BCB 569 Fall 2015 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: TBD (either MBB 1428 or 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: (blackboard)
http://bb.its.iastate.edu/

Reference Texts:
1. Protein Structure and function, Petsko, 2004
2. Introduction to Protein Structure, Branden and Tooze, 1998
3. Computational methods for protein structure prediction and modeling (volume 1 and 2), Xu, Xu, and Liang, 2007
4. Lecture Notes on Computational Structural Biology, Zhijun Wu, 2008
5. Molecular Modeling and Simulation, Tamar Schlick, 2002
8. Textbook of Structural Biology, Liljas et al, 2010
9. Molecular Biophysics, Michael Daune, 1999

Recommended articles: (will be distributed throughout the course)

Learning Outcome:
By the end of this course, students who have successfully completed should have:
• established an essential foundation of structural informatics
- computationally manipulated and analyze molecular structures
- become familiar with the frontier of current research
- gained research experience in
  - literature survey and study of a selected topic
  - hands-on experience in the use of computational methods
  - designing new or improving existing computational methods

**Course Requirements and Grading:**

1. (15%) Quizzes and/or literature reviews.

2. (35%) About 3-5 homework assignments
   - Tentative topics:
     - protein structure and geometry, PDB files, visualization, structure calculations, 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 on it.
   - Project mentoring: Once the topics have been agreed upon with instructors, students will choose one of the instructors as their project advisor and start to meet with him, individually or in small groups regularly to talk about project progress and to receive feedback.
   - Possible project areas/topics:
     - protein structure alignment
     - protein geometry
     - identification of domains
     - modeling
     - tertiary structure prediction
     - protein-protein interaction
     - molecular dynamics
     - statistical potential
     - big data research, etc., etc.
   - Students may choose a different subject area than those listed above. 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 21
- Project proposal presentation: Oct 22, 27
- Project presentation: Dec 8, 10, 17 (7:30-9:30am, final exam slot)
- Project report (4-6 pages) due: Dec 17, 5pm

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.

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 (~3.5 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
   G. Molecule Machines

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

III. Structure Analysis (~2 weeks)
   A. Protein geometry (internal coordinates, solvent-accessible surface etc.)
   B. Identification of domains
   C. Protein structure comparison
   D. Classification of Protein Folds
IV. Structure Prediction (~1 week)  
   A. Sequence Analysis  
   B. Local Structure Prediction  
   C. Homology Modeling  
   D. Threading  
   E. Ab initio Protein Structure Prediction  

V. Modeling and Simulations of Dynamics (~3.5 weeks)  
   A. Protein-Protein and Protein-Nucleic Acid Interactions  
   B. Molecular Dynamics  
   C. Other Sampling Methods (e.g., Replica exchange)  
   D. Coarse-grained models  
   E. Mechanisms and Regulation  

VI. Protein Design and Drug Selection (1 week)  

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.
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<thead>
<tr>
<th>Class No</th>
<th>Date</th>
<th>Lecturer – Subject</th>
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<td>8/25</td>
<td>GS – Introduction to the course</td>
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<tr>
<td>2</td>
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<td>GS – Basic principles and fundamental interactions</td>
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<td>GS – Molecular Architecture</td>
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<td>4</td>
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<td>GS – Structure Representations (internal and Cartesian Coordinates)</td>
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<td>5</td>
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<td>GS – Potential Functions (empirical potentials, statistical potentials)</td>
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<td>Sankar – Lab 1 (Graphics: visualization using PyMol, VMD)</td>
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<td>7</td>
<td>9/15</td>
<td>GS - Geometry Calculations (Basics, Voronoi graphs, Delaunay triangulation, alpha shapes.)</td>
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<td>Hargrove – X-ray Experiments</td>
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<td>Barb – NMR Experiments</td>
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<td>10</td>
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<td>Wu – X-ray Computations</td>
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<td>RJ – Structure Matching</td>
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<td>RJ - Folds &amp; Domains</td>
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<td>RJ – Sequence Analysis</td>
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<td>RJ – Secondary Structures and Sequence-Structure relationship</td>
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<td>RJ – Ab initio Predictions</td>
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<td>10/22</td>
<td>RJ + GS – Proposal presentation (10-15min each)</td>
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<td>RJ + GS – Proposal presentation (10-15min each)</td>
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<td>Walley – Proteomics methods</td>
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<td>GS - Molecular Simulations I</td>
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<td>RJ – Coarse-grained models I</td>
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<td>26</td>
<td>11/19</td>
<td>RJ – Nucleic Acids, Lipids, Regulations, and Images</td>
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<td>27</td>
<td>12/1</td>
<td>RJ – Protein Design</td>
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<td>28</td>
<td>12/3</td>
<td>RJ – Drug Selection</td>
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<td>12/17 (Thurs, 7:30-9:30am, final exam slot)</td>
<td>RJ + GS - Student project presentation</td>
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RJ: Robert Jernigan  
GS: Guang Song
**Academic Honesty**

