Computational Nanomechanics and Nanomaterials
EML 6934 Section 4D83

Class Periods: Monday/Wednesday/Friday, Period 5, 11:45 am – 12:35 pm
Location: MAE-A 327
Academic Term: Spring 2020

Instructor
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Office Hours: Monday/Wednesday/Friday, 10:30 – 11:30 am, NEB 133

Course Description
To elucidate the fundamentals of select modeling techniques in nanomechanics and nanomaterials. Modeling and simulation methods will be covered that span from atomistic to mesoscale domains, with particular focus given to "classical" atomistic modeling techniques such as molecular mechanics, molecular dynamics and Monte Carlo simulations. Applications will focus on studies of the structural and thermomechanical properties of materials.

Course Pre-Requisites / Co-Requisites
No formal pre-requisites.
Students should have a strong undergraduate understanding of mechanics, material science and physics.
Students should be familiar with programming and plotting in Matlab or Python.

Textbooks and Software
Required: Relevant journal papers distributed via Canvas.
Optional: *Introduction to Computational Materials Science*, LeSar, 2013
Optional: *Computer Simulation of Liquids*, Allen and Tildesley, 1989.
Optional: *The Art of Molecular Dynamics Simulation*, Second Edition, Rapaport, 2004.
Optional: *Understanding Molecular Simulation*, Second Edition, Frenkel and Smit, 2002.

Course Topics
1) What is Computational Mechanics and Materials Science?
2) Atomistic Simulations
   a) Basic principles – Thermodynamic properties / Ensembles
   b) Interatomic potentials for different material classes
3) Molecular Dynamics
   a) Force calculation
   b) Extended boundary conditions (temperature and pressure control)
   c) Integration methods
4) Monte Carlo Simulations
   a) Use of random number generators
   b) Isobaric/isothermal applications
5) Molecular Mechanics
   a) Energy minimization techniques
   b) Minimum energy path between states (nudged elastic band method)
6) Brief Overview to Multiscale Modeling
7) Brief Overview of Phase Field Modeling

Assessment Methods
Your grade for this course will be determined based on your performance on homework assignments and a course project report/presentation:

Homework 50%
Homework will be assigned and collected approximately every two weeks during the semester. Most homework assignments will require programming skills in Matlab or Python. The collective purpose of the homework assignments will be for each student to write their own 1 or 2 dimensional atomistic simulation code capable of performing molecular mechanics, molecular dynamics and Monte Carlo simulations using a two-body interatomic potential.

Course Project 50%
Students will be required to complete a course project. The course project could be a critical literature review of a relevant topic in the literature. Or, the course project could employ open-source atomistic simulation codes, such as LAMMPS, to perform relevant calculations. Students will present the results of their work via a written report and an oral presentation (during the regular class period). The course project can be related to, but not duplicate, a student's current research activity. Example project topics include:

- Mechanical behavior of carbon nanotubes
- Efficiency of different thermostats for molecular dynamics simulations
- Application of MD to model thermal conductivity

It is the responsibility of each student to propose a project topic. Topics that are related to the student's area of research are acceptable and encouraged. However, students may not duplicate research results or research publication for credit in this class. Students are encouraged to speak with Professor Spearot prior to submitting a project topic.

Approval
All project topics must be approved by Professor Spearot. Please submit a project title, abstract (~200 words) and an initial reference list electronically by **February 21**.

Report
10-12 pages (1 inch margins, 12 point font, 1.5 line spacing, including figures). Reports are due electronically to Professor Spearot by **April 10**.

Presentation
~15 minutes to be given in class between **April 13 and April 12** (depending on the number of students in the class). Order of student presentations will be determined randomly.

Grading
Project grades will be a composite of both oral (25%) and written (75%) reports.

Grading Scale
An example numerical grading scheme is shown below. This information should only be used as a general guide as the course instructor reserves the right to adjust the final numerical grading demarcations. Course grades will be "curved" if necessary – this decision will not be made until the end of the semester once all homework assignments and course projects are graded.

