MSE 485/CSE 485/PHYS 466: Atomic-Scale Simulations

Fall 2023

Schedule
TR 9:30-10:50am in 305 Materials Science and Engineering Building

Course content
• Course website: courses.engr.illinois.edu/mse485; PDF syllabus
• Code grading: PrairieLearn
• Homework report deposit: GradeScope (entry code K326P6)
• Announcements, discussion forums: Slack; email Prof. Trinkle to be added.

Scope
• 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
• Computational approaches based on molecular dynamics and Monte Carlo
• Limited discussion of quantum simulations (zero temperature and finite temperature methods) and optimization techniques (simulated annealing)

Objectives
Students will be able to
1. explain fundamentals of molecular dynamics: integration algorithms, static and dynamic correlations functions, and their connection to order and transport
2. explain fundamentals of Monte Carlo and random walks: variance reduction, Metropolis algorithms, kinetic Monte Carlo, heat diffusion, Brownian motion
3. apply molecular dynamics and Monte Carlo to relevant material problems, such as
   1. phase transitions (melting/freezing, calculating free energies)
   2. polymers (growth and equilibrium structure)
4. determine proper parameters for a simulation;
5. determine if a simulation result is reliable based on the underlying physical principles in the simulation;
6. systematically analyze data to extract meaningful materials quantities.

Prerequisites

- Thermodynamics of Materials
  - MSE 401, or equivalent (MSE 500)
- Programming experience
  - Python, C, C++, or Fortran

If you have not passed a prerequisite course or are concerned about your background (especially if you have no prior programming experience), please see the instructor before continuing.

Instructor

Dallas R. Trinkle (dtrinkle@illinois.edu; 308 MSEB in the west stairwell).

- Professor and Associate Head (joined Univ. Illinois in 2006)
- Computational materials science
  - Crystalline defects (dislocations, point defects, interfaces) from density functional theory
  - Development of new algorithms, computational tools
  - Solid solution softening / strengthening, pipe diffusion, general theory of diffusion
- Office hours: Thursday 11:00-11:50am; or by appointment.

Teaching assistant: Cunwei Fan (cfan11@illinois.edu) and Rephayah Black (rlb8@illinois.edu)

Teaching approach: Lecture + Hands-on project-based learning

An “active learning” approach where we focus on the course objectives: understanding and applying computational modeling tools to simulate material behavior, determine if a simulation is reliable, and use a systematic approach to computation. You will:

- Develop simulation tools from the ground up
- Practice using computational tools to sample phase space;
- Determine appropriate simulation parameters using systematic techniques;
- Integrate theoretical and computational methods to understand physical phenomena;
- Communicate your results and understanding in written form.

Over the course of the semester, you will implement statistical analysis, molecular dynamics, and Monte Carlo techniques to atomic-scale simulations.

Logistics

- Classes will consist of
  - in-class lecture/discussion about theory and practical aspects
  - demonstrations of computational approaches as appropriate
Homework

Homework will be assigned through the MSE 485 website and assignments are due 11:59 pm the day posted on the MSE 485 website. Late submissions will be penalized by 50% for each day late, unless excused in advance. Your 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 TA grades only your report.

The written 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 neat and organized! More details and an example will be provided. Tables and graphical representations of results need to be generated using some software program such as Python, Excel, TecPlot, MatLab, etc., rather than being hand-drawn. Correct interpretation and implementation of the problem and correct final answers are important.

Projects

In the next few weeks, we will form teams that balance interests, programming ability, and experience. The team will be given (i) a collective grade for a status report 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 of your project at the end of the semester during the time allotted for the final exam.

Prior to the status report, two slides used for this presentation need to 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. Also the final reports and the final presentations need to be submitted electronically. Late submissions will be penalized by 50% for each day late. **If you have any questions about the suitability of your project please get in touch with the instructor.**
Grading

Breakdown:

- **25%** Homework (code)
- **25%** Homework (report)
- **5%** Status report
- **15%** Final presentation
- **15%** Final report
- **5%** Peer review Status report
- **10%** Peer review Final report

Letter grades:

- A+ (>97), A (>93), A- (>90)
- B+ (>87), B (>83), B- (>80)
- C+ (>77), C (>73), C- (>70)
- D+ (>67), D (>63), D- (>60)

Expectations

To succeed in this class, you will need to

- study assigned reading material before coming to class, and formulate questions;
- participate in the class;
- be able to write Python code;
- make sure you understand the homework problems and solutions;
- propose, develop, implement, and present a computational problem together with a team;
- seek out help when you have trouble.

