC, Discussion of MD
5. Monte Carlo
    1. Random Numbers
    2. Monte Carlo

3. Metropolis
4. NVT / GC Monte Carlo
5. Phase Coexistence
6. Finite Size Effects

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.