HON 343: Introduction to Interdisciplinary Computational Science

Credits: 3

Restrictions: None

Course Description:

Computational science is an emerging interdisciplinary field of all the sciences, combined with computer science, and mathematics. This course is to provide the fundamentals of computational as applies to experimental sciences, and introduce a variety of scientific applications. We will examine how scientific investigations involve experiment as well as computing in basic sciences such as physics, chemistry, global change, medicine and particularly biosciences. The student will be offered examples of experimental data, computer simulations, and data analysis.

Course Objectives/Outcomes:

By the end of the semester the students should

1. Understand the definitions and know the basics of computational science.
2. Know the components of computational models in basic sciences such as biology, chemistry, physics, and Earth sciences.
3. Know the principles of experiment, modeling, and simulations in bioscience.
4. Know how to build simple computer models in basic sciences as well as in applied sciences.
5. Understand discrepancies between publications in Science and non-Science.
6. Recognize that computational science plays a major role in science and engineering.
7. Understand computational science as an important tool for scientific investigations.
8. Know the basics of what is involved to analyze scientific data and simulations.
9. Understand the scientific meaning of simulations.
10. Know how to interpret scientific and simulated data.
11. Know how to build simple computer models using experimental data.
12. Understand how to bridge computational science to basic science.

Major Topics Covered:

1. Definition and introduction to computational science
2. Introduction to modeling, simulations, and computational studies
3. How to understand and write papers in computational science
4. Basics of Applications in computational science
5. Data science tools such as data fusion, data interpolation, etc.
6. Data analysis
7. Study cases in computational science
8. Example of computational models
9. Computational Science tools; neuronal simulators
10. Interpretation of scientific and simulated data

Texts and Recommended Readings

1. Lecture notes (Main source of course information, will be posted on blackboard)
2. Introduction to Computational Science; Modeling and Simulation for the Sciences, A Shiflet and G Shiflet
3. **Introduction to Computational Molecular Biology,** Carlos Setubal, Joao Meidanis, **Edition: 2nd Edition, Copyright: PWS Publishing**
4. Computational Cell Biology, Christopher Fall (Editor), Eric Marland (Editor), John Wagner (Editor), John Tyson (Editor), Copyright: Kindle Books
5. **Principles of Computational Cell Biology: From Protein Complexes to Cellular Networks,** Volkhard Helms, Copyright: Wiley-VCH
6. The Book of GENESIS, J. M. Bower and D. Beeman, Exploring Realistic Neural Models with the GEneralNEuralSImulation System, Second edition, Springer-Verlag, New York (1998). (ISBN 0-387-94938-0)
   Book of GENESIS, Exploring Realistic Neural Models with the General Neural Simulation System
   http://www.genesis-sim.org/GENESIS/bog/bog.html
   http://authors.library.caltech.edu/36220/1/bower_2003.pdf
7. Book of XPP
   http://www.math.pitt.edu/~bard/xpp/xpp.html
   http://www.math.pitt.edu/~bard/bardware/xpp_doc.pdf
8. **Yang Keun-Hang**, Franaszczuk Piotr J., and Bergey Gregory K. (2003) The Influences of Somatic and Dendritic Inhibition on the Patterns of Bursting in a Neuronal Circuit Model. ***Biological Cybernetics***, 89:242-253.
9. **Yang Keun-Hang**, Franaszczuk Piotr J., and Bergey Gregory K. (2005) Inhibition Modifies the Effects of Slow Calcium-Activated Potassium Channels on Epileptiform Activity in a Neuronal Network Model. Epub 2004 Dec 21. ***Biological Cybernetics,*** 92:71-81.
10. **Yang Keun-Hang**, Blackwell K.T. (2000) Analog Pattern Matching in a Dendritic Spine Model Based on Phosphorylation of Potassium Channels. ***Network***: Computation in Neural System, 11:281-297.
11. **Yang Keun-Hang**, Franaszczuk Piotr J., and Bergey Gregory K. (2002) The influence of Synaptic Connectivity on the Pattern of Bursting Behavior in Model Pyramidal Cells. ***Neurocomputing***, 44-46:233-242.
12. **Yang Keun-Hang**, Jeanette Hellgren Kotaleski, and Blackwell K.T. (2001) The Role of Protein Kinase C in the Biochemical Pathways in Classical Conditioning. ***Neurocomputing***, 38-40:79-85.
13. **Susan Yang's homepage**
    http://computationalbiology.chapman.edu/refereed-papers.html

Key Bibliography:

- Computational Cell Biology**,** by Volkhard Helms, John Wiley & Sons publishing, 2008
- Fundamental Concepts of Bioinformatics, by Dan E. Krane; Michael L. Raymer, Benjamin-Cummings Pub Co, 2002.

