

BCB 569 Fall 2009 Syllabus

Bioinformatics III: Structural Genome Informatics

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

Course meeting hours and location:

2:10pm – 3:30pm, TR, MBB 1424

Course Instructors:

Robert L. Jernigan

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Office hours: by appointment

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Guang Song

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Course website: (WebCT)

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

Recommended 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. Molecular Modeling and Simulation, Tamar Schlick
4. Lecture Notes on Computational Structural Biology, Zhijun Wu
5. Structural Bioinformatics, Philip Bourne and Helge Weissig
6. Protein Structure Prediction: a practical approach, M. Sternberg, 1996

Recommended articles: (will distribute throughout the course)

Learning Outcome:

- Laying a foundation of the basic topics of structural informatics
- Knowing the frontier of current research in the field
- Gaining research experience in
 - literature survey and study on a selected topic
 - hand-on experience of computational techniques

- designing new or improving existing methods

Course Requirements and Grading:

1. (10%) Reviews of assignment literatures, in-class discussion participation and possibly quizzes.
2. (40%) About 3-4 homework assignments
Tentative topics:
 - a) protein structure and geometry, PDB file, visualization
 - b) structure calculation
 - c) molecular dynamicsHomework 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. 20), 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 (or one of its sub-areas)
protein-protein interaction
molecular dynamics
statistical potential

(Students may choose a different area than listed here. Please talk to one of the instructors)

Key project dates:

Project proposal (1 page) due: Oct 20
Project proposal presentation: Oct 27, 29
Project presentation: Dec 8
Project report (4-6 pages) due: Dec 18

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.

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; survey)

I. Basics (~2.5 weeks)

- A. Protein Structure basics (Book 1, Chapter 1)
- B. PDB format, Visualization (Book 2, chapter 18)
- C. Empirical Force fields (Book 2, chapter 2)
- D. Knowledge-based Energy functions (Book 2, chapter 3)

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 (Book 2, chapter 5)
- B. Classification of Protein Folds (Book 2, chapter 5)
- C. Identification of domains (Book 2, chapter 4)
- D. Protein geometry (internal coordinates, solvent-accessible surface etc.) (Book 2, chapter 6)

IV. Structure Prediction (~2.5 weeks)

- A. Sequence Analysis
- B. Local Structure Prediction (Book 2, chapter 7)
- C. Homology Modeling (Book 2, chapter 10)
- D. Threading (Book 2, chapter 12)
- E. Ab initio protein structure prediction (Book 2, chapter 13)

V. Localization and Interactions (~1 weeks)

- A. Protein localization
- B. Protein-protein interactions (Book 2, chapter 15)

VI. Modeling and Simulations of Dynamics (~2 weeks)

- A. Molecular Dynamics
- B. Coarse-grained models (Elastic network model)

Class No	Date	Lecturer – Subject
1	8/25	GS – Introduction to the course
2	8/27	GS – Structure Basics (amino acids, protein flexibility)
3	9/1	GS – Structure Basics (secondary, tertiary structure)
4	9/3	GS – Structure Basics (PDB and Visualization)
5	9/8	GS – Structure Basics (internal and Cartesian Coordinates)
6	9/10	GS – Structure Basics (empirical potentials)
7	9/15	Hargrove - X-ray Experiments
8	9/17	GS – Structure Basics (statistical potentials)
9	9/22	Wu – X-ray Computations (Class meeting time 2-3pm)
10	9/24	Andreotti – NMR Experiments
11	9/29	Wu - NMR Computations (Class meeting time 2-3pm)
12	10/1	GS - Geometry Calculations (Voronoi graphs, etc.)
13	10/6	RJ – Overview of protein structures and functions
14	10/8	RJ – Structure Matching
15	10/13	RJ - Folds & Domains
16	10/15	RJ – Sequence Analysis
17	10/20	Andrzej Kloczkowski - Secondary Structures
18	10/22	RJ – Ab initio Predictions
19	10/27	RJ + GS – Proposal presentation (10-15min each)
20	10/29	RJ + GS – Proposal presentation (10-15min each)
21	11/3	Zimmermann – Lab 1 (VMD, homology, 2 nd structure)
22	11/5	RJ + Katebi – Lab 2 (docking)
23	11/10	Zhou – Protein localization
24	11/12	Honavar – Protein-Protein interactions
25	11/17	GS - Coarse-grained models
26	11/19	RJ – Coarse-grained models
27	12/1	GS – Molecular Dynamics
28	12/3	RJ – Molecular Dynamics
29	12/8	RJ + GS - Student projects (3 presentations + course evaluations)
30	12/10	RJ + GS - Student project presentation
	Final (12/18)	9:45-11:45am, Student project presentation

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.