CSI 786 *Molecular Dynamics Modeling*
Crosslisted: CHEM 579/PHYS 780
Co-taught: CDS 461 *Molecular Dynamics and Monte Carlo Simulations*
Spring 2021

Classroom: Synchronous meetings on Zoom
Class time: Tuesdays, 4:30 pm - 7:10 pm
Class notes: http://nano.gmu.edu/csi786/index.html

Instructor Name: Estela Blaisten
Office location: Research Hall 221, Fairfax campus
Office hours: By appointment through Zoom
Email address: blaisten@gmu.edu (preferred way of communication)

This class is synchronous, online. *Activities and assignments in this course will regularly use web-conferencing software (Zoom). Students are required to have a laptop/desktop with a functional camera and microphone. In an emergency, students can connect through a telephone call, but video connection is the expected norm.*

Professor Blaisten does not authorize in anyway the recording of any lecture content in this course. Sharing of video lecture or lab content violates student privacy governed by the Family Education Rights and Privacy Act (FERPA). Additionally, any written, video, or audio content built by Prof. Blaisten for CSI 786/CHEM 579/PHYS 780 and CDS 461 instruction that is shared online externally to GMU is a clear and punishable violation of GMU's Honor Code.

Course Description and Goals

The theme of the course is Molecular Dynamics and Monte Carlo methods. These methods are currently orthodox means for simulating molecular-scale models of matter. The methods were originally devised in the 1950's, began to receive widespread attention in the mid-1970's, and are today a fundamental scientific approach to design nano systems, as well as bulk crystals, glasses, liquids, polymers, surfaces, and interfaces. Additionally, the methodology has been adopted by computational biologists, and is today an essential element of bio-oriented research.

By the end of this course, students will be able to

1. apply Molecular Dynamics and Monte Carlo algorithms for solving numerical problems in computational science
2. appraise theoretical foundations of algorithms
3. reinforce practical skills for building computer programs that include common data analysis of the simulation methods learned in class
4. perform elementary atomistic simulations

Prerequisites: Calculus, introductory physics or physical chemistry, and knowledge of a programming language (at the level of CSI 501 or better). An understanding of the basic concepts of ordinary differential equations is helpful.

Required Textbook

Molecular Dynamics Simulation, by J. M. Haile, John Wiley, 1997 (ISBN-13: 978-0-471-18439-3), paperback or hardcopy.

A supplemental textbook is:

Understanding Molecular Simulation, by Daan Frenkel and Berend Smit, Academic Press, 2nd edition, 2002.

Evaluation

Grading scale (points): A (90-100), B (80-89), C (≤79) (with eventual slight variations)

Grading policy (may change slightly):

1) Homework (40%). Each of 8-10 homework will be graded between 1 and 10. Ten is the best. Present homework in a report-like fashion.
2) Individual project: project description (30%).
3) Class participation and attendance, including presentations by students on the material related to the textbook or class notes, on their advances in the individual project, or additional explanations on homework assignments. Included is a final presentation of the individual project to take place on the date of final exam that Registrar assigns to this course (30%).

Late assignments: Late assignments will not be accepted unless due to emergency or work-related compelling reasons for part-time students.

"Re-do" homework policy:

1) Homework graded and returned to you can be revised for a better grade with a penalty on its final grade of minus 1 point.
2) Redo homework should be turned in with the original handout containing the corrections.

Other considerations: If there are any obligations related to religious holidays, please inform the instructor the first week of class

Course schedule for Spring 2021

Subject 1,
Numerical methods in science, stochastic vs. deterministic. Modeling vs. simulation. "Experiments' in the computer

Subject 2,
Newtonian or Hamiltonian dynamics. Phase space. Examples

Subject 3
Distribution functions. Sampling theory. Periodic boundary conditions

Subject 4
Hard spheres model. Models of different bonds. Model potentials.

How to assess predictability.

Subject 5
Finite difference methods for the solution of ordinary differential equations.
Euler method. Algorithms for Molecular Dynamics. Reliability of trajectories.

Subject 6
How to perform Molecular Dynamics and Monte Carlo simulations. Equilibration. Production,
Data analysis of trajectories.

Subject 7
Static properties. Thermodynamic functions. One-slide project presentations (March 16th)

Subject 8
Static properties. Thermodynamic response functions.

Subject 9
Static properties. Entropic functions. Static structure.

Subject 10
Dynamic properties. Time correlation functions. Transport coefficients

Subject 11
Dynamic structure.

Class 12
Projects pre-presentation

Class 13
Projects pre-presentation

Final exam day: Project presentations. Each student does a final presentation of his/her project. This meeting is not an exam, it is part of the individual project and your contribution to class participation.

Course Logistics

The course uses a password protected site for distributing lecture materials and study recommendations. You will need to access the site remotely with a browser (Firefox, Safari, etc):

http://nano.gmu.edu/csi786/index.html

ID/password instructions will be sent by email to your GMU email.

