UNIVERSITY OF CALIFORNIA, MERCED

MSE 119 – Materials Simulations

Spring 2017

Course Details:	Lecture meets	Tuesday 11:30 – 12:20 PM, CLSSRM 286
	Discussion meets	Tuesday 12:30 – 1:20 PM, KOLLIG 202
	Laboratory meets	Thursday12:00 – 2:50 PM, KOLLIG 202
	Total units	3

Instructor: Professor Lilian P. Davila, Ph.D.
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Office hours: Tuesday 3:00 – 4:00 pm and by appointment

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Office and hours: AOA, TBA, Friday 11:00 - noon and by appointment

I. Course Description:

Computer simulations have been used over several decades in many disciplines to improve our understanding of different phenomena. In particular, computational methods have expanded the field of materials science and consequently have impacted nanoscience and nanotechnology research in recent years. Computational materials science has proven to be a valuable "non-destructive" technique for novel research.

This course is an introduction to computational materials science. This course will cover computational methods in materials research and their applications in modern studies. Among such methods are *ab initio*, molecular dynamics (MD), mesoscale, multiscale modeling and finite element methods. Nanostructure and microstructure evolution, and materials properties will also be included. A computational project will be developed throughout the term. Also, relevant cases studies will illustrate the variety of topic studies through contemporary computational materials science research.

II. Course Goals and Outcomes:

Course Goals:

* Learn key concepts and major topics in computer simulations through which materials scientists study and apply methods to understand and predict phenomena and properties.

* Understand the fundamentals of the computational methods that are widely available as well as their strengths and limitations.

* Analyze contemporary computer modeling studies by reviewing case studies. Be able to successfully communicate knowledge gained.

Learning Outcomes:

By the end of this course through readings, discussions, interactions, project experience, research paper, oral presentations and exams students will demonstrate:

* Ability to apply fundamental knowledge needed to understand materials simulations including terminology, key concepts, methods and topics of study. Also, ability to critically evaluate current research literature in the field of materials science and engineering and nanotechnology.

* Knowledge of topics in computational materials science that enable the comparison of similarities and differences among available methods. Ability to select computational method(s) that are appropriate for a given simulation study.

* Ability to analyze contemporary studies and to make connections and decisions based on their scientific merit. Students will also be adept at oral and written communication of research results in their field to expert and non-expert audiences.

III. Format and Procedures:

This course is structured as follows: weekly interactive sessions where lectures, discussions, project, oral presentations and exams will take place. Labs will consist of demonstrations, hands-on work and exercises. <u>Punctuality, attendance, active participation and respectful behavior are expected from all students</u>.

Use of electronic devices during class is disruptive and a discourtesy to fellow students and the instructor, and detracts from the learning environment. Students are requested not to operate electronic devices in the classroom other than for purposes related to the course (note-taking, entry of due dates into a PDA, etc.). Violations of this policy will result in confiscation of the device by the instructor for the duration of the class session. Repeated violations will result in referral for academic discipline.

Lectures (preparation & participation)
<u>Prepare by reading assigned sections for the lecture</u>. Each lecture will begin promptly, a short reading pop-quiz consisting of definitions, key ideas or concepts on case studies will take place in the first 15 minutes of each lecture thus <u>be sure to be on time</u>. Lectures will be interactive – ask questions, participate in lectures and simulation discussion. Lectures will include writing on whiteboard, PowerPoint slides and the use of selected websites in the Internet. *I will do my best to post promptly class materials on the course website via CatCourses*. Bonus points may be awarded for exceptional participation.

Discussions and Midterm
Punctuality, attendance, active participation and thoughtful work are rewarded in this course. You will review material and case studies provided by the instructor. Bring discussion material and notes to class. A midterm will be given as scheduled below based on the material covered to date.

Simulations Project, Paper and Presentation

Each student will develop a computational project a using computer program available to the class. Each student will submit a term paper and present his/her project to the class at the end of the semester.

IV. My Assumptions:

Throughout this course the terms **materials modeling** and **materials simulations** will be used interchangeably. My preference is to use the latter as it is most appropriate and descriptive to the concepts presented in this course.

This course builds on the assumption that students took ENGR 45 (Introduction to Materials). Students are responsible for reviewing basic concepts taught in ENGR 45 as needed to understand computational material presented in this class. Students are expected to exercise intellectual independence in consulting materials outside the class in order to strengthen the depth and breadth of their understanding. Supplemental resources may include consulting other textbooks, Wikipedia, and materials science learning modules on the web that are hosted by professional societies or universities. I believe that to effectively learn the content presented in this course, the students need to prepare for the lectures via the assigned reading material, participate actively, analyze selected case studies via critical thinking, work diligently on their project and use the instructor's office hours effectively.

V. Course Requirements and Grading Procedures:

Reference texts and articles:

- *Computer Simulations of Liquids* by M.P. Allen and D.J. Tildesley
- *Molecular Dynamics Simulation* by J.M. Haile
- *Monte Carlo Methods.1: Basics* by M.H. Kalos and P.A. Whitlock
- *Materials Science for Engineering: An Introduction* by W.D. Callister
- Several cases studies in the form of journals will be provided by the instructor

Required attendance and participation in lectures and discussions:

a. Regular attendance is expected
b. Complete all assigned readings before class. Bring materials to class for discussion.
c. Participate in discussions and classroom activities
d. Turn in completed assignments on time. No late work will be accepted.
e. **Make at least one visit to instructor's office hours per week.**
f. For term report, review drafts with writing tutors on campus for feedback.