*Obtaining help:* The main two ways to obtain help are online at Canvas or in person at office hours. Please do not send email directly to TAs or professors for routine help or absences! In cases of emergencies related to assignments (e.g., illness) you should contact your professor at the earliest possible opportunity.

Formal and Informal Accommodations

I am committed to assisting students requiring special accommodations for circumstances that are registered with the DRES Student Services Department. These formal accommodations should be discussed with me as early as possible in the semester or as soon after DRES approval as possible.

If you are not formally registered with DRES and have anxiety, depression, learning disabilities, or other issues that affect your ability to fully participate and learn in this class, you are encouraged to check-in with me so we can determine together the kind of support you need to thrive in this class. Please set up a meeting with me via email.
Inclusion and Diversity

I value all students regardless of their background, race, religion (creed), ethnicity, gender, gender expression, age, country of origin, disability status, marital status, sexual orientation, or military status, etc., and am committed to providing a climate of excellence and inclusiveness within all aspects of the course. If there are aspects of your culture or identity that you would like to share with me as they relate to your success in this class, I am happy to meet to discuss. Likewise, if you have any concerns in this area of facing any special issues or challenges, you are encouraged to discuss the matter with me (set up a meeting via email) with an assurance of full confidentiality (only exception being mandatory reporting of academic integrity / code violation and sexual harassment). Harassment or discrimination of any kind will not be tolerated.

Anti-Racism and Inclusivity Statement

The intent is to raise student and instructor awareness of the ongoing threat of bias and racism and of the need to take personal responsibility in creating an inclusive learning environment.

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.

Learning Environment

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 Office of the Vice Chancellor for Diversity, Equity and Inclusion (OVCDEI). Based on your report, OVCDEI 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.

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 ODOS 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/confidentiality.

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

**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 FERPA info for more information on FERPA.

**Academic Integrity**

You are bound by the University Honor Code in this course. Any violation of the Honor Code will result in disciplinary action.

Students are responsible for producing their own work. Collaborative interaction is encouraged, but each student must do their own individual prelecture work, and contribute their own work to the group. **Plagiarism will not be tolerated, and verified incidents will result in all parties receiving a zero and formal academic sanctions.** Students are responsible for familiarizing themselves with the definition of and penalties for plagiarism in Section I-401 of the UIUC Student Code. Note that plagiarism includes “copying another student’s paper or working with another person when both submit similar papers without authorization to satisfy an individual assignment.”

**Changes to syllabus**

May occur as deemed necessary by the professor; they will be announced via Canvas and the updated syllabus posted on the course website.

