AME 4970/5970-008: Computational Materials Science (Spring 2024)
Tuesdays and Thursdays 9:00 – 10:15 AM
Felgar Hall, Room 334

Instructor: Dr. Shuozhi Xu
Office: Felgar Hall, Room 236
Email: shuozhixu@ou.edu
Phone: 405-325-1737 (office)
Office Hours: Tuesdays 10:20 – 11:50 AM, Wednesdays 10:20 – 11:50 AM, or by appointment
(students will be notified beforehand if some office hours are to be offered via Zoom)

TA: None

Textbook:
Introduction to Computational Materials Science: Fundamentals to Applications
Richard LeSar, 1st edition, Cambridge University Press, 2013.

Learning Goals:
By the end of the course, students will be able to…
1. Learn about common computational materials science approaches at different length and time scales.
2. Understand the fundamental principles of two approaches: the atomistic simulation method and the phase-field method.
3. Utilize software tools to perform simulations.
4. Develop skills in data analysis and visualization to interpret simulation results.
5. Explore the state-of-the-art developments in computational materials science.

Topics:
1. Common computational materials science approaches (Week 1–2)
2. The atomistic simulation method (Weeks 2–8)
3. Seminars (Week 8–9)
4. The phase-field method (Weeks 11–14)

Grade Distribution:

Students who are registered for AME 4970
Homework (4) 40%
Mid-term exam (2) 30%
Project data submission (1) 8%
Project presentation (1) 12%
[**The final grade of each AME 4970 student will be scaled by 100/90**]

Students who are registered for AME 5970
Homework (4) 40%
Mid-term exam (2) 30%
Project data submission (1) 8%
Project presentation (1) 12%
Report (1) 10%

Grading Policy:
90+ .....A
80-89 .....B
70-79 C
60-69 .....D
-59 .....F

Canvas:
All lectures, homework assignments, solutions, and grades will be posted on Canvas (https://canvas.ou.edu/). The students should submit all homework, the project, and the report to Canvas.

Late Submission and Missed Exam(s):
Unless the instructor gives prior approval, each day (24 hours) of late submission will result in a deduction of 3 points (out of 100 points) for that submission. If your submission is late for more than five days (120 hours), you will get zero point. A missed exam counts as zero and there will be no make-up exam unless a valid excuse from a physician or a university authority is presented to the instructor.

Classroom Policies:
Each class period, each student is expected to bring a laptop, which may be used for programming exercises. Please refrain from doing homework or other activities during class. Turn your cell phones to silent when you enter.

Academic Support:
The Gallogly College of Engineering has the infrastructure in place to help you succeed and to get you the support you need. Make sure you take advantage of the infrastructure available to you. For more information, please visit: https://www.ou.edu/coe/academics/student-support

Academic Integrity Policy:
Academic integrity means honesty and responsibility in scholarship. Academic assignments exist to help students learn; grades exist to show how fully this goal is attained. Therefore, all work and all grades should result from the student's own understanding and effort. Academic misconduct is any act which improperly affects the evaluation of a student's academic performance or achievement. Misconduct occurs when the student either knows or reasonably should know that the act constitutes academic misconduct. For more information, please visit: https://www.ou.edu/integrity/students

Use of Generative AI in Coursework:
Students may use generative AI tools such as ChatGPT, Bing AI, or Bard, to help them learn course content, complete course assignments, or do other course-related tasks. In the meantime, students are expected to provide attribution for any text created using generative AI tools as appropriate.

Reasonable Accommodation Policy:
OU is committed to the goal of achieving equal educational opportunity and full participation for students with disabilities. OU ensures that no "qualified individual with a disability" will be excluded from participation in, be denied the benefits of, or otherwise be subjected to discrimination solely on the basis of disability under any program or activity offered by OU. Therefore, if you have a disability that may prevent the full demonstration of your abilities in this course, please contact me personally as soon as possible so I can provide an appropriate contact to discuss accommodations necessary to ensure full participation and facilitate your educational opportunities. The OU Accessibility and Disability Resource Center (ADRC) provides support services to students with disabilities, see https://www.ou.edu/adrc, or contact the Center at adrc@ou.edu or 405-325-3852.

