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: See Piazza for times and location of the office hours.

Course websites:

- Class schedule, lecture slides/recordings, assignments, links: MSE 404MIC website
- Gradebook: Compass
- Project report deposit: GradeScope
- Quizzes: PRAIRIELEARN
- Announcements, online discussion forums: Piazza

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. 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 expected; Linux/bash familiarity useful but not required.

Instructor: André Schleife (schleife; 204A MSEB).

Teaching Assistants: Joshua Leveillee (leveill2)

Required Text: None.


Special accommodations: To obtain disability-related academic adjustments and/or auxiliary aids, students with disabilities must contact their lecturer and the Disability Resources and Educational Services (DRES, disability.illinois.edu) as soon as possible, and no later than Sep. 1.

Course evaluation:

\[
\text{5 \% \times \text{Attendance} + 10 \% \times \text{Quizzes} + 20 \% \times \text{Project 1 (bash)} + 20 \% \times \text{Project 2 (Quantum Espresso)} + 20 \% \times \text{Project 3 (LAMMPS)} + 25 \% \times \text{Term Project} = \text{Total}}
\]
Numerical total score corresponds to the following final grades:

<table>
<thead>
<tr>
<th>Grade Letter</th>
<th>Score Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>A+</td>
<td>98 – 100</td>
</tr>
<tr>
<td>B+</td>
<td>87.5 – 92</td>
</tr>
<tr>
<td>C+</td>
<td>77.5 – 79</td>
</tr>
<tr>
<td>D+</td>
<td>58.3 – 66</td>
</tr>
<tr>
<td>A</td>
<td>95 – 97</td>
</tr>
<tr>
<td>B</td>
<td>85 – 87</td>
</tr>
<tr>
<td>C</td>
<td>75 – 77</td>
</tr>
<tr>
<td>D</td>
<td>50 – 58</td>
</tr>
<tr>
<td>F</td>
<td>0 – 29</td>
</tr>
<tr>
<td>A–</td>
<td>92.5 – 94</td>
</tr>
<tr>
<td>B–</td>
<td>80 – 84</td>
</tr>
<tr>
<td>C–</td>
<td>66.7 – 74</td>
</tr>
<tr>
<td>D–</td>
<td>30 – 49</td>
</tr>
</tbody>
</table>

Class attendance: The class sessions on Tue and Thu 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.

Lab attendance: The purpose of the lab sessions is to provide students with reserved access to the EWS Lab to work on homework projects. Lab attendance is optional, the instructor will not be present and no lectures 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 GradeScope web site. There the TA will grade the report. 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.

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. Submissions should take the form of a one-sentence topic title and short (maximum 300 word) abstract that (i) summarizes the topic area and its importance, (ii) defines specific objectives and how they will be achieved using computational tools. Early topic identification is encouraged.

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 Excel, TecPlot, MatLab, etc., rather than being hand-drawn. Papers should be structured as a short lab report containing 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 GradeScope web site. Late submissions will not be accepted, but students with legitimate excuses should contact Prof. Schleife well before the due date.

**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. Plagiarism will not be tolerated, and 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”.

**Grade Reporting:** All assessment scores are stored in the gradebook in Compass. Any errors in grade reporting appearing in the gradebook must be reported within 1 week of the grade being posted in the gradebook or by the last day of class, whichever is earlier. If you have a missing grade, contact the instructor.

**Obtaining help:** The main two ways to obtain help are online at Piazza or in person at office hours. You can also speak with your professor briefly after lecture. Please do not send email directly to TAs or professors 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 Forum (Piazza):** This class uses Piazza for all communication between the instructor, TAs, and students. Please visit piazza.com/illinois/fall2018/mse404 to register. The Piazza link will take you to the current class page at any time. Official class announcements will be sent via Piazza, so you must register with an email address that you regularly check. If you desire, you can post anonymously on Piazza or make a private post just to the instructors (this should be done rather than emailing the professor directly). Note that Piazza 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 20. 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.

**Academic Integrity, Harassment, and Discrimination:** You are bound by the University Honor Code in this course. Any violation of the Honor Code will result in disciplinary action. In addition, harassment or discrimination of any kind will not be tolerated. Please report any concerns immediately to your professor.

**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.