Natural Science Inquiry Learning Outcome:

Uses scientific principles and reasoning as a way of knowing the natural world, distinguishing science from non-science.

Chapman University's Students with Disabilities Policy:

In compliance with ADA guidelines, students who have any condition, either permanent or temporary, that might affect their ability to perform in this class are encouraged to inform the instructor at the beginning of the term. The University, through the Disability Services Office, will work with the appropriate faculty member who is asked to provide the accommodations for a student in determining what accommodations are suitable based on the documentation and the individual student needs. The granting of any accommodation will not be retroactive and cannot jeopardize the academic standards or integrity of the course.

Chapman Academic Integrity Policy:

"Chapman is a community of scholars that emphasizes the mutual responsibility of all members to seek knowledge honestly and in good faith. Students are responsible for doing their own work, and academic dishonesty of any kind will be subject to sanction by the instructor and referral to the university's Academic Integrity Committee, which may impose additional sanctions up to and including dismissal. (See the Undergraduate Catalog for the full policy.)" Cheating on exams or plagiarism will not be accepted in any way and will result in zero points for this exam/quiz/homework.

Equity and Diversity

Chapman University is committed to ensuring equality and valuing diversity. Students and professors are reminded to show respect at all times as outlined in Chapman's Harassment and Discrimination Policy: http://tinyurl.com/CUHarassment-Discrimination. Any violations of this policy should be discussed with the professor, the Dean of Students and/or otherwise reported in accordance with this policy.

Students Assessment (100 Points Total)

Attendance and Class Participation	Total: 10 Points (You can miss one class)
2 Exams (12.5 points each)	Total: 25 Points
Homework, Reading Papers, and Reports (5 points each)	Total: 30 Points
Group Project	Total: 10 Points
Final Exam	Total: 30 Points

Attendance Policy:

Students may miss at most one class. Homework and reading assignmentsare officially due one week from the day assigned (Tue/Thu 2:30 PM). Students are required to arrange to turn in all assignments on time whether they attend class or not, except for unforeseen, excused absences. Students are allowed to use their class notes.

Reports and Homework:

Students will be asked to turn in reports during the whole semester for specific lectures (more research oriented) and for guest lectures. Reports should be turned according to the posted dates.

Reports and Homework should be turned electronically. The subject of your email and the file name should reflect what you are submitting. For instance, if Susan Yang is attending HON245 and she is turning in one of her reports or homeworkshe should do the following:

Example: Homework 1
Email Subject would read: HON-Homework1
File name: Susan_Yang_Homework1.doc

Make-up/Late Policy:

Make-ups of exams or labs may only be scheduled with prior consent of the instructor but are generally not permitted. All make-ups must be completed before the next exam. Any homework not completed on time is subject to the following penalties: ≤1 day late = 15% off final score; >1 day-1 week late = 30% off final score, >1 week late = not accepted.

Grading:

Final Grade	Points (from To)
A	95 – 100
A-	90 – 94
B+	85 – 89
B	80 – 84
B-	70 – 79
C+	65 – 69
C	55 – 64
C-	50 – 54
D+	45 – 49
D	40 – 44
D-	30 – 39
F	<30

Incomplete Grade Policy:

The grade of Incomplete may be assigned by an instructor if a student, through circumstances beyond his or her control, has not completed a small portion of a course by the conclusion of the term. The student must request in writing the grade of Incomplete and must propose a date acceptable to the faculty member by which the missing work will be completed. A grade of Incomplete may not be assigned in order to give a student a chance to do more work to improve a grade.