BIOSC 1544 – Simulation and Modeling

Spring, 2023

Instructor Information

Instructor	Email	Office Location & Hours
Jacob D. Durrant	durrantj@pitt.edu	3:30-4:30pm, Fridays, Clapp 102

General Information

Description

BIOSC 1544 is an upper-level course that teaches students how computational structural biology, including simulation and modeling, can be used to solve biological challenges. Topics will include protein structure and modeling, virtual small-molecule screening, molecular dynamics simulations, molecular visualization, and online resources for studying proteins and molecules. A class project will allow students to apply these tools.

Expectations and Goals

Though the focus will be on computational structural biology, the course aims to provide a broad understanding of many computational techniques. Rather than turning you into experts in a specific field, I hope to expose you to a wide variety of comp-bio-related topics. Students will learn through lectures and hands-on assignments involving the online resources discussed in class. Three exams spread throughout the term will assess comprehension.

Prerequisites

Students must have earned a "C" or better in BIOSC 1540 (Computational Biology) and a computer-programming course (CS 0008, 0010, 0011 or 0012). Students in BIOSC 1544 are expected to have a basic understanding of structural biology as well as BASH and Python programming.

Grading

Introduction

Scores on assignments, exams, and participation will determine final grades. If circumstances require us to reschedule any due dates, I will update the Syllabus on Canvas. It is the students' responsibility to consult the latest version of the syllabus to verify all due dates and policies. I reserve the right to update this syllabus as required over the course of the term.

Grade Breakdown

Home Assignments (~50% of Final Grade)

In-class, small-group assignments may accompany some lectures, so students should always bring a reasonably capable laptop computer. If necessary, you might consider checking out a laptop from Hillman Library.

Other lectures will include take-home homework assignments. Feel free to form study groups to discuss these assignments, though you may choose to work on them individually if you prefer. That said, these assignments should include only each student's own work (i.e., simply copying the work of others is cheating). In the past some students have participated in multiple groups and have turned in multiple versions of each assignment. Please submit only one assignment. I will grade only the first I encounter.

All assignments are due at the beginning of the next lecture and should be submitted through Canvas. I won't likely accept assignments after that time.

Not all assignments will have the same number of questions, but each assignment will weigh equally in calculating the final grade. For example, given two different assignments with four and eight questions,

respectively, the second assignment will **not** count twice as much as the first. Rather, both will count equally.

Exams (~45% of Final Grade)

Three closed-book exams will be administered through the online Canvas interface. Exams will be administered in class during the designated class time. Students must complete exams individually, without help from other students. Exams are cumulative, though most questions will address recently presented material. The third exam is scheduled for the last Thursday of the term (April 19th), so there will be no exam scheduled during finals week.

Participation (~5% of Final Grade)

Attendance and participation are critical. To assess participation, I will ask students to contribute exam-style questions. I may well use these questions in actual exams, perhaps in modified form. Students will submit questions through Canvas.

Additional in-class activities (e.g., polls and surveys) may also count towards participation. Although I would like to avoid it if possible, I may take attendance directly on select days if poor class attendance becomes an issue.

Final Grade

I will calculate letter grades according to the following scale: A (≥94%), A- (≥90%), B+ (≥86%), B (≥83%), B- (≥80%), C+ (≥76%), C (≥73%), C- (≥70%), D+ (≥66%), D (≥63%), D- (≥60%), F (<60%). Note that students can only count this class towards the Bioscience major if they earn a "C" grade or better. I reserve the right to curve the grading scheme to benefit the class if I think it's appropriate. I also reserve the right to provide extra-credit points.

Regrading Policy

I'm willing to regrade exam or homework questions. Regrade requests must be made in writing within one week of grading. I'll consider only concise requests expressing well-defined concerns; vague, wordy requests will be rejected without consideration. Upon receiving a regrade request, I reserve the right to regrade the entire assignment or exam, possibly leading to a reduced score overall. Students are thus advised to carefully consult one another and/or their class notes prior to requesting a regrade. That having been said, I welcome legitimate concerns.

