# Computational Nanomechanics and Nanomaterials

EML 6386 Section DSCN

***Class Periods:*** Monday/Wednesday/Friday, Period 7, 1:55 pm – 2:45 pm
***Location:*** MAE-B 238
***Academic Term:*** Spring 2024

***Instructor***

Douglas Spearot, Ph.D.
Email: dspearot@ufl.edu
Phone: 352-392-6747
Office Hours: Monday/Friday, 3:00 – 4:00 pm, MAE-A 310

***Course Description***

To elucidate the fundamentals of select modeling techniques in nanomechanics and nanomaterials. Modeling and simulation methods covered will 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 have some familiarity with numerical methods and 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) Temperature and pressure control
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) Coupled Atomistic Continuum Method
7) Discrete Dislocation Dynamics 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
- Application of MD to model thermal conductivity
- Use of AI to develop interatomic potentials

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 16**.

***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 19**.

***Presentation***
~15 minutes to be given in class between **April 22 and May 3** (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 is a general guide; the course instructor reserves the right to adjust the final numerical grading demarcations. Course grades will be "elevated" if necessary – this decision will not be made until the end of the semester once all exams and homework assignments are graded. Additional information may be found at:
https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx

100–93.4 = A, 93.3–90.0 = A-
89.9–86.7 = B+, 86.6–83.4 = B, 83.3–80.0 = B-
79.9–76.7 = C+, 76.6–73.4 = C, 73.3–70.0 = C-
69.9–66.7 = D+, 66.6–63.4 = D, 63.3–60.0 = D-
60.0-0.0 = E

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

***Students Requiring Accommodations***
Students with disabilities who experience learning barriers and would like to request academic accommodations should connect with the disability Resource Center by visiting https://disability.ufl.edu/students/get-started/. It is important for students to share their accommodation letter with their instructor and discuss their access needs, as early as possible in the semester.

***In-Class Recording***
Students are allowed to record video or audio of class lectures. However, the purposes for which these recordings may be used are strictly controlled. The only allowable purposes are (1) for personal educational use, (2) in connection with a complaint to the university, or (3) as evidence in, or in preparation for, a criminal or civil proceeding. All other purposes are prohibited. Specifically, students may not publish recorded lectures without the written consent of the instructor.

A "class lecture" is an educational presentation intended to inform or teach enrolled students about a particular subject, including any instructor-led discussions that form part of the presentation, and delivered by any instructor hired or appointed by the University, or by a guest instructor, as part of a University of Florida course. A class lecture does not include lab sessions, student presentations, clinical presentations such as patient history, academic exercises involving solely student participation, assessments (quizzes, tests, exams), field trips, private conversations between students in the class or between a student and the faculty or lecturer during a class session.

Publication without permission of the instructor is prohibited. To "publish" means to share, transmit, circulate, distribute, or provide access to a recording, regardless of format or medium, to another person (or persons), including but not limited to another student within the same class section. Additionally, a recording, or transcript of a recording, is considered published if it is posted on or uploaded to, in whole or in part, any media platform, including but not limited to social media, book, magazine, newspaper, leaflet, or third party note/tutoring services. A student who publishes a recording without written consent may be subject to a civil cause of action instituted by a person injured by the publication and/or discipline under UF Regulation 4.040 Student Honor Code and Student Conduct Code.

***University Honesty Policy***
UF students are bound by The Honor Pledge which states, "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://sccr.dso.ufl.edu/process/student-conduct-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.

***Commitment to a Safe and Inclusive Learning Environment***
The Herbert Wertheim College of Engineering values varied perspectives and lived experiences within our community and is committed to supporting the University's core values, including the elimination of

discrimination. It is expected that every person in this class will treat one another with dignity and respect regardless of race, creed, color, religion, age, disability, sex, sexual orientation, gender identity and expression, marital status, national origin, political opinions or affiliations, genetic information, and veteran status.

- Your academic advisor or Graduate Program Coordinator
- HWCOE Human Resources, 352-392-0904, student-support-hr@eng.ufl.edu
- Curtis Taylor, Associate Dean of Student Affairs, 352-392-2177, taylor@eng.ufl.edu
- Toshikazu Nishida, Associate Dean of Academic Affairs, 352-392-0943, nishida@eng.ufl.edu

***Course Evaluations***

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. Summaries of results are available to students at https://gatorevals.aa.ufl.edu/public-results/.

***Software Use and Copyrighted Materials***

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 with regards to grades earned in courses and on individual assignments. For more information, please see: https://registrar.ufl.edu/ferpa.html.

***Campus Resources***

*Health and Wellness*

**U Matter, We Care:** Your well-being is important to the University of Florida. The U Matter, We Care initiative is committed to creating a culture of care on our campus by encouraging members of our community to look out for one another and to reach out for help if a member of our community is in need. If you or a friend is in distress, please contact umatter@ufl.edu so that the U Matter, We Care Team can reach out to the student in distress. A nighttime and weekend crisis counselor are available by phone at 352-392-1575. The U Matter, We Care Team can help connect students to the many other helping resources available including, but not limited to, Victim Advocates, Housing staff, and the Counseling and Wellness Center. Please remember that asking for help is a sign of strength. In case of emergency, call 9-1-1.

**Counseling and Wellness Center:** https://counseling.ufl.edu or 392-1575. You can also call the University Police Department at 392-1111 or dial 9-1-1 for emergencies.

**Sexual Discrimination, Harassment, Assault, or Violence:** If you or a friend has been subjected to sexual discrimination, sexual harassment, sexual assault, or violence contact the Office of Title IX Compliance, located at Yon Hall, Room 427, 1908 Stadium Road, 352-273-1094, title-ix@ufl.edu.

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

**University Police Department:** http://www.police.ufl.edu/ or 392-1111 (dial 9-1-1 for emergencies).

*Academic Resources*

**E-learning technical support:** 352-392-4357 (select option 2) or e-mail Learning-support@ufl.edu; https://lss.at.ufl.edu/help.shtml.

**Career Connections Center:** Career assistance and counseling. Reitz Union, 392-1601; https://career.ufl.edu.

**Library Support:** Various ways to receive assistance with respect to using the libraries or finding resources; http://cms.uflib.ufl.edu/ask.

**Teaching Center:** General study skills and tutoring. Broward Hall, 392-2010 or 392-6420; https://teachingcenter.ufl.edu/.

**Writing Studio:** Help brainstorming, formatting, and writing papers. 302 Tigert Hall, 846-1138; https://writing.ufl.edu/writing-studio/.

**Student Complaints Campus:** https://care.dso.ufl.edu.

**On-Line Students Complaints:** https://distance.ufl.edu/getting-help/.