Schedule: Lecture: Tues/Thurs 2:00 pm – 3:30 pm; Lab: Tues/Thurs 3:30 pm – 5:00 pm; L440 Digital Computing Lab; *Office hours:* André Schleife (Tues/Thurs, 3.30 – 4.00 pm CST).

Course websites:

- Class schedule, lecture slides/recordings, assignments, links: MSE 404MIC website
- Announcements, Online discussion forums: CampusWire
- Project report deposit: see links on MSE 404MIC website
- Quizzes, Reports: PRAIRIELEARN

Course Summary: This half semester course will provide hands-on experience with popular microscopic computational materials science and engineering software through project-based learning in electronic structure calculation (Quantum Espresso) and molecular simulation (LAMMPS). Students will also develop proficiency in the command line interface and bash shell scripting, both of which are oftentimes instrumental for using modern supercomputers. The course will prioritize the physical principles underlying the software to confer an understanding of their applicability and limitations, and hands-on immersive praxis to give students the confidence and expertise to independently use these tools. Aluminum will serve as a pervasive subject of study to expose students to its analysis at different levels of theory in the Computational Materials Science and Engineering (CMSE) paradigm, and illustrate couplings between these different levels of theory and computation in the spirit of ICME (Integrated Computational Materials Engineering).

Prerequisites: Basic familiarity with MATLAB or Python expected; Linux/bash familiarity useful but not required.

Instructor: André Schleife (schleife).

Required Text: None.

Alternative Texts: *Introduction to Linux*, M. Garrels, Third Edition (Fultus Corporation, 2010)
Linux Shell Scripting With Bash, K. O. Burtch (Sams Publishing, 2004)
Learning the bash Shell: Unix Shell Programming, C. Newham (O'Reilly Media, Inc., 2009)
Integrated Computational Materials Engineering (ICME) for Metals: Using Multiscale Modeling to Invigorate Engineering Design with Science, M. F. Horstemeyer (Wiley, 2012)
Quantum-Espresso Manual: http://www.quantum-espresso.org/resources/users-manual
LAMMPS Manual: http://lammps.sandia.gov/doc/Manual.html

Disability-Related Accommodations: To obtain disability-related academic adjustments and/or auxiliary aids, students with disabilities must contact the course instructor and the Disability Resources and Educational Services (DRES, http://disability.illinois.edu) as soon as possible, and no later than Sep. 1. To contact DRES, you may visit 1207 S. Oak St., Champaign, call 333-4603, e-mail disability or go to https://www.disability.illinois.edu. If you are concerned you have a disability-related condition that is impacting your academic progress, there are academic screening appointments available that can help diagnosis a previously undiagnosed disability. You may access these by visiting the DRES website and selecting "Request an Academic Screening" at the bottom of the page.

Course evaluation:

$$6\,\%\times\text{Participation} + 9\,\%\times\text{Quizzes} + 20\,\%\times\text{Project 1 (bash)} + 20\,\%\times\text{Project 2 (Quantum Espresso)} + 20\,\%\times\text{Project 3 (LAMMPS)} + 5\,\%\times\text{Abstract} + 20\,\%\times\text{Term Project} = \text{Total}$$

Numerical total score corresponds to the following final grades:

A+ (98 – 100)	B+ (87.5 – 92)	C+ (77.5 – 79)	D+ (58.3 – 66)
A (95 – 97)	B (85 – 87)	C (75 – 77)	D (50 – 58) F (0 – 29)
A– (92.5 – 94)	B– (80 – 84)	C– (66.7 – 74)	D– (30 – 49)

Class attendance: The class sessions on Tue and Thur will be split between (i) formal lectures covering the theoretical and algorithmic underpinnings of the software, (ii) hands-on introduction to the software packages, and (iii) in-class time to work on projects under supervision of the instructor. Attendance to these classes will contribute to your final grade. More than two unexcused absences will negatively impact your grade. Lectures will also be recorded and subsequently made available for watching by anyone unable to attend the live lecture. Either attending the live lecture or watching the recording immediately afterwards is mandatory and will help to understand the material and to use the software.

Lab attendance: The purpose of the lab sessions is to provide students with a dedicated time to work on homework projects. Lab attendance is optional, the instructor will not be present and no lectures will be delivered, but this time may be used for make-up lectures.

Quizzes: Short, online, multiple-choice quizzes will be issued to gauge understanding and mastery of the course material. These tests are designed to provide the instructor and students with feedback on basic understanding of the theoretical and algorithmic principles underlying the software, and will contribute to the final grade. Quizzes will only be available online, on the PRAIRIELEARN web site for a specified time period and no extensions will be granted.