IT Requirements for the Course

Hardware: You will need access to a Windows, Macintosh, or Linux computer. The lab in RH 249 allows you to work in any of the 24 linux-servers, either in person or remotely through SSH (or Putty). You login with your Mason ID and password:

cdsXX.mesa.gmu.edu, where XX=01 through 24

These RH 249 computers do not share the desktops. Therefore, it is recommended that you take note on what computer you work the first time, and then keep working in that computer for the rest of the semester. To access these workstations you need to install the VPN (Virtual Private Network) and to be logged in to it. For the installation use:

https://its.gmu.edu/service/virtual-private-network-vpn/

Software: Computers in this lab have all the needed software. They have installed compilers for Fortran, C, c++. Python and MatLab. If computers in this lab are not used, students are expected to have access to a programming language software suitable for scientific calculations.

Course Policies: Student Responsibilities

Email: Students are responsible for reading and maintaining the content of university emails sent to their Mason email account. Therefore, students are required to activate their email account and check it regularly. All communications from this course will be sent to students solely through their Mason email account. Alternatively, students may set a "forward" for forwarding any Mason incoming email/message to your preferred email account.

Use of phones, cameras, recording, texting in class is not allowed. Students should turn off the ringing of smart devices (cell phone, alerts apps) while in the Zoom classroom.

- *The use of laptop or a desktop computer is required in this class. You will only be permitted to work on material related to the class, however. Engaging in activities not related to the course (e.g., gaming, email, chat, etc.) will result in a significant reduction in your participation grade.*
- *We will frequently be using the internet as a means to enhance our discussions. We will also be using computers for our in-class writing assignments. Please be respectful of your peers and your instructor and do not engage in activities that are unrelated to the class. Such disruptions show a lack of professionalism and may affect your participation grade.*

Academic integrity: Students are responsible for their own work and must take on the responsibility of dealing explicitly with consequences to any academic integrity violation. Students must adhere to the George Mason University **Honor Code** as it relates to integrity regarding coursework and grades. The Honor Code reads as follows:

"To promote a stronger sense of mutual responsibility, respect, trust, and fairness among all members of the George Mason University community and with the desire for greater academic and personal achievement, we, the student members of the University Community have set forth this: Student members of the George Mason University community pledge not to cheat, plagiarize, steal and/or lie in matters related to academic work."
[See Honor Code website: http://oai.gmu.edu/the-mason-honor-code].

This is very important now [See Academic Integrity website: https://oai.gmu.edu/].

Classroom Conduct: Students must adhere to the Mason Honor Code and be very respectful of all class co-participants. It is recommended that students select a static virtual background for joining the classes. This enhances privacy. It is helpful for the group if each student adds a photo (ID type of photo) to be visible when the conference video is off.

Academic honesty policy of the course: Students are expected to follow the Honor Code at all time and for all activities. Academic dishonesty will not be tolerated in this class. Exams, projects, and homework must reflect individual work. If you have difficulty with the assignments, discuss them with the instructor.

Students with disabilities: Students with disabilities who seek accommodations in a course must be registered with the George Mason University Office of Disability Services (ODS) and inform the instructor, in writing, at the beginning of the semester [See Office of Disability Services website: http://ods.gmu.edu/].

Students that become ill: Students that become ill due to the pandemic should follow the Mason health recommendations and steps to follow: [https://shs.gmu.edu/.

University policies: Students must follow the university policies [See University Policies website: http://universitypolicy.gmu.edu].

Responsible use of computing: Students must follow the university policy for Responsible Use of Computing [See University Policies website: http://universitypolicy.gmu.edu/policies/responsible-use-of-computing].

University calendar: Students should consult the current Academic Calendar [See https://registrar.gmu.edu/calendars/spring-2021 .

University catalog: Students should use the current university catalog [See University Catalog website: http://catalog.gmu.edu].

Student Services

University libraries: University Libraries provide excellent resources for books and journal publications. In addition, there are resources for distance students [See Library website: http://library.gmu.edu/distance].

Writing center: The George Mason University Writing Center staff provides a variety of resources and services (e.g., tutoring, workshops, writing guides, handbooks) intended to support students as they work to construct and share knowledge through writing. (See Writing Center website: http://writingcenter.gmu.edu). ESL Help: The program was designed specifically for students whose first language is not English who feel they might benefit from additional, targeted support over the course of an entire semester.

Counseling and Psychological Services: The George Mason University Counseling and Psychological Services (CAPS) staff consists of professional counseling and clinical psychologists, social workers, and counselors who offer a wide range of services (e.g.,

individual and group counseling, workshops and outreach programs) to enhance students' personal experience and academic performance [See Counseling and Psychological Services website: http://caps.gmu.edu].

Family Educational Rights and Privacy Act (FERPA): The Family Educational Rights and Privacy Act of 1974 (FERPA), also known as the "Buckley Amendment," is a federal law that gives protection to student educational records and provides students with certain rights [See Registrar's Office website: http://registrar.gmu.edu/privacy].