

**Schedule:** T/R 11:00 am – 12:20 pm; 218 Ceramics

**Course websites:**

- Class schedule, lecture slides/recordings, homework assignments, links: [MSE 485 website](#)
- Code grading: [PRAIRIELEARN](#)
- Homework report deposit: [GradeScope](#)
- Gradebook: [Compass](#)
- Announcements, online discussion forums: [Piazza](#)

**Scope:**

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. Students will become familiar with popular techniques to sample phase space, such as molecular dynamics (integration algorithms, static and dynamic correlations functions, and their connection to order and transport) and Monte Carlo and Random Walks (variance reduction, Metropolis algorithms, kinetic Monte Carlo, heat diffusion, Brownian motion). Example applications will include phase transitions (melting-freezing, calculating free energies) and polymers (growth and equilibrium structure). In addition, quantum simulations (zero temperature and finite temperature methods) and optimization techniques (e.g. simulated annealing) will be discussed.

**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.*

**Instructor:** André Schleife ([schleife](#); 204A MSEB).

*Office hours:* By appointment only; Please contact instructor via [Piazza](#) in advance.

**Teaching Assistants:** Chadwick Fan ([cfan11](#)), William Wheeler ([wawheel2](#)), Xiongjie Yu ([xyu40](#)).

*Office hours:* see [Piazza](#) for times and location of the TA office hours.

**Recommended Texts:** *Understanding Molecular Simulation*, D. Frenkel and B. Smit, Second Edition (Academic Press, 2001). *Computational Materials Science*, Richard LeSar, Cambridge University Press, 2013.

**Special accommodations:** To obtain disability-related academic adjustments and/or auxiliary aids, students with disabilities must contact their lecturer and the Disability Resources and Educational Services (DRES, [disability.illinois.edu](#)) as soon as possible, and no later than Sep. 1.

**i>clickers:** Quizzes will be administered in lectures using the i>clickers. The i>clicker remote may be purchased at any of the book stores and must be registered on [Compass](#). The navigation bar on the left of the MSE485 page should have an item “Register my i>clicker”. **You need to register your i>clicker by**

Sep. 8, when the i>clicker roster will be synced for the last time.

Course evaluation:

$$25\% \times \text{Homework (Code)} + 25\% \times \text{Homework (Report)} + 10\% \times \text{In-lecture i>clicker} + 5\% \times \text{Status Report} + 10\% \times \text{Final Presentation} + 15\% \times \text{Final Report} + 5\% \times \text{Peer Review Status Report} + 5\% \times \text{Peer Review Final Report} = \text{Total}$$

**Numerical total score corresponds to the following final grades:**

A+ (97 – 100)	B+ (87 – 89)	C+ (77 – 79)	D+ (67 – 69)		
A (93 – 96)	B (83 – 86)	C (73 – 76)	D (63 – 66)	F (0 – 59)	
A- (90 – 92)	B- (80 – 82)	C- (70 – 72)	D- (60 – 62)		

**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 TAs grade 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.

**Lectures:** Prompt and regular attendance at lectures is required to obtain credit for i>clicker quizzes: 80 % participation, 20 % correctness. Your lowest four i>clicker scores will be dropped.

**Status Report, Final Project Presentation, and Project Report:** 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.*

**Grade Reporting:** All assessment scores are stored in the gradebook in [Compass](#). Any errors appearing in the gradebook must be reported within 1 week of the grade being posted in the gradebook or by the last day of class, whichever is earlier. If you have a missing grade, contact the instructor.

**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 [Piazza](#) 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 exams (e.g., illness) you should contact your professor at the earliest possible opportunity.

**Online Forum (Piazza):** This class uses [Piazza](#) for all communication between the instructor, TAs, and students. Please visit [piazza.com/illinois/fall2017/phys466mse485cse485](http://piazza.com/illinois/fall2017/phys466mse485cse485) to register. The [Piazza](#) link will take you to the current class page at any time. Official class announcements will be sent via [Piazza](#), so you must register with an email address that you regularly check. If you desire, you can post anonymously on [Piazza](#) or make a private post just to the instructors (this should be done rather than emailing the professor directly). *Note that Piazza should be used to communicate with your instructors, rather than email.*

**Office Hours:** TA office hours will be held, see [Piazza](#) 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.

**Absences:** Excused Absence Request Form: [illinois.edu/fb/sec/6866545](http://illinois.edu/fb/sec/6866545)

1. Excuses from assessments will only be given in the following circumstances:
  - (a) Illness.
  - (b) Personal crisis (e.g., car accident, required court appearance, death of a close relative).
  - (c) Required attendance at an official UIUC activity (e.g., varsity athletics, band concert).
2. In all cases you must complete the online Excused Absence Request Form and upload a scan of the official written documentation explaining your absence.
3. In cases (a) or (b) an official excuse letter from the Dean on Duty must be submitted via the online form within 2 weeks of the due date of the missed assessment, but no later than reading day (Dec. 14). In cases of extended or unusual illness, late submission of excuse documentation will be considered. See [Student Assistance Center](#).
4. In case (c) an official letter from the designated university official must be submitted via the online form at least one week prior to the due date of the missed assessment.

5. Notwithstanding the above, at the professor's discretion you may be required to make up any excused work or attend substitute instruction or assessment.

**Academic Integrity, Harassment, and Discrimination:** You are bound by the [University Honor Code](#) in this course. Any violation of the Honor Code will result in disciplinary action. In addition, harassment or discrimination of any kind will not be tolerated. Please report any concerns immediately to your professor.

**Changes to syllabus:** may occur as deemed necessary by the professor; they will be announced.

**Calendar and Topics:** Changes to schedule will be announced; see [MSE 485 website](#) calendar for topics, specific assignments, and to remain up to date.