

MSE 454:

Computational Approaches in Materials Science & Engineering

Course description

Computational approaches are becoming to be a driving force for advances in materials discovery and development. This course will focus on the computational methods and tools used in the MSE community. In the introductory part of the course, students will have broad exposure to the advantages, disadvantages, and pitfalls associated with various methods, the concepts behind the methods, and the basics of numerical modeling and simulation. The hands-on laboratory sessions, homework problems, and class project will provide a first-hand learning experience in modeling.

This course is partially flipped, meaning (1) there are some lectures you must watch and some preparation reading/work to be completed (such as the quizzes) before coming to the class and (2) students make presents (one mini-lecture and final project presentation). This frees up time to work on difficult task in class when the instructor can help with the task as needed. If there are any concerns with this format, please contact Katsuyo Thornton to discuss more details to ensure the class fits your academic plan.

Course Information

Location of Class:	EECS 2331 (CAEN Computer Lab)
Time:	Wednesdays & Fridays 1:30-3PM
Instructor:	Katsuyo Thornton
Office Location:	Zoom (See Canvas for the link)
Telephone:	(734) 615-1498 - the voicemail will be forwarded to my email.
Office Hours:	Will be set based on instructor/student availability
E-Mail:	mse454instructors@umich.edu to contact instructors (include "MSE454" in the subject line)

Prerequisites

The course is primarily intended for seniors meeting the prerequisites (or equivalent) in materials science and related fields and graduate students who are interested in gaining a broad background in computational materials science. Because we build on the materials taught in MSE330, 335, and 365, they are included in the formal prerequisites. However, they are waived for undergraduate students with equivalent background and for graduate students generally. Basic understanding of relevant science (materials science in particular) is required. Most of the work would involve running tools and writing a small MATLAB scripts or modifying them. While programming experience is not required, it is expected that students learn what is needed to carry out the homework and project. Basic mathematics covered in the required math courses (Math 115/116/215/216) is required. We will review and cover some mathematics

(especially partial differential equations), but if some topics look unfamiliar to you, please let me know so I can provide reading materials.

Textbook

There is no required textbook. Reading materials are provided within Canvas. Occasionally, reading materials will be given from papers or books. There will be some books on reserve shortly.

Course Topics and Schedule

See the course schedule on Canvas or pdf.

Grading

Exam	25 percent
Quizzes	5 percent
Homework/Lab Reports	30 percent
Group Project Report	15 percent
Group Final Presentation	10 percent
Project Check-Ins	5 percent
Mini-Presentation	5 percent
Attendance	5 percent
Participation	See below

The project peer evaluations will be used to scale the points for project report and final oral presentation.

Participation will be considered when giving a letter grade, especially in borderline cases.

Exam

An in-class exam will be held on Friday, November 17, 2023, the week before the Thanksgiving break week. The exam will test the basic knowledge about computational methods discussed in the course up to that time. There will be no final exam.

Quizzes

There will be post-lecture quizzes to make sure students grasp important points from the lecture and readings.

Homework assignments

Homework assignments are given every 1-2 weeks, primarily based on the hands-on computational laboratory. All assignments are due at 11:59PM (one minute before midnight) Eastern Time on the due date.

Project

The major emphasis of this course will be on the final project. During the early part of the semester, teams will be formed, and each team will choose a topic of their own.

The project results will be summarized in both a written report (jointly written, but each student leading a specific portion) and an oral presentation (jointly presented). There will be intermediate assignments, including short oral presentations and written progress reports. Again, all assignments are due at 11:59PM (one minute before midnight) Eastern Time on the due date.

Mini-Presentations

Each student will select a topic and present it in class. This could be a tutorial for a tool not covered in the class, a presentation on a published literature (within computational materials science & engineering, or deeper look at a method beyond covered in the class. There will be a sign up for a date, and you must obtain an approval for the topic.

Course Policies

1. The course schedule, course syllabus, and course policy are subject to change. In the event of any changes, a updated information will be posted on the course website.
2. Lecture and laboratory topics are included in the schedule. Reading assignments and homework due dates will be announced in the class.
3. No collaboration is allowed during the exam. Collaboration is encouraged on homework assignments and projects, but students must submit their own work unless otherwise noted.
4. Again, all assignments are due at 11:59PM (one minute before midnight) Eastern Time on the due date. Late submissions without previously obtained approval (with valid reasons) will be penalized following the schedule below:

Up to 12 hours:	10%
Up to 24 hours:	20%
Up to 2 days:	40%
Up to 3 days	60%

6. Late homework beyond 3 days is not accepted without an acceptable reason.
7. Late assignments must be submitted via Canvas, and the timestamp on the site will be used for the penalty calculation.
8. If you are experiencing a technical problem during the submission, email the assignment to the instructor (with an appropriate subject line), which will serve as the time stamp, and when the technical issue is resolved, submit it on Canvas.
9. Students are responsible for keeping themselves updated with the homework assignments, homework dues, exam date(s), and other course work and deadlines.
10. Attendance in class is expected and required, as working individually or in pair during the class is a key part of the course. If you must miss it, please contact the instructor to

notify ahead of the time and ask your classmates to obtain information you may have missed.