Adjustments for Pregnancy/Childbirth Related Issues:
Should you need modifications or adjustments to your course requirements because of documented pregnancy-related or childbirth-related issues, please contact me or ADRC to discuss. Modifications will be made where medically necessary and similar in scope to accommodations based on temporary disability. For more information, please visit: https://www.ou.edu/content/dam/eoo/documents/faqs/faqs-pregnant-and-parenting-students.pdf

Mental Health Support:
The University Counseling Center provides comprehensive mental health services. One of their missions is to provide high quality counseling and crisis intervention to the campus community members, including students. They strive to promote the psychological wellbeing of all members of the university community. They remain committed to the practice of psychology as governed by applicable professional ethics codes and by federal and state laws. For more information, please visit: https://www.ou.edu/ucc

Title IX Resources and Reporting Requirement:
Anyone who has been impacted by gender-based violence, including dating violence, domestic violence, stalking, harassment, and sexual assault, deserves access to resources so that they are supported personally and academically. OU is committed to offering resources to those impacted, including: speaking with someone confidentially about your options, medical attention, counseling, reporting, academic support, and safety plans. If you would like to speak with someone confidentially, please contact OU Advocates (https://www.ou.edu/gec/gender-based-violence/advocates, available 24/7 at 405-615-0013) or another confidential resource (see "Can I make an anonymous report?" on this page: https://www.ou.edu/gec/gender-based-violence/learn-more). You may also choose to report gender-based violence and discrimination through other means, including by contacting the Institutional Equity Office (https://www.ou.edu/eoo, ieo@ou.edu, 405-325-3546) or police (911). Because OU is committed to the safety of you and other students, I, as well as other faculty, Graduate Assistants, and Teaching Assistants, are mandatory reporters. This means that we are obligated to report gender-based violence that has been disclosed to us to the Institutional Equity Office. This includes disclosures that occur in: class discussion, writing assignments, discussion boards, emails and during Student/Office Hours.

Tentative Semester Schedule:

Week	Date	Topic	Notes	Week	Date	Topic	Notes
1	1/16	No class	Bad weather	9	3/12	Seminars	
	1/18	Overview			3/14	Seminars	HW 3 due
2	1/23	Introduction	HW 1 assigned	10	3/19	No class	Spring vacation
	1/25	Atomistics #1			3/21	No class	Spring vacation
3	1/30	Atomistics #2	HW 1 due	11	3/26	Phase-field #1	HW 3 solution
	2/1	Atomistics #3			3/28	Phase-field #2	HW 4 assigned
4	2/6	Atomistics #4	HW 1 solution	12	4/2	Phase-field #3	
	2/8	Atomistics #5			4/4	Phase-field #4	HW 4 due
5	2/13	Atomistics #6	HW 2 assigned	13	4/9	Phase-field #5	
	2/15	Atomistics #7			4/11	Review	HW 4 solution
6	2/20	Atomistics #8	HW 2 due	14	4/16	Mid-term exam #2	Covers phase-field
	2/22	Atomistics #9			4/18	Project presentation via Zoom	
7	2/27	Atomistics #10	HW 2 solution	15	4/23	Project presentation via Zoom	
	2/29	Review	Project assigned		4/25	Project presentation via Zoom	AME 4970 student project due
8	3/5	Mid-term exam #1	Covers atomistics	16	4/30	Project presentation via Zoom	AME 5970 student report due
	3/7	Seminars	HW 3 assigned		5/2	Project presentation via Zoom	AME 5970 student project due

Zoom link: https://oklahoma.zoom.us/j/97026199957?pwd=RlRpOFlKbys2Q1F0eXRQalkvNG0vUT09 (only users with an OU Zoom account can join)
Final exam: None
Project data: Submissions may be formatted as plain text files or Excel spreadsheets. Alternatively, a Google Drive link, a Dropbox link, or other cloud storage service links may be submitted on Canvas.
Project presentations: Students who are registered for AME 4970 will do the presentations first, because of the OU policy on the pre-finals week's schedule for undergraduate courses.
Project data and presentation slides: different due dates for AME 4970 and AME 5970 students
Report: NOT required for AME 4970 students. Each AME 5970 student is required to submit a report reviewing the application of computational materials science (including materials informatics) in a specific research field (e.g., his/her own research field). A single PDF file is required for submission. For details, see the slides for the first class.