Computational Materials Science and Engineering
MSE 498 AF
Fall 2015

Instructor: Prof. A.L. Ferguson
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CRN: 61159 (3 credit hours)
url: https://courses.illinois.edu/schedule/2015/fall/MSE/498

Lecture: L440 DCL ◆ 11 am – 12:20 pm ◆ Tue, Thu

Lab: L440 DCL ◆ 5–7 pm ◆ Wed

Office Hours: 204 MSEB ◆ 12:30–1:30 pm ◆ Tue

Course Summary

This new course will provide hands-on experience with popular computational materials science and engineering software through a series of projects in: electronic structure calculation (Quantum Espresso), molecular simulation (LAMMPS), finite element modeling (OOF2), and phase modeling (Thermo-Calc). Students will also develop proficiency in bash shell scripting, and data analysis and visualization in MATLAB. The course will familiarize students with a broad survey of software tools in computational materials science, scientific computing, and prioritize the physical principles underlying the software to confer an understanding of their applicability and limitations.

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)
A. Gilat, V. Subramaniam *MATLAB: An Introduction with Applications (4th ed.)* (John Wiley & Sons, 2011)
S. Otto, J.P. Denier *An Introduction to Programming and Numerical Methods in MATLAB* (Springer, 2005)
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
OOF2 Manual: www.ctcms.nist.gov/~langer/oof2man/
Thermo-Calc Manual: www.thermocalc.com/res/Manuals/Thermo-Calc_UsersGuide.pdf

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 Wed lab session 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 periodically 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 6 homework projects associated with each module (bash, MATLAB, Quantum Espresso, LAMMPS, OOF2, Thermo-Calc). 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, but need not necessarily 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	5%
Project 1A (bash)	7.5%
Project 1B (MATLAB)	7.5%
Project 2 (Quantum-Espresso)	15%
Project 3 (LAMMPS)	15%
Project 4 (OOF2)	15%
Project 5 (Thermo-Calc)	15%
Term Project	15%

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 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
   (i) What is computational materials science and engineering?
   (ii) The **bash shell**
   (iii) Data analysis using **MATLAB**
II. Electronic structure calculations: **Quantum-Espresso**
III. Molecular dynamics: **LAMMPS**
IV. Finite element modeling: **OOF2**
V. Phase equilibria: **Thermo-Calc**

Revised Schedule

Class	Date	Day	Module	Topic	Type	Due
1	Aug 25	T	I	CMSE / bash	*L*	
2	Aug 27	Th	I	bash	*L*	
3	Sep 1	T	I	MATLAB	*L/H*	
4	Sep 3	Th	I	MATLAB	*L/H*	
5	Sep 8	T	II	Quantum-Espresso – Theory	*L*	
6	Sep 10	Th	II	Quantum-Espresso – Practice	*L*	Q I, P IA & IB
7	Sep 15	T	II	Walkthrough	*H*	
8*	Sep 17	Th	II	Walkthrough / Project	*H*	
9	Sep 22	T	II	Project	*H*	
10	Sep 24	Th	II	Project	*H*	
11	Sep 29	T	III	LAMMPS – Theory	*L*	
12	Oct 1	Th	III	LAMMPS – Practice	*L*	Q II, P II
13	Oct 6	T	III	Walkthrough	*H*	
14	Oct 8	Th	III	Walkthrough / Project	*H*	
15	Oct 13	T	III	Project	*H*	
16	Oct 15	Th	III	Project	*H*	
17	Oct 20	T	IV	OOF2 – Theory	*L*	
18	Oct 22	Th	IV	OOF2 – Practice	*L*	Q III, P III
19	Oct 27	T	IV	Walkthrough	*H*	
20	Oct 29	Th	IV	Walkthrough / Project	*H*	
21	Nov 3	T	IV	Project	*H*	
22	Nov 4	W	IV	Project	*H*	
23	Nov 5	Th	V	Thermo-Calc – Theory	*L*	
*	Nov 10	T		NO CLASS		
*	Nov 12	Th		NO CLASS		Q IV, P IV + Topic
24	Nov 17	T	V	Thermo-Calc – Practice	*L*	
25	Nov 18	W	V	Walkthrough	*H*	
26	Nov 19	Th	V	Walkthrough / Project	*H*	
	Nov 24	T		THANKSGIVING BREAK		
	Nov 26	Th		THANKSGIVING BREAK		
27	Dec 1	T	V	Project	*H*	
28	Dec 3	Th	V	Project	*H*	
29*	Dec 8	T	–	Wrap-Up	*L/H*	
	Dec 10	Th		*Reading Day*		Q V, P V
	Dec 18			*End of Final Exam Period*		Report

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

Make-up classes to be held during lab time slot **Wed 5-6:20 pm** in the usual room (L440 DCL)