11. Any grading errors must be reported to the instructor within seven days (including the weekend) after the graded homework is returned. They must be reported through Canvas email with a note describing the error to your original assignment. The use of Canvas in this case provides the time stamp for the submission. Please follow up if you do not hear back within a reasonable time.

Reference Books

Although there are numerous books on the subjects discussed in class, I selected several books that are available online or at the Art, Architecture and Engineering Library. They are not intended to be required readings. Rather, they are intended to help you gain further understanding of the topics covered in the course, as well as providing a starting point for topics outside of the course coverage. Other references will be provided time to time during the semester.

- R. J. LeVeque, Finite Difference Methods for Ordinary and Partial Differential Equations Steady-State and Time-Dependent Problems, SIAM (2007).

<https://epubs-siam-org.proxy.lib.umich.edu/doi/book/10.1137/1.9780898717839>

- E. Atkinson, An Introduction to Numerical Analysis, Wiley (1989).
- E. Süli and D.F. Mayers, An Introduction to Numerical Analysis, Cambridge University Press (2003).

<https://www-cambridge-org.proxy.lib.umich.edu/core/books/an-introduction-to-numerical-analysis/FD8BCAD7FE68002E2179DFF68B8B7237>

- Frankel and B. Smit, Understanding Molecular Simulation, Academic Press (1996).

<https://www-sciencedirect-com.proxy.lib.umich.edu/book/9780122673511/understanding-molecular-simulation>

- David Potter, Computational Physics, Wiley (1977). On reserve.
- William H. Press, Saul A. Teukolsky, William T. Vetterling, and Brian P. Flannery, Numerical Recipes, second edition, Cambridge University Press (1993).
<http://numerical.recipes>
- Raabe, Computational Materials Science: The Simulation of Materials Microstructures and Properties, Wiley (1998).

<https://onlinelibrary-wiley-com.proxy.lib.umich.edu/doi/book/10.1002/3527601945>

- C. Zienkiewicz and R. L. Taylor, Finite Element Method, Vol. 1

<https://app.knovel.com/web/toc.v/cid:kpFEMIBFEA/>

- Mark F. Horstemeyer, Integrated Computational Materials Engineering (ICME) for Metals: Using Multiscale Modeling to Invigorate Engineering Design with Science, Wiley, (2012).

<https://onlinelibrary-wiley-com.proxy.lib.umich.edu/doi/book/10.1002/9781118342664>

Additional Useful Information to Support Your Success:

Additional useful information is provided in Module 1. Please be sure to read all of the pages contained.

Attributions and Copyright:

Attributions for content are listed as necessary. When an attribution is not mentioned, content was created by the instructor, Katsuyo Thornton, who will hold the copyright 2023. *Please contact the instructor if you wish to share any course materials* (that do not have a specific attribution) with individuals not in the class. This includes, lecture files, lecture outlines, assignments, quiz, and exam questions, and YouTube links to the course lectures. Thank you for your cooperation.

MSE 454 Tentative Course Topics and Schedule (as of 8/31/23)

Week	Class #	Mod #	Date		Topic	Note
1	1	1	8/30/23	W	Course Information; Overview	
1	2	2	9/1/23	F	Basics in Computation & Programming	
2	3	2	9/6/23	W	Let's learn MATLAB or Python IDE	Project Interest Due
2	4	2	9/8/23	F	Cellular Automata (CA) Lecture/Lab with MATLAB	
3	5	3	9/13/23	W	Partial Differential Equations and Other Math Topics (including Fourier Trans.)	Project team formation
3	6	3	9/15/23	F	Finite Difference Methods	CA due
4	7	3	9/20/23	W	Finite Difference Methods Lab (Diffusion)	
4	8	4	9/22/23	F	Phase Field Method	Project check
5	9	4	9/27/23	W	Phase Field (PF) Method Lab	Diffusion due
5	10	5	9/29/23	F	Finite Element Method (FEM)	Project check
6	11	5	10/4/23	W	FEM Lab (COMSOL)	PF due
6	12	6	10/6/23	F	Density Functional Theory (DFT)	Project check
7	13	6	10/11/23	W	DFT Lab	FEM due
7	14	7	10/13/23	F	Computational Thermodynamics	Project check
8	15	7	10/18/23	W	Thermo-Calc Lab	DFT due
8	16	8	10/20/23	F	Molecular Dynamics	Project check
9	17	9	10/25/23	W	Monte Carlo Method	Thermo due
9	18	9	10/27/23	F	Monte Carlo Lab	Project check
10	19	9	11/1/23	W	Kinetic Monte Carlo Method	
10	20		11/3/23	F	Project Review/Workshop	MC due
11	21	10	11/8/23	W	MGI/ICME and PRISMS Center (John Allison)	
11	22	11	11/10/23	F	PRISMS Software Lab	
12	23		11/15/23	W	Exam Review	
12	24		11/17/23	F	Exam	Exam
13			11/22/23	W	No class - Thanksgiving break	
13			11/24/23	F	No class - Thanksgiving break	
14	25	12	11/29/23	W	Introduction to Data Science in MSE	
14	26	13	12/1/23	F	Special Topics	
15	27		12/6/23	W	Project Presentations	Last class
16	FINAL REP.		12/13/23	W	Final Paper Due at 6PM	Final paper