Withdrawal Policy

If you are unable to stay current with the material, regardless of the reason, consider withdrawing from the course. Please consult the official academic calendar to learn when the add/drop period ends and when the monitored withdrawal form must be submitted to the Dean's Office.

G Grades

In some rare cases, extenuating personal circumstances arising after the withdrawal deadline may prevent students from finishing the course. Per SAS guidelines, if such students have been attending the course and making regular progress, they may petition for a G grade (University of Pittsburgh Undergraduate Bulletin, 1999-2002, p.29). If you find yourself in this situation, send me a request in writing that documents your reason(s) for the grade-change request. You will have to complete the course work before the G grade can be removed.

Course Materials

Required Materials

This course does not require a textbook. I will post links to online resources, articles from the scientific literature, etc., on Canvas to support what we discuss in class. I may draw exam questions from this posted material, in addition to what we cover in class.

Course Website

Course materials, an up-to-date syllabus, and a discussion board will be available through Canvas, https://canvas.pitt.edu/. Contact the computer help desk at (412) 624-HELP if you need help with the Canvas system.

Course Schedule

Lectures are on Mondays and Wednesdays, from 3:00 to 4:15 PM, in 144 Cathedral of Learning. I may change the topics/schedule below based on the needs/interests/pace of the class. Always consult Canvas for an up-to-date syllabus.

Date	Topic	Exercises Assigned	Exercises Due
Jan. 9th	Review Syllabus Comp Bio: General Overview UNIX Command Line (Intro)		
Jan. 11th	Basic Python	UNIX	
Jan. 16th	No Class (Martin Luther King Day)		
Jan. 18th	High-Performance Computing #1	Python	UNIX
Jan. 23rd	High-Performance Computing #2 Careers in Comp Bio	Candidate exam questions	Python
Jan. 25th	Machine Learning Discuss Questions re. Exam #1	Machine learning: scikit-learn	Candidate exam questions
Jan. 30th	EXAM 1		
Feb. 1st	Intro to Proteins & Ligands Review Exam #1		Machine learning: scikit-learn
Feb. 6th	Ligand/Protein Binding	BINANA (with reading)	
Feb. 8th	Cheminformatics 1	RDKit: Cheminformatics	BINANA (with reading)
Feb. 13th	Cheminformatics 2	PubChem Searching	RDKit: Cheminformatics
Feb. 15th	Small-Molecule Drugs	Chemical Properties	PubChem Searching
Feb. 20th	Small-Molecule Models	Gypsum-DL (reading) Candidate exam questions	Chemical Properties
Feb. 22nd	Ligand-Based CADD	RDKit: QSAR	Gypsum-DL (reading) Candidate exam questions
Feb. 27th	Catch-up Day (Python Packages, Command-line Programs) Discuss Questions re. Exam #2	TBA (likely Python related)	RDKit: QSAR

Date	Topic	Exercises Assigned	Exercises Due
Mar. 1st	EXAM 2		
Mar. 6th	**No Class (Spring Break)**		
Mar. 8th	**No Class (Spring Break)**		
Mar. 13th	Determining Protein Structures Review Exam #2		TBA (likely Python related)
Mar. 15th	Search & Visualize Proteins	UniProt and PDB Searching, Visualization, Prot2Prot	
Mar. 20th	Alignment and Homology Models	AlphaFold/SWISS-MODEL	UniProt and PDB Searching, Visualization, Prot2Prot
Mar. 22nd	Druggable Proteins	FPocketWeb	AlphaFold/SWISS-MODEL
Mar. 27th	Protein Simulations 1	MD Engine	FPocketWeb
Mar. 29th	Protein Simulations 2	NAMD and VMD	MD Engine
Apr. 3rd	CADD and Protein Flexibility	Molecular Dynamics Simulations and Drug Discovery (Reading)	NAMD and VMD
Apr. 5th	Computational Alchemy	Open-Source Browser-Based Tools for Structure-Based Computer-Aided Drug Discovery (Reading)	Molecular Dynamics Simulations and Drug Discovery
Apr. 10th	Structure-Based CADD	Webina docking	Open-Source Browser-Based Tools for Structure-Based Computer-Aided Drug Discovery
Apr. 12th	Lead optimization	Lead optimization: DeepFrag Candidate exam questions	Webina docking
Apr. 17th	Career day Discuss Questions re. Exam #3		Lead optimization: DeepFrag Candidate exam questions
Apr. 19th	EXAM 3		

Some lectures may not take the entire 1.25 hours. If so, students should get together in groups after the lecture to work on their homework assignments.

