BIOSC1630 Computational Biology Seminar

Course Syllabus
Fall 2020 (Term 2211)
Wednesdays / 1:15 - 3:45 pm

Instructor: Dr. Burak Kaynak

Room: WEB Based Class

Office hours: TBD

Course Content/Description: This course focuses on reading and analyzing primary research literature in the field of computational biology with an emphasis on effective techniques for communicating about the associated science both in writing and orally. You are provided a set of journal articles focusing on current topics in computational structural biology. We will discuss the articles in the following way: On most weeks 2-3 students will be in charge of presenting the background and first figures, then we will discuss and prepare slides for the remaining parts either in groups or together in class. You are expected to read each article carefully before class and participate fully in the discussions.

This is also a writing-intensive course that fulfills the requirement for a writing course in your major. You will have some shorter writing assignments, and then you will write and revise a literature review paper centering on a computational structural biology research article. Formats will be announced. You will put it into context by using at least two more primary literature articles. You will be expected to include in your paper significant background about the biological question being investigated, the current state of knowledge about the topic, a discussion of critical *computational* techniques and findings leading to our understanding, and your suggestions for future work.

- You will choose one substantial primary literature article that interests you. You will cover this paper in detail.
  - You are encouraged to choose your article within the scope of the topics discussed in class. However, you may choose it from a different area of computational biology as long as it encompasses recent computational techniques in that area.
  - The article must either be current (within the last year or two) or seminal.
  - Your article must be approved by the instructor.
- You will choose at least two more primary literature articles that help explain your focus article.
  - One article must have been published before your focus article.
  - The other article may have been published at any time.
  - You will cover in detail at least one computational method and finding in each of these articles.
- You may use additional primary literature articles in brief and review articles to help with your introduction and conclusions.

Finally, you will prepare and revise a talk on your focus primary literature article.

Requisites: PREQ: BIOSC 1540 Computational Biology (minimum grade of 'C') and ENGCOMP 0200; LSEVEL: Junior or Senior

Course schedule:

Date	Class	What is Due?
Class 1 Aug. 19	• Introduction to the course • Identifying, reading, and analyzing primary literature • Preparing slides (slides with bullets, assertion-evidence slides)	• Familiarize with research topics in computational structural biology
Class 2 Aug. 26	• Review article (class discusses and prepares slides) • Giving effective oral presentations	• Read article 1
Class 3 Sept. 2	• Journal article 2 (Group A presents first figures followed by class producing the remaining slides) • Paragraph structure (Issue and Point)	• Read article 2 • Group A prepares presentation • Write a paragraph for the article that will be announced
Class 4 Sept. 9	• Journal article 3 (Group B presents first figures followed by class producing the remaining slides) • Peer review of paragraphs looking for Issue and Point	• Read article 3 • Group B prepares presentation • Write a paragraph for article 2
Class 5 Sept. 16	• Journal article 4 (Group C presents first figures followed by class producing the remaining slides) • Peer review of paragraphs looking for Issue and Point	• Read article 4 • Group C prepares presentation • Write a paragraph for article 3
Class 6 Sept. 23	• Journal article 5 (Group D presents first figures followed by class producing the remaining slides) • Avoiding plagiarism	• Read article 5 • Group D prepares presentation • Write topic proposal with reference list
Class 7 Sept. 30	• Journal article 6 (Group E presents first figures followed by class producing the remaining slides)	• Read article 6 • Group E prepares presentation • Write a paragraph for article 5
Class 8 Oct. 7	• Journal article 7 (Group F presents first figures followed by class producing the remaining slides)	• Read article 7
Oct. 8 **Thursday**		• Write first draft (partial) and upload it by 5 pm
Oct. 14	NO CLASS	

Class 9 Oct. 21	• Practice talks in groups • More on giving effective presentations	• Prepare 10 min talk on your paper
Class 10 Oct. 28	• Practice talks in groups • More on the structure of a review paper	• Prepare 10 min talk on your paper
Oct. 29 **Thursday**		• Write second draft (full) and upload it by 5 pm
Class 11 Nov. 4	• Final talks	• Revise talk • Peer review two papers
Class 12 Nov. 11	• Final talks	• Revise talk
Class 13 Nov. 18	• Final talks	• Revise talk
Thanksgiving Break		
Nov. 30 **Monday**		• Revise paper to produce final version and upload it by 11:59 pm

Grading: Your final grade will be determined on the basis of your total points earned for the semester. A total of 250 points are possible using the following criteria:

Group Presentation *(each presenter graded separately)*	15 points
Method Paragraphs	20 points
Proposal/ref list	12 points
First draft	15 points
Second draft	35 points
Peer review	14 points
Final Talk	40 points
Final paper	60 points
Participation *(3 points/class)*	39 points
Total	250 points

At a minimum 90% and above will be an A- or better, 80% and above will be a B- or better, and 70% and above will be a C or better. Late assignments will be docked 10% per day unless excused for a documented reason that is outside of your control.

