ASEN 6519: Molecular Simulation of Materials

Spring 2023

Class meetings: Tue/Thu 11:30 AM - 12:45 PM AERO N250

Instructor:

Prof. Sanghamitra Neogi
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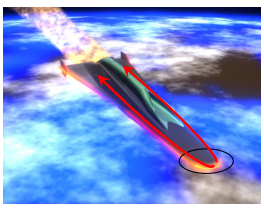
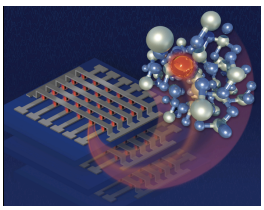
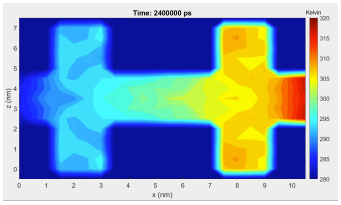
Course Description, Objective, and Outcomes:

When the relevant transformation of a material or a structure occurs over length scales on the order of atomic spacings and time scales on the order of the period of atomic vibrations, one cannot rely on continuum descriptions of materials to accurately describe the phenomena. Dynamic restructuring of materials surfaces or interfaces, oxidation of microstructures in composite materials or ceramics at high-temperatures or in highly chemically-active environments are some examples of such phenomena. The theoretical formulations can be complex and often cannot fully describe the physical mechanisms responsible for the transformations. At the same time, performing experiments can be challenging as well as expensive.

Numerical techniques offer the remarkable opportunity to predict atomic level phenomena and provide guidance to experimental studies. Molecular modeling and simulations thus emerged as an essential tool for not only predicting the materials performance in diverse environments but designing novel materials with desired functionalities and performance. Predictive modeling of materials at the atomic scale is of great interest in a broad range of technological applications, including electronic, optoelectronic, energy conversion, renewable energy harvesting, chemical-sensing, bio-medical and quantum devices.

The objective of this course is to expose students to the theory and implementation of numerical techniques for modeling behavior of materials at the atomic level. The numerical technique of focus will be classical molecular dynamics simulations. One of the main applications that will be discussed in this course is the analysis of heat conduction properties of materials. If we can control heat conduction in materials, we will be able to design leading edges of aerospace vehicles that are capable of flying at supersonic and hypersonic speeds, engineer thermoelectric materials with improved efficiency for deep space explorations and design next generation radiation-hard microelectronics based on wide and ultra-wide-band-gap semiconductors. In this course, you will

- Learn the theory behind molecular dynamics (MD) simulations.
- Write your own MD code to perform simulations.
- Critically assess published results from MD simulations for technical correctness and physical relevance.
- Analyze MD results to obtain physically measurable parameters.
- Design your class project to model materials in different environmental conditions.
- Learn to use the open-source software, LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), to model atomic level phenomena accurately.

Logistics:

A. Office hours

Tue/Thu 02:00 - 03:00 PM, otherwise by appointment.

B. Class Time

There are two 75-mins meetings per week. The time will include formal lecturing, computer demonstrations, and group work. You are responsible for all material discussed in class, whether you attended or not. Class schedule is posted on Canvas, subject to change.

C. Prerequisites

Students are expected to have taken an undergraduate thermodynamics course. Background knowledge in hamiltonian formulation of classical mechanics, statistical mechanics, and solid state physics will be helpful but is not required. Experience with computer programming is going to be helpful but extensive previous experience is not required. It is strongly recommend to work in a Linux-based platform. Students are free to program in a language of their choice, however it is advised to use Python/Matlab/Fortran for coding/scripting purposes. Some of the assignments will be based on using the LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) software.

D. Website

Course materials are available on Canvas.

E. Reading Material

The textbook for the course will be

- *Statistical Mechanics: Theory and Molecular Simulation*, Mark E. Tuckerman, Oxford, 2010
  eBook available online through CU Boulder Libraries;
  Link: https://ebookcentral.proquest.com/lib/ucb/detail.action?docID=3053587.

The following books may be useful for reference. You will also be provided with notes and papers from the literature during the semester.

