Computational Materials Science and Engineering (Microscale)
MSE 404 MICRO
Fall 2017

Instructor: Prof. A.L. Ferguson   **TA:** Bryce Thurston
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CRN: 66895 (1.5 credit hours)

www: https://courses.illinois.edu/schedule/2017/fall/MSE/404

Lecture: L440 DCL ◆ 2–3:30 pm ◆ Tue, Thu

Lab: L440 DCL ◆ 3:30–5 pm ◆ Tue, Thu

Office Hours: 204 MSEB ◆ 8:45-9:45 am ◆ Thu
L440 DCL ◆ 3:30–5 pm ◆ Thu

Dates: 08/28/17 – 10/20/17 (first half of fall semester)

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; familiarity with Linux/bash useful but not required.

Required Text

None.

Secondary Texts

M. Garrels *Introduction to Linux (3rd ed.)* (Fultus Corporation, 2010)
K.O. Burtch *Linux Shell Scripting With Bash* (Sams Publishing, 2004)
C. Newham *Learning the bash Shell: Unix Shell Programming* (O'Reilly Media, Inc., 2009)
M.F. Horstemeyer *Integrated Computational Materials Engineering (ICME) for Metals: Using Multiscale Modeling to Invigorate Engineering Design with Science* (Wiley, 2012)

Quantum-Espresso Manual: www.quantum-espresso.org/users-manual
LAMMPS Manual: http://lammps.sandia.gov/doc/Manual.html

Attendance

Class: 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 the T,Th classes will contribute to your final grade. More than two unexcused absences will negatively impact your grade.**

Lab: 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.

Assessment

As a hands-on class, competence and proficiency will be assessed through (i) class projects associated with each course module, (ii) short online quizzes, and (iii) a student-defined term project. **There will be no written midterm or final examinations.**

Quizzes: Short, online multiple-choice Compass 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 for a specified time period. Solutions will be immediately posted after the quiz closes, and **accordingly no extensions can 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 via Compass by the deadline stated in the brief. **Late submissions will not be accepted,** *but students with legitimate excuses should contact Prof. Ferguson well before the due date.*

Term Project: 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. Ferguson will be available to discuss and advise topic selection. Submissions should take the form of a one-sentence topic title and short (≤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 – Term project reports should be 5-8 pages in length (excl. figures and bibliography; 12-pt font, 1-inch margins, single-spaced). Papers should be structured as a short lab report containing the following sections: Abstract, Introduction, Methods, Results and Discussion, Conclusions, Bibliography. Prof. Ferguson 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. **Late submissions will not be accepted,** *but students with legitimate excuses should contact Prof. Ferguson 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 all parties receiving a zero and 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".

Exams: None.

Grading

Breakdown: Attendance...5%
Quizzes...10%
Project 1 (bash)...20%
Project 2 (Quantum-Espresso).........20%
Project 3 (LAMMPS)............................ 20%
Term Project.. 25%

Letter Grades: Letter grades will be based on final aggregate student scores, with numerical cutoffs specified by the instructor. However, students with aggregate scores >95% are guaranteed *at least* an A, >85% *at least* a B, and >75% *at least* a C (i.e. cutoffs for these letter grades will not be higher than these values).

Office Hours

The instructor and/or TA will be available to discuss any aspects of the syllabus, material, software, quizzes, or homework projects directly after class, or during the scheduled office hours.

Compass

Course announcements, grades, quizzes, projects, and files will be posted via Compass (https://compass2g.illinois.edu). Online quizzes and projects submitted will be submitted via this portal. It is students' responsibility to check Compass for announcements and updates.

Course Coverage

I. **Introduction: CMSE / ICME**

Computation as the "third pillar" of science; multi-scale and multi-physics computation; drivers in academia, industry, and public policy; computational materials science and engineering (CMSE) and integrated computational materials engineering (ICME) resources and software tools

II. **Scripting in scientific computing: bash shell**

Scientific Linux and EWS workstations; command line interface (CLI) and graphical user interface (GUI); common bash commands; bash utilities (expr, ssh/scp, sftp, vim, wget); installing software from source; bash scripting through worked examples; awk

III. **Electronic structure calculations: Quantum-Espresso**

Theory: review of quantum mechanics – Schrodinger, Hartree, Hartree-Fock, DFT; particle in a box; hydrogen atom and electronic orbitals; basis set expansion; many-electron problem; Slater determinants; exchange and correlation; Hohenberg-Kohn Theorems; Kohn-Sham equations; exchange-correlation functionals; pseudopotentials; Bloch Theorem; plane wave basis set; reciprocal space; Brillouin Zone; k-points sampling; band structure plots; successes and failures of DFT; post-DFT methods

Praxis (Quantum Espresso): functionality; documentation and tutorials; installation; parallel performance; high-level overview of running QE from the command line; input/output files; convergence criteria; visualization

Walkthrough: H_2 molecule – ab initio prediction of energy and bond length

Project: Al xtal – convergence, energy, lattice parameter, bulk modulus, and band structure

IV. **Molecular dynamics: LAMMPS**

Theory: molecular dynamics as a "computational microscope"; applications in academia and industry; history and milestones; Laplace's Demon / clockwork universe; quantum effects; initial configuration and velocity; interaction potentials / force fields; Verlet algorithm; MD in various ensembles – thermostats and barostats; periodic boundary conditions; Ewald summation; specialized MD variants; successes and failures of MD; MD software packages

Praxis (LAMMPS): availability; installation; documentation; performance; anatomy of a LAMMPS simulation; visualization in OVITO

Walkthrough: Al xtal – cohesive energy, lattice parameter, and crack propagation

Project: Al xtal – Young's modulus and Peierls stress

Tentative Schedule

Class	Date	Day	Module	Topic	Type	Due
1	Aug 29	T	I	Introduction / bash	*L*	
2	Aug 31	Th	I	bash	*L*	
3	Sep 5	T	II	Quantum-Espresso – Theory	*L*	
4	Sep 7	Th	II	Quantum-Espresso – Practice	*L*	Q I, P I
*	Sep 12	T		**NO CLASS**		
5	Sep 14	Th	II	Walkthrough	*H*	
6	Sep 19	T	II	Walkthrough / Project	*H*	
7	Sep 21	Th	II	Project	*H*	
8*	Sep 26	T	II	Project	*H*	
9	Sep 28	Th	III	LAMMPS – Theory	*L*	
10	Oct 3	T	III	LAMMPS – Practice	*L*	Q II, P II, Term Project Topic
*	Oct 5	Th		**NO CLASS**		
11	Oct 10	T	III	Walkthrough	*H*	
12*	Oct 12	Th	III	Walkthrough / Project	*H*	
13	Oct 17	T	III	Project	*H*	
14	Oct 19	Th	III	Project	*H*	
	Oct 23	M				Q III, P III
	Oct 26	Th				Term Project

* Prof. Ferguson on travel these dates, appropriate arrangements TBA.