CAP5515: COMPUTATIONAL MOLECULAR BIOLOGY

SYLLABUS

- **Semester:** Spring 2010
- **Schedule:** Tue 9:35-10:25, Thu 9:35-11:30
- **Location:** CSE 107
- **Professor:** Alper Üngör
  E534 CSE Building
  ungor@cise.ufl.edu
  `http://www.cise.ufl.edu/~ungor`
- **Office hours:** Tue 13:00-15:00
- **Web-page:** `http://www.cise.ufl.edu/class/cap5515sp10`
- **Prerequisites:** COP 3530 or equivalent, or Instructor's permission

Computational Biology and Bioinformatics are rooted in life sciences as well as computer and information sciences and technologies. Both of these interdisciplinary approaches draw from specific disciplines such as mathematics, physics, computer science and engineering, biology, and behavioral science. Bioinformatics applies principles of information sciences and technologies to make the vast, diverse, and complex life sciences data more understandable and useful. Computational biology uses mathematical and computational approaches to address theoretical and experimental questions in biology. Although bioinformatics and computational biology are distinct, there is also significant overlap and activity at their interface.

Bioinformatics: Research, development, or application of computational tools and approaches for expanding the use of biological, medical, behavioral or health data, including those to acquire, store, organize, archive, analyze, or visualize such data.

Computational Biology: The development and application of data-analytical and theoretical methods, mathematical modeling and computational simulation techniques to the study of biological, behavioral, and social systems.

This course will survey the fundamental concepts in computational molecular biology, including

Protein Modeling	*Alpha Shapes*	*Molecular & Skin Surfaces*
Protein Docking	*Scoring Functions*	*Interfaces & Interactions*
Protein Folding	*Structure Predition*	*Motion planning*
Protein Data Bank	*Drug Design*	*Molecular Visualization*
Structure Determination	*X-ray Crystallography*	*NMR Spectroscopy*

Coursework

Grades will be based on paper presentations (25%), commentaries (15%), an exam (25%), a semester project (25%), and a book review (10%).

- **Paper Presentations:** There will be paper (selected from top journals and recent conferences) presentations by the students. Each student is expected to give at least two such presentations through out the semester. The presenters will also write a review (minimum two page) on each paper.

- **Commentaries:** Students are expected to give feedback on each other's presentations. Each student will write a short commentary (roughly one page) on each presentation. I will grade these commentaries and also use them as feedback to grade the presentations.

- **Project:** Each student is expected to complete a small scale research project which could be a survey, a software implementation, or formulating and solving a theoretical problem. A one-page project proposal should be submitted by the sixth week of the semester. Final project reports are due by the last week of the semester. Projects will be presented on the last two weeks of the semester.

- **Book Review:** James Watson's well-known book, The Double Helix, is a required reading for the class and each student is expected to write a short critique of it. This report is due on the week after the Spring Break.

- **Attendance:** Class participation is strongly encouraged as it contributes to part of your grade (through commentaries).

- **Exam:** There will be an in-class comprehensive exam tentatively scheduled on Apr 8.

Course Material

- **Recommended Textbooks:**

  1. *The Double Helix: A Personal Account of the Discovery of the Structure of DNA*, James D. Watson, 1968.

  2. *Molecular Modeling: Basic Principles and Applications*, 2nd Ed., Hans-Dieter Höltje, Wolfgang Sippl, Didier Rognan, Gerd Folkers, September 2003

  3. *Structural Bioinformatics*, Philip Bourne, Helge Weissig, 2002. Wiley-Liss.

  4. *Introduction to Protein Structure*, Carl Branden, John Tooze, Garland Publishing, 2nd Ed., January 1999.

  5. *Molecular Modelling: Principles and Applications*, 2nd edition, Andrew R. Leach, Published by Pearson Education EMA, January 2001.

  6. *Introduction to Algorithms (2nd ed).*, T.H. Cormen, C.E. Leiserson, R.L. Rivest, and C. Stein, (MIT Press and McGraw-Hill, 2001).

- **Conferences:** RECOMB, WABI, PSB, CSB, ISMB/ECCB, ...

- **Journals:**

  1. *Journal of Computational Biology*

  2. *Bioinformatics*

  3. *Proteins: Structure, Function, and Bioinformatics*

- Also watch the class web page for other survey and research papers, links, etc.

Other Issues

- **Announcements:** Students are responsible following the announcements on the course web-page (`http://www.cise.ufl.edu/class/cap5515sp10`). Schedule updates regarding the homeworks, exams and office hours will appear on the web-page.

- **Accommodations for Students with Disabilities:** Students requesting classroom accommodation must first register with the Dean of Students Office. The Dean of Students Office will provide documentation to the student who must then provide this documentation to the Instructor when requesting accommodation.

- **The University's Honesty Policy:** All students admitted to the University of Florida have signed a statement of academic honesty committing themselves to be honest in all academic work and understanding that failure to comply with this commitment will result in disciplinary action. This statement is a reminder to uphold your obligation as a student at the University of Florida and to be honest in all work submitted and exams taken in this class and all others.
  The following links contain additional information relating to academic honesty:
  - `http://lss.at.ufl.edu/services/turnitin/resources.html`
  - `http://www.dso.ufl.edu/judicial`