- *Computer Simulation of Liquids*, M. P. Allen and D. J. Tildesly, Oxford, 1989, ISBN 9780198556459.
- *Introduction to Modern Statistical Mechanics*, D. Chandler, Oxford, 1987, ISBN 9780195042771.

F. Grades

Homework (40%), two mid-term exams (25%), class participation (5%), and project (30%);

(a) Homework assignments: 40%

There will be six homework assignments in the course. There will be pencil and paper problems and programming assignments. Students are encouraged to work together but must submit their own work for grading. If applicable, you must indicate in your submission who you worked with. For programming assignments, documentation within the code is strongly recommended. It is necessary than your final submitted code runs without giving an error, to receive credit.

Homework will be due on **Fridays at 11:59 PM** and should be submitted to Canvas. Please put all files (code, text documents, scanned files) into one zip file with the naming scheme (last- name)HW(homework number).zip. For example, neogiHW4.zip. Recommended file types are: pdf, jpg, png etc for documents and figures. Homework submitted by 8 AM the day after it is due will be penalized 25%. Homework submitted by midnight of the day after it is due will be penalized 50%. Homework submitted after that time will result in a grade of zero.

(b) Project presentations and reports: 30%

Details will be provided in class. The deadline policies will be similar to homework submission policies.

(c) Participation: 5%

The students will be required to provide peer review for presentations. More details will be provided in class.

Any grading disputes will be handled by the instructor. Any request for a grade change should be made to the instructor, in writing, **within one week after the graded work is returned**. Your entire submission will be subject to regrading. Students are advised to read and adhere to the Honor Code at the University of Colorado at Boulder.

(d) Exam dates (tentative):

- **Mid-term Exam 1:** Thursday, March 7
- **Mid-term Exam 2:** Thursday, April 13
- **Final Project Presentations:** Wednesday, May 10 4:30 PM–7:00 PM or before. We might need the entire time till 7:00 PM, please make your travel arrangements accordingly.

Tentative List of Course Topics:

1. Introduction to molecular simulation
   (a) Model systems
   (b) Empirical potentials
   (c) Finite systems: Consideration of boundary conditions
2. Review of classical mechanics
   (a) Newton's laws of motion
   (b) Phase space: Visualizing classical motion
   (c) Hamiltonian formulation of classical mechanics
3. Introduction to classical statistical mechanics
   (a) The laws of thermodynamics
   (b) The ensemble concept: connection between the macroscopic and the microscopic worlds
   (c) Types of statistical ensembles
4. The microcanonical ensemble and introduction to molecular dynamics
   (a) Conditions for thermal equilibrium
   (b) Initialization
   (c) Equations of motion, energy calculations
   (d) Integrating the equations of motion: Finite difference methods
5. The canonical (constant-temperature) ensemble
   (a) Energy fluctuations in the canonical ensemble
   (b) Determining structure and thermodynamics in real gases and liquids
   (c) Constant-temperature molecular dynamics

6. Classical time-dependent statistical mechanics
    (a) Externally driven systems and linear response theory
    (b) Application of linear response theory: Transport coefficients
    (c) Calculating time correlation functions from molecular dynamics
    (d) The nonequilibrium molecular dynamics approach

There might be lectures on advanced topics in addition to the above content, mainly on modeling thermal properties of materials.

Classroom Behavior

Both students and faculty are responsible for maintaining an appropriate learning environment in all instructional settings, whether in person, remote or online. Those who fail to adhere to such behavioral standards may be subject to discipline. Professional courtesy and sensitivity are especially important with respect to individuals and topics dealing with race, color, national origin, sex, pregnancy, age, disability, creed, religion, sexual orientation, gender identity, gender expression, veteran status, political affiliation or political philosophy. For more information, see the classroom behavior policy, the Student Code of Conduct, and the Office of Institutional Equity and Compliance.

Requirements for COVID-19

As a matter of public health and safety, all members of the CU Boulder community and all visitors to campus must follow university, department and building requirements and all public health orders in place to reduce the risk of spreading infectious disease. CU Boulder currently requires COVID-19 vaccination and boosters for all faculty, staff and students. Students, faculty and staff must upload proof of vaccination and boosters or file for an exemption based on medical, ethical or moral grounds through the MyCUHealth portal.

