AME 4970/5970: Computational Materials Science (Spring 2026)
Tuesdays and Thursdays 12:00 – 1:15 PM
Felgar Hall, Room 319

Instructor: Dr. Shuozhi Xu
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Email: shuozhixu@ou.edu
Phone: 405-325-1737 (office)
Office Hours: Tuesdays 10:00 – 11:30 AM, Thursdays 10:00 – 11:30 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.

Prerequisite for AME 4970:
AME 3723 or MATH 3401

Prerequisite for AME 5970:
AME 3723 or MATH 3401

Learning Outcomes:
1. Identify and compare ≥8 computational materials methods across length/time scales, producing a chart that correctly classifies each and lists ≥2 pros/cons per method.
2. Explain governing equations/assumptions for atomistic simulations, density functional theory, and phase-field method, and correctly solve 4–6 multi-step problems.
3. Create a reproducible LAMMPS workflow (inputs + scripts) to simulate benchmark systems and compute ≥2 material properties that match reference values within a tolerance of ±10%.
4. Implement a Quantum ESPRESSO-based workflow to simulate a benchmark system, ensuring that at least 2 calculated properties meet a ±10% accuracy threshold compared to literature standards.
5. Implement in MATLAB a phase-field simulation, demonstrate numerical verification, and quantify microstructural metrics with a goodness-of-fit ≥ 0.9.
6. Produce publication-quality figures and a short memo interpreting trends from atomistic, density functional theory, or phase-field simulation outputs, plus a 12-minute presentation that introduces one's own project work.

Topics:
1. Common computational materials science approaches (Week 1)
2. The atomistic simulation method (Weeks 2–7)
3. Seminars (Week 8)
4. Density functional theory (Weeks 10–11)
5. The phase-field method (Weeks 11–14)

Grade Distribution:
Homework (4) 20%
Mid-term exam (2) 40%
Project data submission (1) 20%
Project presentation (1) 20%
[*AME 4970 students will work on one project while AME 5970 students will work on two projects.*]

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

Canvas:
All lectures, homework assignments, project, solutions, and grades will be posted on Canvas (https://canvas.ou.edu/). The students should submit their answers to homework assignments and project 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 5 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 Policy:
Each class period, each student is expected to bring a laptop, which may be used for programming exercises. Please refrain from working on homework or other activities during class, and silence your cell phones upon entering. Attendance will not be taken, but active participation is highly encouraged.

Generative AI Policy:
Use of generative AI is not permitted during exams. However, for all other tasks (homework assignments, project etc) in this course, you:

- May use any free Generative AI tools, including those provided to you by the university, such as Copilot (https://itsupport.ou.edu/TDClient/30/Unified/KB/ArticleDet?ID=3173) and AI tools with Adobe Creative Cloud (https://itsupport.ou.edu/TDClient/30/Unified/Requests/ServiceDet?ID=46, available in campus computer labs). This will allow everyone in the course to have the same access to Generative AI.
- Are expected to cite your usage of Generative AI, including any direct quotes or paraphrasing of ideas/content generated by AI, per the class's citation guidelines.

Deviating from the acknowledgement guidelines described here may be considered a violation of the academic integrity policy of this course.

Final Exam Preparation Period:
Pre-finals week will be defined as the seven calendar days before the first day of finals. Faculty may cover new course material throughout this week. For specific provisions of the policy please refer to OU's Final Exam Preparation Period policy: https://www.ou.edu/registrar/academic-records/academic-calendars/final-exam-policies

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

Reasonable Accommodation Policy:
OU is committed to the goal of achieving equal educational opportunity and full educational participation for students with disabilities. If you have not yet established services through the Accessibility and Disability Resource Center (ADRC), but have a documented disability and require accommodations, please complete ADRC's pre-registration form (https://cm.maxient.com/reportingform.php?UnivofOklahoma&layout_id=350) to begin the registration process. ADRC facilitates the interactive process that establishes reasonable accommodations for students at OU. For more information on ADRC registration procedures, please contact ADRC at (405)325-3852 or adrc@ou.edu, or visit www.ou.edu/adrc for more information. If you have already established reasonable accommodations with ADRC, please log into iAdvise to request your semester accommodations as soon as possible and contact me privately, so that we have adequate time to arrange your approved academic accommodations. Note: disabilities may include, but are not limited to, mental health, chronic health, physical, vision, hearing, learning and attention disabilities, pregnancy-related. ADRC can also support students experiencing temporary medical conditions.

Religious Observance:
It is the policy of the University to excuse the absences of students that result from religious observances and to reschedule examinations and additional required classwork that may fall on religious holidays, without penalty. [See Faculty Handbook (https://www.ou.edu/provost/faculty-affairs/faculty-handbook) 3.15.2]

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 ADRC at 405/325-3852 and/or the Institutional Equity Office at 405/325-3546 as soon as possible. Also, see the Institutional Equity Office FAQ on Pregnant and Parenting Students' Rights (https://www.ou.edu/content/dam/eoo/documents/faqs/faqs-pregnant-and-parenting-students.pdf) for answers to commonly asked questions.

Mental Health Support Services:
Support is available for any student experiencing mental health issues that are impacting their academic success. Students can either been seen at the University Counseling Center (UCC) located on the second floor of Goddard Health Center or receive 24/7/365 crisis support from a licensed mental health provider through TimelyCare (https://www.ou.edu/studentaffairs/resources/timelycare). To schedule an appointment or receive more information about mental health resources at OU please call the UCC at 405-325-2911 or visit UCC (https://www.ou.edu/ucc), located at 620 Elm Ave., Room 201, Norman, OK 73019.

