BSC 4933/6932, Fall 2017: Computational Biology

Instructor Sameer Varma

Office: ISA 6205
Phone: 974-9288
Email: svarma@usf.edu
Office hours: 5:00-6:00 PM, Tuesday/Thursday in ISA 6205 or by appointment

Lectures/Lab 3:30 - 4:45 PM, Tuesday & Thursday in Room ISA 4010

Website Canvas

Description

This course provides a general overview of the data-analytical and theoretical methods, mathematical modeling and computational simulation techniques available to study biological systems. Course content is tailored for biology majors, who have successfully taken Physics II and Calculus II, and also serves as a bridge to enroll in more advanced courses offered by the physics and chemistry departments. The course focusses on and provides a more in-depth understanding of (1) systems biology, which deals with the mathematically modeling of cellular processes, like signaling pathways and gene regulation; and (2) biomolecular simulations, which deals with predicting the structure, dynamics and activities of biomolecules. The course also provides hands-on experiences in mathematical modeling and conducting and analyzing biomolecular simulations.

Objectives

1. Introduce biology majors, undergraduates as well as graduate students, to the various computer simulation approaches used in biological research.
2. Provide a fundamental understanding of how molecular simulation techniques are used for predicting the structure, dynamics and activities of biomolecules.
3. Provide in-depth understanding of how predictive mathematical models are constructed for describing complex signaling pathways and gene regulatory networks.
4. Provide hands-on experience in simulation/modeling software like MATLAB and GROMACS.

Outcomes and expectations

1. Develop a broad understanding of the various computer simulation approaches used in biological research.
2. Understand and learn to use molecular simulation techniques for predicting the structure, dynamics and activities of biomolecules.
3. Learn to mathematically model cellular processes, like signaling and gene regulation, and obtain optimum solutions to coupled ODE based models.

Syllabus

Date	Topic	Notes
Aug 22	Course Overview, **Visualization of 3D structures**	
Aug 24	*No Class* — Assignment: Unix tutorials 1-5 at http://www.ee.surrey.ac.uk/Teaching/Unix/	Assignment
Protein structure prediction		
Aug 29	Homology modeling	
Aug 31	Threading and *ab initio* approaches	
Molecular simulations		
Sep 5	Equations of motion	
Sep 7	Algorithms for integrating equations of motion	
Sep 12	Potential energy functions and force fields	HW 1 due
Sep 14	Thermodynamics and statistical mechanics	
Sep 19	Exam 1: Aug 22- Sep 12	
Sep 21	Thermodynamics and statistical mechanics	
Sep 26	Algorithms for boundary conditions	
Sep 28	Lab: Introduction to Gromacs software	
Oct 3	Lab: Molecular dynamics simulations	
Oct 5	Lab: Basic analysis of molecular dynamics simulations	
Kinetic modeling		
Oct 10	Reaction kinetics/energetics, unimolecular/bimolecular reactions	
Oct 12	Opposing/concurrent/consecutive reactions	HW 2 due
Oct 17	Steady state approximation and enzyme kinetics	
Oct 19	Exam 2: Sep 14 - Oct 12	
Oct 24	Oscillating reactions	

Date	Topic	Notes
Oct 26	Modeling biological pathways	
Oct 31	Stochastic modeling and the chemical master equation	
Nov 2	Gene network models	
Nov 7	Lab: Solve ODEs using Matlab	HW 3 due
Nov 14	Lab: Solve ODEs using Matlab	
Nov 16	Lab: Modeling biological pathways	Lab project due
Nov 21	Reading day	
Nov 23	Thanksgiving	
Nov 28	Review of lab project	
Nov 30	Exam 3: Oct 17 - Nov 16	

Note: This is a tentative syllabus. You will be notified of any changes to this schedule.