Each assignment or project is to be the product of your own intellectual efforts.

The class will follow Iowa State University’s policy on academic dishonesty. Anyone suspected of academic dishonesty will be reported to the Dean of Students Office. [http://www.dso.iastate.edu/ja/academic/misconduct.html](http://www.dso.iastate.edu/ja/academic/misconduct.html)

Anyone found responsible will receive an automatic F in the course.

**Disability Accommodation**

Iowa State University complies with the Americans with Disabilities Act and Sect 504 of the Rehabilitation Act. If you have a disability and anticipate needing accommodations in this course, please contact (instructor name) to set up a meeting within the first two weeks of the semester or as soon as you become aware of your need. Before meeting with us, you will need to obtain a SAAR form with recommendations for accommodations from the [Disability Resources Office](http://www.dso.iastate.edu), located in Room 1076 on the main floor of the Student Services Building. Their telephone number is 515-294-7220 or email disabilityresources@iastate.edu. Retroactive requests for accommodations will not be honored.

**Dead Week**

This class follows the Iowa State University Dead Week policy as noted in section 10.6.4 of the Faculty Handbook [http://www.provost.iastate.edu/sites/default/files/uploads/fh/Faculty%20Handbook%20August%202014%20final.pdf](http://www.provost.iastate.edu/sites/default/files/uploads/fh/Faculty%20Handbook%20August%202014%20final.pdf)

**Harassment and Discrimination**

Iowa State University strives to maintain our campus as a place of work and study for faculty, staff, and students that is free of all forms of prohibited discrimination and harassment based upon race, ethnicity, sex (including sexual assault), pregnancy, color, religion, national origin, physical or mental disability, age, marital status, sexual orientation, gender identity, genetic information, or status as a U.S. veteran. Any student who has concerns about such behavior should contact his/her instructor, Student Assistance at 515-294-1020 or email dso-sas@iastate.edu, or the Office of Equal Opportunity and Compliance at 515-294-7612.

**Religious Accommodation**

If an academic or work requirement conflicts with your religious practices and/or observances, you may request reasonable accommodations. Your request must be in writing, and your instructor or supervisor will review the request. You or your instructor may also seek assistance from the Dean of Students Office or the Office of Equal Opportunity and Compliance.
Contact Information

If you are experiencing, or have experienced, a problem with any of the above issues, email academicissues@iastate.edu.
Appendix: titles of Past Course Projects

- Using Tertiary structure prediction combined with enzyme digestion pattern to find suitable structural candidate for HIV-1 antigens
- A heuristic to annotate Denovo Assembled Transcriptome using a Protein Structure Classification Database
- Identifying Protein Sub-Families using Mixture Model-based Clustering
- Non-native interactions on splicing-related protein fluctuation dynamics and conformation changes
- Finding Patterns in DNA Sequences: A Linear-Runtime Greedy Approach
- Protein-Protein Deformable Docking
- Structure Modeling and Visualization of DNA Origami
- Mixtures of Kinase Phosphorylation Motifs
- Protein fold classification incorporating additional evolutionary information from phylogenetic profiles

- Identifying Conserved Structural Features in Biological Datasets Using Sequence Information
- Principal Curve for Geometrical Feature Extraction in MD Trajectory
- A Domain Determination Method based on Internal Distance Change Matrix deprived from ENM
- Homology Modeling of Enzymes from the Degradation and Synthesis of Ketone Bodies
- Conformation Transitions of GroEL by Coarse Grained MD Simulation
- ANALYSIS OF RESIDUE INTERACTIONS INVOLVED IN PROTEIN CONFORMATIONAL SWITCHING