Title IX Resources and Reporting Requirement:
OU faculty are committed to creating a safe learning environment for all members of our community, free from gender and sex-based discrimination, including sexual harassment, domestic and dating violence, sexual assault, and stalking, in accordance with Title IX. There are resources available to those impacted, including: speaking with someone confidentially about your options, medical attention, counseling, reporting, academic support, and safety plans. If you have (or someone you know has) experienced any form of sex or gender-based discrimination or violence and wish to speak with someone confidentially, please contact OU Advocates (https://www.ou.edu/advocacyandeducaon/ou-advocates, available 24/7 at 405-615-0013) or UCC. Because OU is committed to the safety of you and other students, and because of our Title IX obligations, 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 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. You may also choose to report directly to the Institutional Equity Office. After a report is filed, the Title IX Coordinator will reach out to provide resources, support, and information and the reported information will remain private. For more information regarding the University's Title IX Grievance procedures, reporting, or support measures, please visit Institutional Equity Office (https://www.ou.edu/eoo) at 405-325-3546.

Emergency Protocol:
During an emergency, there are official university procedures (https://www.ou.edu/campussafety/policy-and-procedures) that will maximize your safety.
Severe Weather: If you receive an OU Alert to seek refuge or hear a tornado siren that signals severe weather,

1. Look for severe weather refuge location maps located inside most OU buildings near the entrances.
2. Seek refuge inside a building. Do not leave one building to seek shelter in another building that you deem safer. If outside, get into the nearest building.
3. Go to the building's severe weather refuge location. If you do not know where that is, go to the lowest level possible and seek refuge in an innermost room. Avoid outside doors and windows.
4. Get in, Get down, Cover up
5. Wait for official notice to resume normal activities.

Additional Weather Safety Information is available through the Department of Campus Safety: https://www.ou.edu/campussafety/divisions#management

Fire Alarm: If you receive an OU Alert that there is danger inside or near the building, or the fire alarm inside the building activates:

1. LEAVE the building. Do not use the elevators.
2. KNOW at least two building exits
3. ASSIST those that may need help
4. PROCEED to the emergency assembly area
5. ONCE safely outside, NOTIFY first responders of anyone that may still be inside building due to mobility issues.
6. WAIT for official notice before attempting to re-enter the building.

For more information, watch the video for OU Fire Safety on Campus: https://vimeo.com/125093634

The University of Oklahoma Active Threat Guidance:
OU embraces a Run, Hide, Fight strategy for active threats on campus. This strategy is well known, widely accepted, and proven to save lives. To receive emergency campus alerts, be sure to update your contact information and preferences in the account settings section at https://one.ou.edu.
RUN: Running away from the threat is usually the best option. If it is safe to run, run as far away from the threat as possible. Call 911 when you are in a safe location and let them know from which OU campus you're calling from and location of active threat.
HIDE: If running is not practical, the next best option is to hide. Lock and barricade all doors; turn of all lights; turn down your phone's volume; search for improvised weapons; hide behind solid objects and walls; and hide yourself completely and stay quiet. Remain in place until law enforcement arrives. Be patient and remain hidden.
FIGHT: If you are unable to run or hide, the last best option is to fight. Have one or more improvised weapons with you and be prepared to attack. Attack them when they are least expecting it and hit them where it hurts most: the face (specifically eyes, nose, and ears), the throat, the diaphragm (solar plexus), and the groin.
Please save OUPD's contact information in your phone.
NORMAN campus: For non-emergencies call (405) 325-1717. For emergencies call (405) 325-1911 or dial 911.
TULSA campus: For non-emergencies call (918) 660-3900. For emergencies call (918) 660-3333 or dial 911.

Tentative Semester Schedule:

Week	Date	Topic	Notes	Week	Date	Topic	Notes
1	1/20	Overview		9	3/16	No class	Spring vacation
	1/22	Introduction			3/20	No class	Spring vacation
2	1/27	Atomistics #1	HW 1 assigned	10	3/24	DFT #1	HW 3 assigned
	1/29	Atomistics #2			3/26	DFT #2	
3	2/3	Atomistics #3	HW 1 due	11	3/31	DFT #3	HW 3 due
	2/5	Atomistics #4			4/2	Phase-field #1	
4	2/10	Atomistics #5	HW 1 solution released	12	4/7	Phase-field #2	HW 3 solution released; HW 4 assigned
	2/12	Atomistics #6			4/9	Phase-field #3	
5	2/17	Atomistics #7	HW 2 assigned	13	4/14	Phase-field #4	HW 4 due
	2/19	Atomistics #8			4/16	Phase-field #5	
6	2/24	Atomistics #9	HW 2 due	14	4/21	Review	HW 4 solution released
	2/26	Atomistics #10			4/23	Mid-term exam #2	Covers DFT and phase-field
7	3/3	Review	HW 2 solution released	15	4/28	Project presentations for AME 4970 students	Project data/slides due at mid-night for the presenters
	3/5	Mid-term exam #1	Covers atomistics		4/30	Project presentations for AME 4970 students	Same as above
8	3/10	Seminar	Project assigned	16	5/5	Project presentations for AME 4970 students	Same as above
	3/12	Seminar			5/7	Project presentations for AME 5970 students	Same as above

Final exam: None

Project: Two options:

- Work on a project I will assign on March 10 (Week 8), OR
- Work on your own project, e.g., your own research project in your graduate study. But
  - It must be related to Computational Materials Science, AND
  - Email me a short description (2–3 sentences) of your planned project and have me approve it by March 24 (Week 10)

Project presentations: AME 4970 students 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: Due at mid-night on the same day as the presentations.

- **Project data:** Submissions may be formatted as plain text files or Excel spreadsheets. Alternatively, a Google Drive link, a Dropbox link, a OneDrive link, or other cloud storage service links may be submitted.
- **Project presentation slides:** Submissions may be in PDF, PowerPoint, or any appropriate format