Reference textbooks

1. Systems Biology - by Klipp, Liebermeister, Wierling & Kowald, Wiley, 1st Edition, 2009
2. Principles of Physical Chemistry - by Lionel Raff, Prentice Hall, 1st edition, 2011.
3. Understanding Molecular Simulations: From Algorithms to Applications - by Frenkel & Smit, Academic Press, 1st edition, 2001
4. Statistical Mechanics, Theory and Molecular Simulation - by Tuckerman, Oxford University Press, 1st Edition, 2010.
5. Molecular Modeling for Beginners, Alan Hinchliffe, Wiley and sons, 2003 (https://www.coulomb.univ-montp2.fr/perso/lucyna.firlej/MasterPro/MMFB.pdf)

Grading

Exam 1	23
Exam 2	23
Exam 3	23
Homework	15
Lab project	16
Total:	100

NOTE: ***There is no exam drop policy.***

The following scheme will be used to assign letter grades:

A+	>= 95	A	>= 90
B+	>= 85	B	>= 80
C+	>= 75	C	>= 70
D+	>= 65	D	>= 60
F	< 60		

Finals: There is no exam in the finals week.

Make-up exam policy: The only acceptable reasons for requesting to make-up assignments or exams are (1) medical (individual or immediate family only), legal (accident or court case; individual only), or funerary (immediate family only). Make ups will only be given at the consent of the instructor and require written documentation concerning the nature of the absence including a signed note from an involved professional. Documentation must be submitted to the instructor within two days from the scheduled exam or assignment for consideration of a make-up. The format and time of the make-up is at the discretion of the instructor.

Incomplete Grade Policy: USF policy states that incomplete grades (I) cannot be assigned unless a student is passing the course at the time of the incomplete and has completed the majority of the work in the course (e.g., A student who passes one exam but is absent for half the semester is not eligible). If an incomplete grade is assigned, it is the responsibility of the instructor to complete the Incomplete Grade Contract (CMMB Office), describing the work to be completed by the student and the time frame of its completion. After satisfactory completion of the work, the instructor must fill out a Change of Grade form (CMMB Office). If the work requirements of the contract are not satisfactorily completed within one semester, the "I" grade will be changed on the student's transcript to an "F" grade.

Academic Conduct

Collegial conduct toward the instructor and classmates is expected at all times. Disruption of academic process' is defined by the University as an act or words of a student in a classroom or teaching environment which, in the reasonable estimation of a faculty member, (a) directs attention from the academic matter at hand (e.g., noisy distractions; persistent, disrespectful or abusive disruptions of lecture, exam, or academic discussions) or (b) presents danger to the health, safety, or well being of the faculty member or students. Breach of these guidelines can result in dismissal from the classroom and an F grade.

Cellular phones: Making or receiving calls, text messaging, and taking photos with a cell phone during lectures are extremely distracting and prohibited in this class. As a courtesy to your fellow students and instructor, please keep cell phones and pagers switched completely off for the duration of this class.

Attendance: Attendance is highly recommended. In case of absence, it is the students' responsibility to consult with other students in the class concerning what was missed.

Religious observance: Students who anticipate the necessity of missing a scheduled exam(s) due to the observation of a major religious holiday must provide notice of the date(s) to me, in writing, by the second class meeting.

Recording lectures: You may make audio recordings of lectures for personal use. The sale of written or recorded lectures is forbidden.

Academic dishonesty: If you are found cheating on any exam, you may receive an "FF" grade for the entire course. This grade represents "failure due to cheating" and becomes a permanent part of your transcript.

Sexual Misconduct/Sexual Harassment Reporting: USF is committed to providing an environment free from sex discrimination, including sexual harassment and sexual violence (USF System Policy 0−004). The USF Center for Victim Advocacy and Violence Prevention is a confidential resource where you can talk about incidents of sexual harassment and gender−based crimes including sexual assault, stalking, and domestic/relationship violence. This confidential resource can help you without having to report your situation to either the Office of Student Rights and Responsibilities (OSSR) or the Office of Diversity, Inclusion, and Equal Opportunity (DIEO), unless you request that they make a report. Please be aware that in compliance with Title IX and under the USF System Policy, educators must report incidents of sexual harassment and gender−based crimes including sexual assault, stalking, and domestic/relationship violence. If you disclose any of these situations in class, in papers, or to instructors personally, we are required to report it to OSSR or DIEO for investigation. Contact the USF Center for Victim Advocacy and Violence Prevention: (813) 974−5757.

Disability

Students in need of academic accommodations for a disability may consult with the office of Services for Students with Disabilities to arrange appropriate accommodations. Students are required to give reasonable notice (typically 5 working days) prior to requesting an accommodation.