BCB 569 Fall 2011 Syllabus

Bioinformatics III: Structural Genome Informatics

(Also cross listed in BBMB/ComS/CprE/Math)

Course meeting hours and location:

2:10pm – 3:30pm, TR,
Location: MBB 1424

Course Instructors:

Robert L. Jernigan
Office: 112 Office & Lab
Office hours: by appointment
Contact: jernigan@iastate.edu, 294-3833

Guang Song
Office: 107 Atanasoff Hall
Office hours: by appointment
Contact: gsong@iastate.edu, 294-1696

Course website: (WebCT)

http://www.celt.iastate.edu/webct/

Reference Texts:

1. Protein Structure and function, Petsko, 2004
2. Computational methods for protein structure prediction and modeling (volume 1 and 2), Xu, Xu, and Liang, 2007
3. Lecture Notes on Computational Structural Biology, Zhijun Wu, 2008
4. Molecular Modeling and Simulation, Tamar Schlick, 2002
5. Structural Bioinformatics, 2nd Edition, Jenny Gu and Philip Bourne, 2009
6. Protein Structure Prediction: a practical approach, M. Sternberg, 1996
7. Textbook of Structural Biology, Liljas et al, 2010
8. Molecular Biophysics, Michael Daune, 1999

Recommended articles: (will be distributed throughout the course)

Learning Outcome:

- Establishing an essential foundation of structural informatics
- Being familiar with the frontier of current research
- Gaining research experience in

- literature survey and study on a selected topic
- hand-on experience of computational techniques
- designing new or improving existing computational methods

Course Requirements and Grading:

1. (10%) Quizzes and/or literature reviews.

2. (40%) About 3-5 homework assignments
   Tentative topics:
   protein structure and geometry, PDB file, visualization, structure calculation, molecular dynamics
   Homework policy:
   1. Late homework: one day late: 25% deduction; not accepted beyond one day
   2. Homework re-grade requests must be submitted in the written form within one week after a grade is received.

3. (50%) Final project and presentation
   What is expected: summarize and review one research area, propose a new approach, implement the proposed approach, write a final report and give a presentation.

   Project mentoring: Once the topics have been decided (proposal due Oct. 19), students will choose one of the instructors as their project advisor and start to meet with him in small groups regularly to talk about project progress and receive feedback.

   Possible project areas/topics:
   protein structure alignment
   protein geometry
   identification of domains
   modeling
   secondary structure prediction
   tertiary structure prediction
   protein-protein interaction
   molecular dynamics
   statistical potential
   etc., etc.
   Students may choose a different area than listed here. Please talk to one of the instructors. Students should not use their current/past research as the project topic, but are welcome to work on a topic related to their research.

   Key project dates:
   Project proposal (1 page) due: Oct 18
   Project proposal presentation: Oct 20, 25

Project presentation: Dec 6, 8, 15
Project report (4-6 pages) due: Dec 15

Project proposal should include: a definition of the problem, why the problem is significant, the current state (what is known about the problem), description of the proposed approach, justification of the proposed approach, how the results are to be evaluated, expected finding of proposal work, significance of the results to be obtained (where they can be used).

Project presentation and report should address each of the above issues in more details, and in addition, present results and discussions.

4. Grading scale:
The tentative grading scale is as follows: 93% = A, 90% = A-, 87% = B+, 83% = B, 80% = B-, 77% = C+, 73% = C, 70% = C-, 67% = D+, 63% = D, 60% = D-. The instructors may adjust this grading scale downward at the end of the semester, but that will not be determined until the overall course grades are calculated at the end of the semester.

List of topics:

0. Introduction to course (go over the syllabus; may start on protein structure)

I. Basics (~2.5 weeks)
- A. Protein Structure basics (Book 1, Chapter 1)
- B. PDB format
- C. Visualization and Graphics
- D. Empirical Force fields
- E. Knowledge-based Energy functions
- F. Nucleic Acid Structures

II. Structure Determination and Refinement (~2 weeks)
- A. X-ray Crystallography
- B. NMR (Nuclear Magnetic Resonance)

III. Structure Analysis (~2 weeks)
- A. Protein structure comparison
- B. Classification of Protein Folds
- C. Identification of domains
- D. Protein geometry (internal coordinates, solvent-accessible surface etc.)

IV. Structure Prediction (~2.5 weeks)
- A. Sequence Analysis
- B. Local Structure Prediction
- C. Homology Modeling
- D. Threading

E. Ab initio Protein Structure Prediction

V. Modeling and Simulations of Dynamics (~2 weeks)
A. Molecular Dynamics
B. Coarse-grained models

VI. Mechanisms, Localization and Interactions (~1 weeks)
A. Mechanisms and Regulation
B. Protein Localization
C. Protein-Protein Interactions

Lab sessions

There will be a few lab sessions in this course during which you will have hand-on experience on learning and using some important software and tools. Make sure to **bring your laptop** with you when you come to class during the lab sessions.

Class No	Date	Lecturer – Subject
1	8/23	GS – Introduction to the course
2	8/25	GS – Structure Basics (amino acids, protein flexibility)
3	8/30	GS – Structure Basics (secondary, tertiary structure, PDB)
4	9/1	GS – Structure Basics (internal and Cartesian Coordinates)
5	9/6	Zimmermann – Lab 1 (Graphics: visualization using PyMol, VMD)
6	9/8	GS – Structure Basics (empirical potentials)
7	9/13	GS – Structure Basics (statistical potentials)
8	9/15	GS – Geometric Calculations (I)
9	9/20	Hargrove – X-ray Experiments
10	9/22	Andreotti – NMR Experiments
11	9/27	Wu – X-ray Computations (3:40-5pm)
12	9/29	Wu - NMR Computations (3:40-5pm)
13	10/4	RJ – Structure Matching
14	10/6	GS - Geometry Calculations II (Voronoi graphs, Delaunay triangulation, alpha shapes.)
15	10/11	RJ - Folds & Domains
16	10/13	RJ – Sequence Analysis
17	10/18	RJ – Secondary Structures and Sequence-Structure relationship
18	10/20	RJ + GS – Proposal presentation (10-15min each)
19	10/25	RJ + GS – Proposal presentation (10-15min each)
20	10/27	Zimmermann – Lab 2 (homology modeling)
21	11/1	RJ – Ab initio Predictions
22	11/3	Katebi + Yennamalli (Raghu) – Lab 3 (docking)
23	11/8	Dobbs – Protein-Protein interactions
24	11/10	RJ – Nucleic Acids, Lipids, Regulations, and Images
25	11/15	RJ – Coarse-grained models (I)
26	11/17	RJ – Coarse-grained models (II)
27	11/29	GS – Molecular Dynamics
28	12/1	GS – Lab 4: Molecular Dynamics
29	12/6	RJ + GS - Student projects (3 presentations + course evaluations)
30	12/8	RJ + GS - Student project presentation
	(Final exam slot – 12/15?)	RJ + GS - Student project presentation

RJ: Robert Jernigan
GS: Guang Song

Academic Honesty

Each assignment is to be the product of your own intellectual efforts. Anyone caught cheating will receive an automatic F in the course.

Disability

If you have a documented disability and anticipate needing accommodations in this course, please meet with your instructor during the first week of class. Request that the Disabilities Resources staff send a SAAR form verifying your disability and specifying the accommodations you will need.