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

Fall 2019

Schedule

TR 9:30-10:50am in 3217 Everitt Laboratory

Course content

- Course website: courses.engr.illinois.edu/mse485; PDF syllabus
- Code grading: PrairieLearn
- Homework report deposit: GradeScope
- Announcements, gradebook, and online discussion forums: Canvas

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; @DallasTrinkle; 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: by appointment only; quick discussions after class as appropriate

Teaching assistant: Han-Yi Chou (grading; hchou10@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 experi-
ence. 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 through Canvas.

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 Canvas) 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.
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 code, reports, and projects. Collaborative interaction is encouraged, but each student must do their own implementation, perform all calculations themselves, and write their own reports. **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

<table>
<thead>
<tr>
<th>Lecture day</th>
<th>Reading</th>
<th>Topic</th>
<th>notes</th>
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<tbody>
<tr>
<td>T Aug 27</td>
<td></td>
<td>Orientation, Introduction, Statistics I</td>
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<tr>
<td>R Aug 29</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 Sep 03</td>
<td>Stat. mech, Frenkel Smit (Chapter 2), LeSar (Appendix D, G)</td>
<td>Correlation, Bias; Python</td>
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<tr>
<td>R Sep 05</td>
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<td>Statistical mechanics</td>
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<td>T Sep 10</td>
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<td>Molecular dynamics, boundary conditions and measurement</td>
<td>HW1 due 9/13 upload</td>
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<td>R Sep 12</td>
<td>MD 1, MD 2, Frenkel Smit (Chapter 4), LeSar (Chapter 3)</td>
<td>Molecular dynamics, forces, time propagation</td>
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<tr>
<td>T Sep 17</td>
<td>Potentials, Frenkel Smit (Appendix F), LeSar (Chapter 5)</td>
<td>Molecular dynamics: Code, force fields</td>
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<tr>
<td>R Sep 19</td>
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<td>Molecular dynamics: force fields II</td>
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<tr>
<td>T Sep 24</td>
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<td>Molecular dynamics: correlation functions</td>
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<td>R Sep 26</td>
<td>Correlations</td>
<td>Pair correlation functions</td>
<td>HW2 due 9/27</td>
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<td>T Oct 01</td>
<td>Dynamics, MD ensembles, Frenkel Smit (Chapter 6, Appendix B, C, E), LeSar (Chapter 6)</td>
<td>Linear response and correlations; Fourier interpolation</td>
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<td>R Oct 03</td>
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<td>Thermostats</td>
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<td>T Oct 08</td>
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<td>Random numbers and psuedorandom number generators</td>
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<td>R Oct 10</td>
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<td>Tests for pseudorandom number generators</td>
<td>HW3 due 10/11</td>
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<td>T Oct 15</td>
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<td>Non-uniform distributions</td>
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<td>R Oct 17</td>
<td>Monte Carlo intro, Sampling, Importance Sampling, Random walk, Frenkel Smit (Chapter 3), LeSar (Chapter 7)</td>
<td>Variance reduction</td>
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<td>T Oct 22</td>
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<td>Metropolis algorithm</td>
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<td>R Oct 24</td>
<td>Alternate MC schemes, Frenkel Smit (Chapter 13, 17)</td>
<td>Alternate Monte Carlo schemes</td>
<td>HW4 due 10/25</td>
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<td>Kinetic MC, Frenkel Smit (Chapter 8), LeSar (Chapter 9)</td>
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<td>Lattice MC, Advanced MC, LeSar (Chapter 7)</td>
<td>MC and Ising model</td>
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<td>T Nov 05</td>
<td>Free energy, Frenkel Smit (Chapter 7, 11)</td>
<td>Free energy techniques</td>
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<td>Frankel Smit (Chapter 15)</td>
<td>Constraints in MD</td>
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<td>T Nov 12</td>
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<td>Constraints: polymers</td>
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<td>R Nov 14</td>
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<td>R Nov 28</td>
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<td>T Dec 03</td>
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<td>R Dec 12</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.

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