The CU Boulder campus is currently mask-optional. However, if public health conditions change and masks are again required in classrooms, students who fail to adhere to masking requirements will be asked to leave class, and students who do not leave class when asked or who refuse to comply with these requirements will be referred to Student Conduct and Conflict Resolution. For more information, see the policy on classroom behavior and the Student Code of Conduct. If you require accommodation because a disability prevents you from fulfilling these safety measures, please follow the steps in the "Accommodation for Disabilities" statement on this syllabus.

If you feel ill and think you might have COVID-19, if you have tested positive for COVID-19, or if you are unvaccinated or partially vaccinated and have been in close contact with someone who has COVID-19, you should stay home and follow the further guidance of the Public Health Office (contacttracing@colorado.edu). If you are fully vaccinated and have been in close contact with someone who has COVID-19, you do not need to stay home; rather, you should self-monitor for symptoms and follow the further guidance of the Public Health Office (contacttracing@colorado.edu). In this course, please let your instructor know if you are going to be absent. You do not need to state the nature of your illness.

Accommodation for Disabilities

If you qualify for accommodations because of a disability, please submit your accommodation letter from Disability Services to your faculty member in a timely manner so that your needs can be addressed. Disability Services determines accommodations based on documented disabilities in the academic environment. Information on requesting accommodations is located on the Disability Services website. Contact Disability Services at 303-492-8671 or dsinfo@colorado.edu for further assistance. If you have a temporary medical condition, see Temporary Medical Conditions on the Disability Services website.

Preferred Student Names and Pronouns

CU Boulder recognizes that students' legal information doesn't always align with how they identify. Students may update their preferred names and pronouns via the student portal; those preferred names and pronouns

are listed on instructors' class rosters. In the absence of such updates, the name that appears on the class roster is the student's legal name.

Honor Code

All students enrolled in a University of Colorado Boulder course are responsible for knowing and adhering to the Honor Code. Violations of the Honor Code may include, but are not limited to: plagiarism, cheating, fabrication, lying, bribery, threat, unauthorized access to academic materials, clicker fraud, submitting the same or similar work in more than one course without permission from all course instructors involved, and aiding academic dishonesty. All incidents of academic misconduct will be reported to Student Conduct & Conflict Resolution (honor@colorado.edu); 303-492-5550). Students found responsible for violating the Honor Code will be assigned resolution outcomes from the Student Conduct & Conflict Resolution as well as be subject to academic sanctions from the faculty member. Additional information regarding the Honor Code academic integrity policy can be found on the Honor Code website.

Sexual Misconduct, Discrimination, Harassment and/or Related Retaliation

CU Boulder is committed to fostering an inclusive and welcoming learning, working, and living environment. University policy prohibits sexual misconduct (harassment, exploitation, and assault), intimate partner violence (dating or domestic violence), stalking, protected-class discrimination and harassment, and related retaliation by or against members of our community on- and off-campus. These behaviors harm individuals and our community. The Office of Institutional Equity and Compliance (OIEC) addresses these concerns, and individuals who believe they have been subjected to misconduct can contact OIEC at 303-492-2127 or email cureport@colorado.edu. Information about university policies, reporting options, and support resources can be found on the OIEC website.

Please know that faculty and graduate instructors have a responsibility to inform OIEC when they are made aware of any issues related to these policies regardless of when or where they occurred to ensure that individuals impacted receive information about their rights, support resources, and resolution options. To learn more about reporting and support options for a variety of concerns, visit Don't Ignore It.

Religious Holidays

Campus policy regarding religious observances requires that faculty make every effort to deal reasonably and fairly with all students who, because of religious obligations, have conflicts with scheduled exams, assignments or required attendance. In this class, you should make arrangements with the instructors at least two weeks in advance, so that appropriate accommodations can be made.

See the campus policy regarding religious observances for full details.

Other Policies Please be respectful of others during class time. This includes turning off your cell phone before class and not talking during class unless you have the floor. Details about all of the university policies can be found on the web at `https://www.colorado.edu/academicaffairs/policies-customs-guidelines`.