Computational Materials Science and Engineering (Macroscale)
MSE 404 MACRO
Fall 2017

Instructor:	Prof. A.L. Ferguson 204 MSEB (217) 300-2354 alf@illinois.edu	**TA:**

CRN: 66897 (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 ◆ 9-10 am ◆ Tue
L440 DCL ◆ 3:30–5 pm ◆ Thu

Dates: 10/23/17 – 12/13/17 (second half of fall semester)

Course Summary

This half semester course will provide hands-on experience with popular macroscopic computational materials science and engineering software through project-based learning in finite element modeling (OOF2) and phase equilibria calculations (Thermo-Calc). Students will also develop proficiency in data analysis and visualization in MATLAB. 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

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)

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 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 (MATLAB, 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 and address the macroscale, 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 (MATLAB)	20%
Project 2 (OOF2)	20%
Project 3 (Thermo-Calc)	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. Data analysis and visualization: MATLAB

MATLAB interface; ethos and data structures; calling functions; documentation and help; loading data; plotting (line, bar, histogram, scatter, surf); statistical data analysis (Pearson's correlation coefficient, permutation test, bootstrap, multiple linear regression, Akaike information criterion, cross validation, Student's t-test)

III. Finite element modeling: OOF2

Theory: finite element method (boundary value problems on complex domains); utility and applications; "divide and conquer" (meshing, properties, basis, solving); basis functions; weak solution and Galerkin method; error quantification and control; 1D heat conduction example and comparison to analytical solution; software packages

Praxis (OOF2): history; GUI and CLI interfaces; availability (nanoHUB); workflow (units, skeletons, meshes, equations, solvers, visualization, analysis, activity, messages)

Walkthrough: Stresses on a bimetallic strip

Project: 1D heat conduction + stress field around exterior crack in Al xtal

IV. Phase equilibria: Thermo-Calc

Theory: phase diagrams; experimental determination / computational prediction; phase diagram projections; thermodynamic potentials; equilibrium conditions; Euler's Theorem; CALPHAD procedure; Gibb's phase rule; lever rule; one and two-component phase equilibria; multicomponent equilibria; applications; software packages

Praxis (Thermo-Calc): availability; history; manual and documentation; applications; databases; Gibbs free energy contributions; numerical optimization

Walkthrough: Al/Si phase diagram (Gibbs curves, T-x projection, phase fractions) + Al/Si/Mg phase diagram (T-x_{Mg} projection, x_{Al}-x_{Si}-x_{Mg} projection)

Project: computational design of carbon and stainless steels

Tentative Schedule

Class	Date	Day	Module	Topic	Type	Due
1	Oct 24	T	I	Introduction / MATLAB	*L*	
2	Oct 26	Th	I	MATLAB	*L*	
3*	Oct 31	T	II	OOF2 – Theory	*L*	
4*	Nov 2	Th	II	OOF2 – Practice	*L*	Q I, P I
5	Nov 7	T	II	Walkthrough	*H*	
6	Nov 9	Th	II	Walkthrough / Project	*H*	
7	Nov 14	T	II	Project	*H*	
8	Nov 16	Th	II	Project	*H*	Term Project Topic
	Nov 21	T		**THANKSGIVING BREAK**	*L*	
	Nov 23	Th		**THANKSGIVING BREAK**	*L*	
9	Nov 28	T	III	Thermo-Calc – Theory		
10	Nov 30	Th	III	Thermo-Calc – Practice		Q II, P II
11	Dec 5	T	III	Walkthrough	*H*	
12*	Dec 7	Th	III	Walkthrough / Project	*H*	
13*	Dec 12	T	III	Project	*H*	
14‡	Dec 14	Th	III	Project	*H*	Q III, P III
	Dec 18	Th				Term Project

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

‡ READING DAY – optional class to provide time for project work in the computer lab.