100–93 = A, 92.9–90 = A-, 89.9–87 = B+, 86.9–83 = B, 82.9–80 = B-, 79.9–77 = C+, 76.9–73 = C
72.9–70 = C-, 69.9–67 = D+, 66.9–63 = D, 62.9–60 = D-, 60-0 = F

Additional information regarding letter grades and associated grade points may be found at: https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx.

Attendance Policy, Class Expectations, and Make-Up Policy
Class attendance is highly recommended, but is not mandatory. Excused absences for homework submission must be consistent with university policies in the undergraduate catalog and require appropriate documentation. Homework extensions will be provided for excused absences in which notification is provided before the assignment date.
https://catalog.ufl.edu/ugrad/current/regulations/info/attendance.aspx

Students Requiring Accommodations
Students with disabilities requesting accommodations should first register with the Disability Resource Center (352-392-8565, https://www.dso.ufl.edu/drc) by providing appropriate documentation. Once registered, students will receive an accommodation letter, which must be presented to the instructor when requesting accommodation. Students with disabilities should follow this procedure as early as possible in the semester.

Course Evaluation
Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available at https://gatorevals.aa.ufl.edu/students/. Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their Canvas course menu under GatorEvals, or via https://ufl.bluera.com/ufl/. Summaries of results are available to students at https://gatorevals.aa.ufl.edu/public-results/.

University Honesty Policy
UF students are bound by The Honor Pledge, "We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honor and integrity by abiding by the Honor Code." On all work submitted for credit by students at the University of Florida, the following pledge is either required or implied: "On my honor, I have neither given nor received unauthorized aid in doing this assignment." The Honor Code (https://www.dso.ufl.edu/sccr/process/student-conduct-honor-code/) specifies a number of behaviors that are in violation of this code and the possible sanctions. Furthermore, you are obligated to report any condition that facilitates academic misconduct to appropriate personnel. If you have any questions or concerns, please consult with the instructor in this class.

Software Use
All faculty, staff, and students of the University are required and expected to obey the laws and legal agreements governing software use. Failure to do so can lead to monetary damages and/or criminal penalties for the individual violator. Because such violations are also against University policies and rules, disciplinary action will be taken as appropriate. We, the members of the University of Florida community, pledge to uphold ourselves and our peers to the highest standards of honesty and integrity.

Student Privacy
There are federal laws protecting your privacy regarding grades earned in courses and on individual assignments. For more information, please see:
http://registrar.ufl.edu/catalog0910/policies/regulationferpa.html

Campus Resources

Health and Wellness

U Matter, We Care
If you or a friend is in distress, please contact umatter@ufl.edu or 352-392-1575 so that a team member can reach out to the student.

Counseling and Wellness Center
http://www.counseling.ufl.edu/cwc or 352-392-1575; or contact the University Police Department: 352-392-1111 or 9-1-1 for emergencies.

Sexual Assault Recovery Services (SARS)
Contact the Student Health Care Center at 352-392-1161.

University Police Department
Contact UFPD at 352-392-1111 (or 9-1-1 for emergencies) or http://www.police.ufl.edu/.

Academic Resources

E-learning technical support
Call 352-392-4357 (select option 2) or e-mail to Learning-support@ufl.edu. You may also find answers to common problems at https://lss.at.ufl.edu/help.shtml.

Career Resource Center
Located in the Reitz Union and offers career assistance and counseling. Call 352-392-1601 or https://www.crc.ufl.edu/.

Library Support
Information on various ways to receive assistance using the libraries or finding resources. http://cms.uflib.ufl.edu/ask.

Teaching Center
Located in Broward Hall and provides general study skills and tutoring. Call 352-392-2010 or 352-392-6420 or https://teachingcenter.ufl.edu/.

Writing Studio
Located at 302 Tigert Hall. Provides help brainstorming, formatting, and writing papers. Call 352-846-1138 or https://writing.ufl.edu/writing-studio/.

On-Campus Student Complaints
https://www.dso.ufl.edu/documents/UF_Complaints_policy.pdf.

On-Line Students Complaints
http://www.distance.ufl.edu/student-complaint-process.