CHEM GA 2671 - SPECIAL TOPICS PHYSICAL CHEMISTRY: COMPUTATIONAL LAB (MS)
AKA: DIVE IN TO COMPUTATIONAL PHYSICAL CHEMISTRY
FALL 2022

Class Time/Room: Tuesday, 2PM-4:30 PM. Computer lab, 541 LaGuardia Place

Instructor: Glen Hocky   hockyg@nyu.edu
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Office Hours: Glen Hocky   TBD
Nicodemo Mazzaferro   TBD

Office hours start the second week of classes.

Course Overview: The goal of this class is to prepare you to use computational tools for chemistry research. It will also lay a foundation for data science and scientific computing more generally. A short lecture portion will introduce concepts behind what we are doing, but the primary emphasis of the class will be on *doing*. The goal by the end of the class is that you can jump into using new tools with ease and confidence.

Specific skills developed in the class: Some skills you will definitely come away with in this class are: (a) use of command line tools and general understanding of linux/unix based architectures, plus running and submitting jobs on high performance computing resources (b) software version control with git and github, (c) AI guided programming with Copilot (did not exist before 2022!), (d) python and jupyter notebooks for data analysis, including use of numpy, matplotlib, pandas, scipy, scikitlearn, (e) molecular dynamics simulations of proteins (with gromacs or amber), (f) molecular dynamics simulations for materials (with LAMMPS or HOOMD-Blue), (g) analyzing MD simulation results using python libraries (mdtraj or MDAnalysis), (h) enhanced sampling simulations with PLUMED, (i) quantum calculations in python, using wavefunction or DFT (with PySCF or Psi4), (j) visualizing molecular structures (primarily with VMD)

Course communication: Like in a research lab, we will use s**lack** for communication. You will be invited to the slack specific to the class. *Please install the slack application on your computer.*

Slack has different "channels" for different topics. Please post your questions and discussions in public channels so that everyone can work together.

Course websites: Course material and assignments will be available on from the group *github* website, and will be announced in slack.

Textbook: There is no textbook for this class, only internet resources will be required

Lectures: The first 20-30 minutes of each lab section will be used Recitations will be used to review key concepts, as well as to go over exams and past homework in more detail. They may also be used to introduce extra material, such as in the first recitation. You need to be registered for one of the recitation sections.

Office hours: There will be regularly scheduled office hours if you wish to discuss topics with me in person. You will also have access to me and all of your classmates' knowledge through slack.

Purpose of office hours. What is the point of office hours? Many people never attend office hours, or they do so only right before or right after an exam. But office hours can be so much more than for emergencies! This is a great chance for us to get to know each-other better. It is also a good time to clear up confusions you (or we) have about the material. We never want people to feel like they are behind. It's also a great time to discuss how the course material relates to your other interests, or to discuss more advance topics. So please consider attending as many office hours as you can from the beginning!

Course assignments: The only assignments will be completion of the labs. For each lab, you will turn in a git repository of a certain format that includes a jupyter notebook or other documents explaining your results and perhaps answering various questions.

Class Attendance: This is a laboratory class, even though it is on the computer. Attendance is mandatory unless you get specific permission. Each week you will be paired with another class member (or two) to work with, which is another reason that attendance is crucial.

Respect and inclusion: Another goal of this course is to create a learning environment that is inclusive and fosters contributions from all students. No one in the course should be made to feel uncomfortable because of the identity or background. If you feel like your performance in the class is being impacted by your experiences outside of class, please don't hesitate to come and talk with me.

Grading: Each lab will be equally weighted. It is expected that you will complete the entire lab with high quality figures and explanations. All labs must be fully completed by the end of the semester. I will give feedback each week or two to let you know if the lab is or is not complete.

It is therefore imperative that you keep up with the labs from week to week so that you can get feedback and make sure that you get an A on each one.

An unexcused absence will lose half-credit on that lab and so two unexcused absences will likely not result in a passing grade.

Academic Integrity and Plagiarism: As you know, we take academic honesty very seriously at NYU. The instructors for this course have no tolerance for plagiarism or cheating. The NYU policy on plagiarism will be enforced. Students who fail to conform to NYU's standards on academic integrity will be subject to stringent disciplinary action. Inform yourself in advance of proper academic conduct. In brief (and quoting from the College of Arts & Science policy), "Academic honesty means that the work you submit – in whatever form – is original." When in doubt, ask. Please consult: http://cas.nyu.edu/page/academicintegrity

Since there are no exams, and you will be working together and using resources from the internet, I do not expect this to be an issue. Still, you should turn in your own work.

Disability Disclosure Statement: Academic accommodations are available for students with disabilities. Please contact the Moses Center for Students with Disabilities (212-998-4980 or mosescsd@nyu.edu) for further information. Students who are requesting academic accommodations are advised to reach out to the Moses Center as early as possible in the semester for assistance.

Labs overview

Lab 1 (Sept 6)
Lab 2 (Sept 13)
Lab 3 (Sept 20)
Lab 4 (Sept 27
Lab 5 (Oct 4)

No class week of Oct 10, time to catch up on any earlier labs that need correcting
Lab 6 (Oct 18)
Lab 7 (Oct 25)
Lab 8 (Nov 1)
Lab 9 (Nov 8)
Lab 10 (Nov 15)
Lab 11 (Nov 22)
Lab 12 (Nov 29)
Lab 13 (Dec 6)
Lab 14 (Dec 13)