Projects: The primary assessment vehicles are homework projects associated with each module (bash, Quantum Espresso, LAMMPS). Students will be provided a detailed brief describing the specific goals and deliverables for each project, and are expected to perform analyses using the software package and produce a short report detailing their findings. Students will submit the project deliverables by the deadline stated in the MSE 404MIC website. The *only format* 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 and you must submit through the link on the MSE 404MIC website. The report will be graded. You may submit each report a maximum of two times; only the latest submission will be graded. Late submissions will not be accepted, but students with legitimate excuses should contact Prof. Schleife well before the due date. If you cannot fully complete the project, you should submit the incomplete report, so you can get partial credit.

Term Project: Computational materials science and engineering is a field with increasing importance in research and industry; to provide experience with applying the tools of computational modeling to materials science and engineering, students will design, and perform a short individual research project on a student-defined topic in computational materials science and engineering (CMSE) or integrated computational materials engineering (ICME). Projects must be computational in nature and address the microscale, but need not use one of the tools covered in the course.

Topic: Prof. Schleife will be available to discuss and advise topic selection. Early topic identification is encouraged. Submissions should take the form of a one-sentence topic title and short (maximum 300 word) abstract. Make sure that your abstract provides direct and explicit answers to these questions (https://www.darpa.mil/work-

with-us/heilmeier-catechism):

- What are you trying to do? Articulate your objectives using absolutely no jargon.
- How is it done today, and what are the limits of current practice?
- What is new in your approach and why do you think it will be successful?
- Who cares? If you are successful, what difference will it make?
- What are the risks?
- How many hours of pure simulation time will it take?
- How long will data analysis take?
- What are the mid-term and final "exams"/"criteria" to check for success?

Each of these eight bullet points, and the project title, are worth one point if addressed and zero points if not addressed in your abstract. In addition, you will receive feedback on the content and tips for the implementation, which does not affect whether you will or won't be awarded these points.

Report: Written reports are assigned to practice the communication of engineering concepts in writing. Term project reports should be 5-8 pages in length (excl. figures and bibliography; 12-pt font, 1-inch margins, single-spaced). Reports should be neat and organized, hand-written or typed. Tables and graphical representations of results should be generated using some software program such as Python, Excel, TecPlot, MatLab, etc., rather than being hand-drawn. Reports should be structured using the following sections: Abstract, Introduction, Methods, Results and Discussion, Conclusions, Bibliography. Prof. Schleife will be available to discuss and advise term projects and production of the report. Term projects will be graded on (i) design of computational materials research project (20 %), (ii) appropriate and competent use of computational tools (50 %), and (iii) clarity of the report (30 %). It is imperative to start work sufficiently early to perform the project and compose the report. You must submit the report through the link on the MSE 404MIC website. Late submissions will not be accepted, but students with legitimate excuses should contact Prof. Schleife well before the due date. If you cannot fully complete the project, still submit the incomplete report, so you can get partial credit.

Plagiarism: Students are responsible for producing their own quiz answers and project reports. Collaborative interaction in small groups is encouraged, but each student must perform all calculations themselves, and write their own reports. In particular, each students is required to produce their own figures and write their own text. This means that exact copies will be considered plagiarism and plagiarism will not be tolerated. Verified incidents will result in formal academic sanctions. Students are responsible for familiarizing themselves with the definition of and penalties for plagiarism in Section I-401 of the UIUC Student Code. Note that plagiarism includes "copying another student's paper or working with another person when both submit similar papers without authorization to satisfy an individual assignment".

Obtaining help: The main two ways to obtain help are online at CampusWire or during class or office hours. You can also speak with your professor briefly after lecture. Please do not send emails for routine help or absences. In cases of emergencies related to exams (e.g., illness) you should email your professor at the earliest possible opportunity.

Online Discussion Forum: This class uses CampusWire for all communication between the instructor and students. You will receive an email invite to register and should let the instructor know if you have not received this email by the first day of class. The CampusWire link will take you to the current class page at any time. Official class announcements will be sent via CampusWire, so you must register with an email address that you regularly check. If you desire, you can post anonymously on CampusWire or make a private post just to the instructors (this should be done rather than emailing the professor directly). *Note that CampusWire should be used to communicate with your instructors, rather than email.*

Absences: Excused Absence Request Form: forms.illinois.edu/sec/1175532

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 Oct 19. 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.