Missed class: If you miss a class for reasons out of your control, relevant documentation must be provided. You will be required to turn in a written summary of the journal article for that week. If you miss giving any of your presentations, you will need to be rescheduled. If you miss any day of final talks, you will be required to read one of the papers and write a summary within one week of missing class.

Academic Integrity Policy: Cheating/plagiarism will not be tolerated. Students suspected of violating the University of Pittsburgh Policy on Academic Integrity (http://www.as.pitt.edu/faculty/policy/integrity.html) will be required to participate in the outlined procedural process as initiated by the instructor.

Violation of the Academic Integrity Code requires the instructor to submit an Academic Integrity Violation Report to the Dean's Office.

Any attempt to submit work that is not the student's own work is a violation of academic integrity. If I find that a writing assignment contains evidence of plagiarism, the level of severity will determine whether the sanction is an F in the course, a 0 score on the assignment, or partial credit on the assignment. **A second academic integrity offense in the course will result in an automatic grade of F.**

Turnitin: Students agree that by taking this course all required assignments may be subject to submission for textual similarity review to Turnitin.com for the detection of plagiarism. All submitted papers will be included as source documents in the Turnitin.com reference database solely for the purpose of detecting plagiarism of such papers. Use of Turnitin.com page service is subject to the Usage Policy and Privacy Pledge posted on the Turnitin.com site.

E-mail: Although e-mail will not be used routinely in this class for communication, occasionally I may send out an e-mail notice using the University e-mail addresses available through Canvas. Such notices are also posted as Announcements on Canvas.

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. 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.

Disability Resources: If you have a disability for which you are, or may be, requesting an accommodation, you are encouraged to contact both the instructor for this course and the Office of Disability Resources and Services, 140 William Pitt Union, 412-648-7890 (phone)/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.

Syllabus Supplement outlining this course as offered during a *Flex@Pitt* semester:

- This course is labeled as a WEB Based Class in PeopleSoft, therefore it will be 100% online regardless of University operating posture. Grades will be assigned as outlined in the grading section of the syllabus.
- This course will use Canvas, Zoom and Panopto.
- Course materials will be available on Canvas, regardless of the University operating posture.
- This course will be conducted synchronously via Zoom and recorded for asynchronous viewing.
- Office hours will be determined in the first class and take place through Zoom, regardless of the University operating posture.
- The zoom links for both classes and office hours will be accessed through Canvas.
- Any course adjustments will be announced on Canvas as needed.
- General discussions and Q&A's should be held through Discussion Board through Canvas. For other personal matters, the best way to contact me, regardless of the University operating posture, is at *buk5@pitt.edu*.

Article List:

#	Date	Article
1	Aug. 26	Nussinov R., Tsai C. J., Allostery in Disease and in Drug Discovery, *Cell* 153 (2) (2013) 293. http://dx.doi.org/10.1016/j.cell.2013.03.034
2	Sept. 2	Kaynak B. T., Bahar I., Doruker P., Essential site scanning analysis: A new approach for detecting sites that modulate the dispersion of protein global motions, *Comput. Struct. Biotec.* 18 (2020) 1577. https://doi.org/10.1016/j.csbj.2020.06.020
3	Sept. 9	Hollingsworth S.A., Kell, B., Valant C. *et al.* Cryptic pocket formation underlies allosteric modulator selectivity at muscarinic GPCRs. *Nat Commun* 10 (2019) 3289. https://doi.org/10.1038/s41467-019-11062-7
4	Sept. 16	Ponzoni L., Peñaherrera D. A, Oltvai Z. N., Bahar I., Rhapsody: predicting the pathogenicity of human missense variants, *Bioinformatics* 36 (10) (2020), Pages 3084–3092, https://doi.org/10.1093/bioinformatics/btaa127
5	Sept. 23	Kurkcuoglu Z., Bonvin A.M.J.J. Pre- and post-docking sampling of conformational changes using ClustENM and HADDOCK for protein-protein and protein-DNA systems. *Proteins* 88 (2020) 292. https://doi.org/10.1002/prot.25802
6	Sept. 30	Adhikari U, Mostofian B., Copperman J. et al., Computational Estimation of Microsecond to Second Atomistic Folding Times, *J. Am. Chem. Soc.* 141 (16) (2019) 6519. https://doi.org/10.1021/jacs.8b10735
7	Oct. 7	Singharoy A., Maffeo C., Delgado-Magnero K. H. *et al.* Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism, *Cell* 179 (5) (2019) 1098. https://doi.org/10.1016/j.cell.2019.10.021