**Calendar**

Suggested readings are from

<table>
<thead>
<tr>
<th>Lecture day</th>
<th>Reading</th>
<th>Topic</th>
<th>notes</th>
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</thead>
<tbody>
<tr>
<td>T Aug 22</td>
<td>Orientation, Introduction, Statistics I</td>
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<tr>
<td>R Aug 24</td>
<td>Statistical errors, Frenkel Smit (Chapter 4 and Appendix D), LeSar (Appendix G)</td>
<td>Statistics and Errors</td>
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<tr>
<td>T Aug 29</td>
<td>Stat. mech, Frenkel Smit (Chapter 2), LeSar (Appendix D, G)</td>
<td>Correlation, Bias; Python and example notebook</td>
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<td>R Aug 31</td>
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<td>Statistical mechanics</td>
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<tr>
<td>T Sep 5</td>
<td>MD 1, MD 2, Frenkel Smit (Chapter 4), LeSar (Chapter 3)</td>
<td>Molecular dynamics, boundary conditions and measurement; forces, time propagation</td>
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<tr>
<td>R Sep 7</td>
<td>Potentials, Frenkel Smit (Appendix F), LeSar (Chapter 5)</td>
<td>Molecular dynamics: Code, force fields</td>
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<tr>
<td>T Sep 12</td>
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<td>Molecular dynamics: force fields II</td>
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<td>R Sep 14</td>
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<td>Molecular dynamics: correlation functions</td>
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<tr>
<td>T Sep 19</td>
<td>Correlations</td>
<td>Pair correlation functions</td>
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<tr>
<td>R Sep 21</td>
<td>Dynamics, MD ensembles, Frenkel Smit (Chapter 6, Appendix B, C, E), LeSar (Chapter 6)</td>
<td>Thermostats</td>
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<td>T Sep 26</td>
<td>Monte Carlo intro</td>
<td>Intro to Monte Carlo</td>
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<tr>
<td>R Sep 28</td>
<td>Sampling</td>
<td>Random numbers and psuedorandom number generators</td>
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<tr>
<td>T Oct 3</td>
<td>Importance Sampling, Random walk, Frenkel Smit (Chapter 3), LeSar (Chapter 7)</td>
<td>Non-uniform distributions</td>
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<td>R Oct 5</td>
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<td>Variance reduction</td>
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<td>T Oct 10</td>
<td>Alternate MC schemes, Frenkel Smit (Chapter 13, 17)</td>
<td>Alternate Monte Carlo schemes</td>
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<td>R Oct 12</td>
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<td>Brownian dynamics</td>
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<td>T Oct 17</td>
<td>no class</td>
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<tr>
<td>R Oct 19</td>
<td>no class</td>
<td>HW4/pdf due 10/20 upload</td>
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<tr>
<td>Lecture day</td>
<td>Reading</td>
<td>Topic</td>
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<td>T Oct 24</td>
<td>Kinetic MC, Frenkel Smit</td>
<td>Kinetic Monte Carlo</td>
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<td>(Chapter 8), LeSar (Chapter 9)</td>
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<td>R Oct 26</td>
<td>Lattice MC, Advanced MC,</td>
<td>MC and Ising model</td>
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<td>LeSar (Chapter 7)</td>
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<td>T Oct 31</td>
<td>no class</td>
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<td>R Nov 2</td>
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<td>Phase transitions and critical slowing down</td>
<td>HW5/pdf due 11/03 upload</td>
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<td>T Nov 7</td>
<td>Frankel Smit (Chapter 15)</td>
<td>Ewald summation</td>
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<td>R Nov 9</td>
<td>Free energy, Frenkel Smit</td>
<td>Free energy techniques</td>
<td>Project proposal draft</td>
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<td>(Chapter 7, 11)</td>
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<td>due 11/10</td>
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<td>T Nov 14</td>
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<td>Constraints in MD + Constraints: polymers</td>
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<td>R Nov 16</td>
<td>Project proposal presentations</td>
<td>Peer review due 11/17</td>
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<td>T Nov 26</td>
<td>no class (fall break)</td>
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<tr>
<td>R Nov 28</td>
<td>no class (fall break)</td>
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<tr>
<td>T Nov 28</td>
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<td>Quantum mechanics for electrons</td>
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<tr>
<td>R Nov 30</td>
<td>Quantum mechanics for electrons</td>
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<td>HW6/pdf due 12/01 upload</td>
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<td>T Dec 5</td>
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<td>Review and questions</td>
<td>Final report due 12/6</td>
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<td>R Dec 7</td>
<td>no class (reading day)</td>
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<tr>
<td>F Dec 8</td>
<td>1:30-4:30pm</td>
<td>Final presentations (exam week)</td>
<td>slides due 10:00am</td>
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<tr>
<td>R Dec 14</td>
<td>no class</td>
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<td>Peer review due 12/14</td>
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**Accessing library resources**

The Univ. Illinois library has access to a huge variety of electronic resources; this plus additional online resources will be our references. Many can be accessed from the library’s website, or via the campus VPN. Alternatively, you can take advantage of the library proxy. This is done by appending `proxy2.library.illinois.edu` to the web address; when reloaded, you will be asked for Univ. Illinois authentication, and then will be able to access the resource as if you were on campus. In general, this authentication is required only once per session. So, the website


would become

http://journals.aps.org.proxy2.library.illinois.edu/prl/abstract/10.1103/PhysRevLett.113.025504
Alternatively, install the Proxy Bookmarklet which makes it extremely easy to use the proxy. I highly recommend this method.