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 404MIC website calendar for exact schedule, assignments, and to remain up to date.

COVID Statement: Following University policy, all students are required to engage in appropriate behavior to protect the health and safety of the community. Students are also required to follow the campus COVID-19 protocols.

Students who feel ill must not come to class. In addition, students who test positive for COVID-19 or have had an exposure that requires testing and/or quarantine must not attend class. The University will provide information to the instructor, in a manner that complies with privacy laws, about students in these latter categories. These students are judged to have excused absences for the class period and should contact the instructor via email about making up the work.

Students who fail to abide by these rules will first be asked to comply; if they refuse, they will be required to leave the classroom immediately. If a student is asked to leave the classroom, the non-compliant student will be judged to have an unexcused absence and reported to the Office for Student Conflict Resolution for

disciplinary action. Accumulation of non-compliance complaints against a student may result in dismissal from the University.

Emergency Response Recommendations: Emergency response recommendations can be found at the following website:
http://police.illinois.edu/emergency-preparedness/. I encourage you to review this website and the campus building floor plans website within the first 10 days of class:
http://police.illinois.edu/emergency-preparedness/building-emergency-action-plans/.

Sexual Misconduct Reporting Obligation: The University of Illinois is committed to combating sexual misconduct. Faculty and staff members are required to report any instances of sexual misconduct to the University's Title IX Office. In turn, an individual with the Title IX Office will provide information about rights and options, including accommodations, support services, the campus disciplinary process, and law enforcement options.

A list of the designated University employees who, as counselors, confidential advisors, and medical professionals, do not have this reporting responsibility and can maintain confidentiality, can be found here: wecare.illinois.edu/resources/students/#confidential.

Other information about resources and reporting is available here: wecare.illinois.edu.

Academic Integrity: The University of Illinois at Urbana-Champaign Student Code should also be considered as a part of this syllabus. Students should pay particular attention to Article 1, Part 4: Academic Integrity. Read the Code at the following URL: http://studentcode.illinois.edu/.

Academic dishonesty may result in a failing grade. Every student is expected to review and abide by the Academic Integrity Policy: https://studentcode.illinois.edu/article1/part4/1-401/. Ignorance is not an excuse for any academic dishonesty. It is your responsibility to read this policy to avoid any misunderstanding. Do not hesitate to ask the instructor(s) if you are ever in doubt about what constitutes plagiarism, cheating, or any other breach of academic integrity.

Religious Observances: Illinois law requires the University to reasonably accommodate its students' religious beliefs, observances, and practices in regard to admissions, class attendance, and the scheduling of examinations and work requirements. You should examine this syllabus at the beginning of the semester for potential conflicts between course deadlines and any of your religious observances. If a conflict exists, you should notify your instructor of the conflict and follow the procedure at https://odos.illinois.edu/community-of-care/resources/students/religious-observances/ to request appropriate accommodations. This should be done in the first two weeks of classes.

Family Educational Rights and Privacy Act (FERPA): Any student who has suppressed their directory information pursuant to Family Educational Rights and Privacy Act (FERPA) should self-identify to the instructor to ensure protection of the privacy of their attendance in this course. See https://registrar.illinois.edu/academic-records/ferpa/ for more information on FERPA.

Anti-Racism and Inclusivity Statement: The Grainger College of Engineering is committed to the creation of an anti-racist, inclusive community that welcomes diversity along a number of dimensions, including, but not limited to, race, ethnicity and national origins, gender and gender identity, sexuality, disability status, class, age, or religious beliefs. The College recognizes that we are learning together in the midst of the Black Lives Matter movement, that Black, Hispanic, and Indigenous voices and contributions have largely

either been excluded from, or not recognized in, science and engineering, and that both overt racism and micro-aggressions threaten the well-being of our students and our university community.

The effectiveness of this course is dependent upon each of us to create a safe and encouraging learning environment that allows for the open exchange of ideas while also ensuring equitable opportunities and respect for all of us. Everyone is expected to help establish and maintain an environment where students, staff, and faculty can contribute without fear of personal ridicule, or intolerant or offensive language. If you witness or experience racism, discrimination, micro-aggressions, or other offensive behavior, you are encouraged to bring this to the attention of the course director if you feel comfortable. You can also report these behaviors to the Bias Assessment and Response Team (BART) (https://bart.illinois.edu/). Based on your report, BART members will follow up and reach out to students to make sure they have the support they need to be healthy and safe. If the reported behavior also violates university policy, staff in the Office for Student Conflict Resolution may respond as well and will take appropriate action.