I will also be available during this time should you have any questions about the homework assignments, key online resources, relevant techniques, etc. Participating in after-lecture group and classroom discussions will likely be critical for success.

Additional Information and Resources

E-Mail Communication

Each student is issued a University e-mail address (username@pitt.edu) upon admittance. This e-mail address may be used by the University for official communication with students. Students are expected to read e-mail sent to this account on a regular basis. Failure to read and react to University communications in a timely manner does not absolve the student from knowing and complying with the content of the communications. The University provides an e-mail forwarding service that allows students to read their e-mail via other service providers (e.g., Hotmail, AOL, Yahoo). Students that choose to forward their e-mail from their pitt.edu address to another address do so at their own risk. If e-mail is lost as a result of forwarding, it does not absolve the student from responding to official communications sent to their University e-mail address. To forward e-mail sent to your University account, go to http://accounts.pitt.edu, log into your account, click on **Edit Forwarding Addresses**, and follow the instructions on the page. Be sure to log out of your account when you have finished. (For the full E-mail Communication Policy, go to www.bc.pitt.edu/policies/policy/09/09-10-01.html.)

The subject line of all emails sent to Dr. Durrant should start with "BIOSC 1544." I receive a large number of emails; if you use this subject prefix, I'll know to prioritize your message.

Academic Integrity

Cheating/plagiarism will not be tolerated. Students suspected of violating the University of Pittsburgh Policy on Academic Integrity, from the February 1974 Senate Committee on Tenure and Academic Freedom reported to the Senate Council, will be required to participate in the outlined procedural process as initiated by the instructor. A minimum sanction of a zero score for the quiz or exam will be imposed. View the complete policy at www.cfo.pitt.edu/policies/policy/02/02-03-02.html.

Students agree that by taking this course, all required papers may be subject to plagiarism detection using iThenticate or some other automated system. All submitted papers may be included as source documents in the iThenticate (or other) reference database to detect plagiarism of such papers.

Turning in assignments created using artificial intelligence or other automated writing tools as if they are your own is cheating. Using such methods to generate ideas (as part of your brainstorming process) or to give suggestions for improvement is not cheating.

COVID-19 Precautions

It is extremely important that you abide by the public health regulations, the University of Pittsburgh's health standards and guidelines, and Pitt's Health Rules. These rules have been developed to protect the health and safety of all of us. For the most up-to-date information and guidance, please visit coronavirus.pitt.edu and check your Pitt email for updates before each class.

If you are required to isolate or quarantine, become sick, or are unable to come to class, contact me as soon as possible to discuss arrangements.

Classroom Recording

Students may not record classroom lectures, discussions, and/or activities without my written permission. Any recordings I approve must only be used by the authorized student, for their own private use.

Disability Resources

If you have a disability for which you are or may be requesting an accommodation, you are encouraged to contact both your instructor and the Office of Disability Resources and Services, 140 William Pitt Union, 412-648-7890/412-624-3346 (Fax), as early as possible in the term. Disability Resources and Services will verify your disability and determine reasonable accommodations for this course. For more information, visit www.studentaffairs.pitt.edu/drsabout.

Office Hours Statement

It is the responsibility of the faculty member as a courtesy and convenience to students to hold office hours (source: www.pitt.edu/~provost/ch3_off_hrs.htm). Most administrative offices are open from 8:30 a.m. to 5:00 p.m., Monday through Friday. A few offices, such as the College of General Studies, have extended hours. In addition, according to the **Academic Integrity Guidelines**, under *I. Faculty Obligations, Point 2*, faculty are "To be available at reasonable times for appointments with students, and to keep such appointments" (source: www.as.pitt.edu/faculty/policy/integrity.html).