Course Policies:

1. **Turn in completed assignments in class. No late work will be accepted.**
2. **No makeup exams will be given.** Missed exams will be prorated, provided the absence was due to illness documented by a physician's statement.
3. Unless you are instructed otherwise, you may discuss assignments and project topics with other students in the class, but submitted work must be your own. The UCM Code of Academic Conduct will be strictly enforced (see below).
4. Students are expected to abide by the UC Merced Principles of Community (see http://studentaffairs.ucmerced.edu/principles-community).

Grading:

The table below summarizes the weight and total points for each portion of the course. All scores will be posted on CatCourses. It is your responsibility to check that scores are recorded accurately.

Element of Course	**Percentage (Approx.)**
Attendance and Discussion	15%
Homework	25%
Midterm	25%
Project: Term Paper (simulations project) & Individual Presentation	25% 10%
Total	**100%**

Final grades will be determined by the percentage of the total course points earned throughout the semester. All scores will be posted on CatCourses.

Grading Scale: The flavor of letter grade (+, even, -) will be decided by the instructor when mid-semester and remainder grades are assigned, based on the student performance throughout the semester.

Percentage of Course Points (Approx.)	**Number of Course Points**	**Grade**
> 80 %	> 800	A-, A, A+
60-79%	600 - 790	B-, B, B+
40-59%	400 - 590	C-, C, C+
30-39%	300 - 390	D
< 30%	< 300	F

VI. Academic Integrity:

a. **Each student in this course is expected to abide by the University of California, Merced's Academic Honesty Policy.** Any work submitted by a student in this course for academic credit will be the student's own work. For this course, collaboration is allowed in the following instances: discussions and modeling project.

b. You are encouraged to study together and to discuss information and concepts covered in lecture and the sections with other students. You can give "consulting" help to or receive "consulting" help from such students. However, this permissible cooperation should never involve one student having possession of a copy of all or part of work done by someone else, in the form of an e mail, an e mail attachment file, a diskette, CD or a hard copy. ***Should copying occur,*** *both the student who copied work from another student and the student who gave material to be copied will both automatically receive a zero for the assignment*. Penalty for violation of this Policy can also be extended to include failure of the course and University disciplinary action.

c. During **examinations**, you must do your own work. Talking or discussion is not permitted during the examinations, nor may you compare papers, copy from others, or collaborate in any way. *Any collaborative behavior during the examinations will result in failure of the exam, and may lead to failure of the course and University disciplinary action*.

d. The UCM Academic Honesty Policy is available online at the Office of Student Life website: http://studentlife.ucmerced.edu under Student Judicial Affairs.

VII. Accommodations for Students with Disabilities:

The University of California Merced is committed to ensuring equal academic opportunities and inclusion for students with disabilities based on the principles of independent living, accessible universal design and diversity. I am available to discuss appropriate academic accommodations that may be required for student with disabilities. Requests for academic accommodations are to be made during the first three weeks of the semester, except for unusual circumstances. Students are encouraged to register with Disability Services Center to verify their eligibility for appropriate accommodations.

VIII. Tentative Weekly Schedule: This is <u>*Subject to Change*</u> to accommodate for necessary adjustments (i.e. guests, student needs, cancelled classes, etc.) over the course of the semester. *Any changes to the schedule will be announced in class and CatCourses site*.

Wk.	Dates	Topic & Learning Goals	Learning Outcomes	Readings: Chapters/ Handouts	Assessments: Homework, Midterm, Paper, Presentation
1	Jan 17 ------- Jan 19	Introduction/logistics ------- Lab		Syllabus	Organization Intro to software
2	Jan 24 ----- Jan 26	Background ------- Intro: LAMMPS		Handout	Discussion Lab: demo/exercises
3	Jan 31 ----- Feb 2	Background, *ab initio* ------------ Case Study		Handout	Discussion, homework Lab: demo/exercises/projects
4	Feb 7 ----- Feb 9	Monte Carlo (MC) ------------ Case Study		Handout	Discussion, homework Lab: demo/exercises/projects
5	Feb 14 ----- Feb 16	Molecular Dynamics (MD) --------------- Case Study		Handout	Discussion, homework Lab: demo/exercises/projects
6	Feb 21 ----- Feb 23	Mesoscale Mod. -------------- Case Study		Handout	Discussion, homework Lab: demo/exercises/projects
7	Feb 28 ----- March 2	Multiscale Mod. ------------ Case Study		Handout	Discussion, homework Lab: demo/exercises/projects
8	March 7 ----- March 9	Finite-Element (FEM) ------------- Case Study		Handout	Discussion, homework **Midterm**
9	March 14 ----- March 16	Mod. Phase Sep. ------------- Case Study		Handout	Discussion, homework Lab: demo/exercises/projects
10	March 21 ----- March 23	Nano/Microstr, Mater. Props ------------- Case Study		Handout	Discussion, homework Simulation project
11	March 27-30	*Spring Recess*		Handout	*No class*
12	April 4 ----- April 6	Learning by doing (LBD) LBD		Handout	Simulation project Simulation project
13	April 11 ----- April 13	LBD ------------ LBD		Handout	Simulation project, work: paper Simulation project, work: paper
14	April 18 ----- April 20	LBD ------------ LBD		Handout	Simulation project, work: paper Simulation project, work: paper
15	April 25 ----- April 27	Review Feedback		Handout	Simulation project, work: paper Simulation project, work: paper
16	May 2 ----- May 4	Review In-class presentation			Review paper, get feedback **Final (individual) paper due**
17	May 11	8:00 – 11:00 am, CLSSRM 286			**Oral (group) presentations due** Course evaluations due