Schedule: M/W/F 3:00 pm – 3:50 pm; 305 MSEB

Course websites:
- Class schedule, lecture slides/recordings, homework assignments, links: MSE 485 website
- Gradebook: Compass
- Announcements, online discussion forums: Piazza

Scope:
This class connects simulation results and properties of materials (structural or thermodynamic quantities), as well as numerical algorithms and systematic and statistical error estimations. Students will become familiar with 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), phase transitions (melting-freezing, calculating free energies), polymers (growth and equilibrium structure), quantum simulation (zero temperature and finite temperature methods), optimization techniques (e.g. simulated annealing).

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.

Prerequisites: MSE401 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.

Instructor: André Schleife (schleife; 204A MSEB).
Office hours: By appointment only; Please contact instructor via Piazza in advance.

Teaching Assistants: William Wheeler (wawheel2), Xianhao Xin (xin2).
Office hours: see Piazza for times and location of the TA office hours.


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 Aug. 28.

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

Course evaluation:

\[ 50\% \times \text{Homework} + 10\% \times \text{In-lecture i>clicker} + \\
10\% \times \text{Project Proposal} + 15\% \times \text{Final Presentation} + 15\% \times \text{Final Report} = \text{Total} \]
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 at 11.59 pm on the day posted on the MSE 485 website. Late submissions will be penalized by 50% for each day late. Your solutions must be submitted electronically via the Homework Upload link: Choose “MSE” as course subject and “485” as course number, then pick the respective assignment to upload. 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. In addition, you must also submit the code that you wrote in order to generate the data in the report. This code needs to be submitted ready to run either as one single ZIP file, or as an “iPython notebook”. The TAs grade the report and code. You may submit each report a maximum of two times; only the latest submission will be graded.

These 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 (50%). Reports should be neat and organized! 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 (50%). Point breakdown for the written report:

- 1: Correct interpretation of the problem
- 2: Correct final answer(s) in the report
- 2: Code is ready to run and reproduces the data/conclusions in the report
- 1: Presentation quality
- 1: Clarity of explanation
- 1: Clear drawings and diagrams
- 1: Correct use of symbolic work
- 1: Use of units on numerical answers

**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.

**Project Proposal, Final Project Presentation, and Project Report**: In 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 project proposal 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. We expect this project 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**: Instead of a written report, we expect you to develop an iPython notebook to explain your project. This should include graphics, literature links, and potentially web references. With your permission, we may use these notebooks in futures 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 proposal presentations, the one-slide proposal used for this presentation needs to be uploaded using the Homework Upload link. Also the final reports and the final presentations need to be uploaded using the Homework Upload link. 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;
· 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/fall2015/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/1b/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. 10). 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.