ME:6255 Multiscale Computational Science and Engineering (3 s.h.)
Spring, 2024

Catalog Description: Computational science and engineering methods at different spatial and temporal scales. Molecular methods, including quantum mechanical calculation, molecular dynamics, and Monte Carlo methods. Continuum methods, including finite element, peridynamics, and mesh-free particle methods. Hierarchical and concurrent multiscale modeling. Reinforcement learning methods and their applications. Agent-based modeling. Quantum computing and quantum algorithms. Artificial intelligence-assisted modeling and simulations.

Prerequisites: Finite element, elementary numerical analysis, or equivalent background in computational science and engineering.

Instructor: Professor Shaoping Xiao, 2416B SC, shaoping-xiao@uiowa.edu

Student Hours: MWF 2:30 PM – 3:20 PM @ 2416B SC
Please email me if you need to make an appointment outside of these hours.

Lecture time: MWF 8:30 – 9:20 AM @ 2133 SC

Textbook: Lecture notes and reading materials provided by the instructor @ ICON

Course Goals: The course's main objective is to introduce the basic concepts of computational methods at the nano/micro/macro scales for various research domains. Students are exposed to the forefront of computational science and engineering.

Learning Objectives:

1. Gain an understanding of molecular methods and their applications.
2. Understand how to apply the Cauchy-Born rule and its extensions in quasicontinuum methods when using continuum mechanics at the nano/micro scales.
3. Understand the basic ideas of hierarchical and concurrent multiscale methods for coupling molecular dynamics with continuum mechanics.
4. Learn about the forefront of computational science and engineering, including agent-based modeling and reinforcement learning.
5. Understand the applications of neural works in multiscale computational science and engineering.
6. Understand quantum computing and quantum algorithms.

Topics:

1. Quantum mechanical calculations.
2. Molecular dynamics
3. Finite element methods, peridynamics, mesh-free methods, etc.
4. Agent-based modeling for social science, public health, earth systems, etc.
5. Automaton theory and model checking
6. Learning-based methods for robotics, control, and complex systems
7. Scale-bridging, either hierarchically or concurrently, between various scales
8. Artificial intelligence and machine learning in modeling and simulations
9. Quantum computing and applications of quantum algorithms

Grading Homework 30%; Midterm 20%; Presentations 10%; Projects 40%

Free Speech and Expression: The University of Iowa supports and upholds the First Amendment protection of freedom of speech and the principles of academic and artistic freedom (https://freespeech.uiowa.edu). We are committed to open inquiry, vigorous debate, and creative expression inside and outside the classroom.

Classroom expectations: The learning activities in this course benefit from you coming to class prepared and participating. I have found this is the best way to engage with the material, and it allows all of us to learn from one another. The expected classroom behaviors are outlined in the Code of Student Life (https://dos.uiowa.edu/policies/code-of-student-life). Please be aware that failure to follow behavior expectations may be addressed by me and may also result in discipline under the Code of Student Life policies governing E.5 Disruptive Behavior or E.6 Failure to Comply with University Directive.

Attendance: Please plan to attend every class. However, I recognize that illness or other extenuating circumstances can arise to make this difficult. If you cannot participate in a class, please let me know, and I can work with you regarding making up missed work such as assignments, quizzes, and classroom attendance. If you know you will miss an examination due to illness, religious holy days, military service obligations, or other unavoidable circumstances or other sponsored University activities (https://opsmanual.uiowa.edu/students/absences-class), please let me know as soon as possible. We can work together to have you make up the examination. I may require documentation in the case of a brief illness. Some specific instructions are described below.

Illness, Unavoidable Circumstances, and University Sponsored Activities: Please communicate with me at your earliest convenience.

Holy Days: You may notify me in writing of any such religious Holy Day conflicts within the first days of the semester and no later than the third week.

Military Service Obligations: Please discuss the expected possibility of missing class with me as soon as possible.

