

Computational Nanomechanics and Nanomaterials

EML 6934 Section 1F75

Class Periods: Monday/Wednesday/Friday, Period 7, 1:55 – 2:45 pm

Location: MAE-B 211

Academic Term: Spring 2017

Instructor

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Office Hours: Monday/Wednesday/Friday, 2:45 – 3:45 pm, NEB 133

Course Description

To provide students with an overview of select atomistic 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.

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 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/due approximately every two or three weeks. The collective goal of the homework assignments will be to write a set of atomistic simulation programs in Matlab using a two-body potential for a 1D chain of atoms. No late homework assignments will be accepted without prior approval.

Course Project 50%

Students will be required to complete a course project. The course project will involve a literature review of a specific topic that has significant relevance to atomistic/multiscale simulation. The student is encouraged to use the open-source atomistic simulation package LAMMPS to perform simulations relevant to their chosen project. Computing time on HiPerGator will be established if necessary. Project results will be disseminated via a written report and an oral presentation (during the regular class period at the end of the semester). 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 24**.

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 7**.

Presentation

~15 minutes to be given in class between **April 12 and April 19**. 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.

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

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 feedback on the quality of instruction in this course by completing online evaluations at: <https://evaluations.ufl.edu/evals>. Evaluations are typically open during the last two or three weeks of the semester, but students will be given specific times when they are open. Summary results of these assessments are available to students at: <https://evaluations.ufl.edu/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>.