Accommodations for Students with Disabilities: The University is committed to providing an educational experience that is accessible to all students. If you have a diagnosed disability or other disabling condition that may impact your ability to complete the course requirements as stated in the syllabus, please seek accommodations through Student Disability Services (SDS https://sds.studentlife.uiowa.edu/students), which is responsible for making Letters of Accommodation (LOA) available to you. The LOA will specify what reasonable course accommodations you are eligible for and those I should provide. It would be very helpful if you could provide me an LOA as early in the semester as possible (at least two weeks prior to the scheduled activity for which an accommodation is sought). Additional information can be found on the SDS website (https://sds.studentlife.uiowa.edu).

Academic Integrity: As students enrolled in courses offered by the College of Engineering, you are expected to follow the College's Code of Academic Honesty (ttps://engineering.uiowa.edu/current-students/advising-and-academic-information/academic-policies-and-procedures/academic-0). Whether collaborations are allowed on assignments shall be specified on my syllabus. If you have questions about these boundaries or need clarification, please let me know.

Non-discrimination Statement: To make the campus a comfortable zone for your living and study, the University of Iowa prohibits discrimination and harassment on the basis of race, creed, color, religion, national origin, age, sex, pregnancy, disability, genetic information, status as a U.S. veteran, served in

the U.S. military, sexual orientation, gender identity, associational preferences, or any other classification that deprives a person of consideration as an individual (https://opsmanual.uiowa.edu/community-policies/human-rights). For more information, you may contact the Office of Institutional Equity (https://diversity.uiowa.edu/division/oie). It would be helpful if you could share your pronouns and chosen/preferred names in MyUI, which is accessible to instructors and advisors.

Sexual Harassment /Sexual Misconduct and Supportive Measures: The University of Iowa prohibits all forms of sexual harassment, sexual misconduct, and related retaliation. The Policy on Sexual Harassment and Sexual Misconduct (https://opsmanual.uiowa.edu/community-policies/sexual-harassment-and-sexual-misconduct) governs actions by students, faculty, staff, and visitors. Incidents of sexual harassment or sexual misconduct can be reported to the Title IX and Gender Equity Office (https://osmrc.uiowa.edu/report-problem-0) or to the Department of Public Safety (https://police.uiowa.edu). Please be aware that students impacted by sexual harassment or sexual misconduct may be eligible for academic supportive measures and can learn more by contacting the Title IX and Gender Equity Office. Information about confidential resources can be found at https://osmrc.uiowa.edu/confidential-resources. If needed, you can watch this video (https://www.youtube.com/watch?v=Jfjo6v6_b3Y) for an explanation of these resources.

Mental Health: It would be normal to feel overwhelmed and/or struggle to meet course expectations. I would like to encourage you to be mindful of your mental health and seek help as a preventive measure. You are welcome to talk to me for assistance with specific class-related concerns. For additional support and counseling, you may contact the University Counseling Service (UCS) http://counseling.uiowa.edu.

Basic Needs and Support for Students: We've all needed help in something at some point in our lives. Student Care & Assistance provides assistance to University of Iowa students experiencing a variety of crisis and emergency situations, including but not limited to medical issues, family emergencies, unexpected challenges, and basic sourcing needs such as food and shelter. You can find more information on the resources related to basic needs at this website, https://basicneeds.uiowa.edu/resources/. You also can contact Student Care & Assistance in the Office of the Dean of Students (Room 135 IMU, dos-assistance@uiowa.edu, or 319-335-1162) for support and assistance with resources.

DEI statement: It is my intention that all students, regardless of their diverse backgrounds and perspectives, are well-served by this course. We aim to address students' learning needs both in and out of the classroom, recognizing that the diversity students bring to this class is a valuable resource and strength. We reject all forms of prejudice and discrimination, including but not limited to those based on age, color, disability, gender, gender identity, gender expression, national origin, political affiliation, race, religion, sexual orientation, and veteran status. As a community, we prioritize respect for all. Both students and I are expected to commit to creating an environment that encourages inquiry and self-expression while understanding and respecting different viewpoints. Your suggestions for improving the course's effectiveness, whether for you, other students, or student groups, are encouraged and appreciated.

Please check more details @ https://provost.uiowa.edu/student-course-policies.