Tentative Course Schedule
Physics 323/623: Computational Biophysics Lab

Time: Tuesday, 3:00-4:50 pm

Date	Topic	Reading Assignment (Read prior to coming to lab; it is expected that students will have completed lecture readings, as well)	Laboratory Assignments Due (due by the beginning of lab on due date)	Leader
Tues Aug 29	Lab 1: Physical models: amino acid and protein structure	*amino acid web sites; Chapter 3, section 3.10; *Richardson 1981 review		JSF
Tues Sep 5	Lab 2: Visualization of proteins: VMD and PDB	Chapter 3, section 3.10; *Richardson 1981 review; *VMD and PDB web pages; *Eglin xtal paper	Lab 1 due	JSF
Tues Sep 12	Lab 2/3: Visualization of proteins revisited	*Eglin xtal and NMR papers; Richardson 1994		JSF
Tues Sep 19	Lab 3: Visualization of proteins revisited (cont)	*Eglin xtal and NMR papers; Richardson 1994	Lab 2 due	JSF
Tues Sep 26	Lab 4: Introduction to MatLab and molecular forces	MatLab book (read Chapter 1 and bring to class); Jackson Chapter 2 (2.1-2.14)	Lab 3 due	JSF
Tues Oct 3	Lab 4: Molecular forces (MatLab) (cont)	MatLab book (read Chapter 1 and bring to class); Jackson Chapter 2 (2.1-2.14)		JSF
Tues Oct 10	(cancelled—work on lecture take-home midterm)			
Tues Oct 17	Lab 5: Helix-coil transition; distances; dihedrals (MatLab)	Chapter 3 (all) (Bring MatLab book to class)	Lab 4 due	FRS
Tues Oct 24	How to read a scientific paper	*Eglin research paper	Lab 5 due	JSF/FRS
Tues Oct 31	Lab 6: Introduction to DEAC cluster, Linux operating system; editing and queuing	*DEAC cluster web pages	~2 page paper: eglin c background, including sequence, structure, function, molecular dynamics	FRS
Tues Nov 7	Lab 7: Dynamics in explicit solvent: setting up the eglin simulations	*MD introduction paper; *NAMD web pages	~2 page paper: MD review of work on eglin c and CI2	FRS
Tues Nov 14	Lab 7 (cont): NAMD trajectory analysis (MatLab, CHARMM and VMD)		Methods paper: dynamics in explicit solvent	FRS/JSF

Tues Nov 21	Student presentations		Putting it together, first draft: (Introduction, Methods, Results, Discussion, thus far)	students
Tues Nov 28	Student presentations			students
Tues Dec 5			Final paper due (including free energy calculations); discussion to include comparison to other student results and to literature)	

*Reading assignments for labs:

- Amino acid web sites: http://wbiomed.curtin.edu.au/teach/biochem/tutorials/AAs/AA.html; http://www.rothamsted.ac.uk/notebook/courses/guide/aa.htm
- Richardson review, 1981: Anatomy and Taxonomy of Protein Structure, J. S. Richardson (1981, as pp. 167-339 in volume 34 of Advances in Protein Chemistry published by Academic Press); electronic version: http://kinemage.biochem.duke.edu/~jsr/index.html
- Richardson 1994: Richardson JS. Introduction: protein motifs. FASEB J. 1994 Dec;8(15):1237-9.
- VMD and PDB web pages: http://www.ks.uiuc.edu/Research/vmd; www.rcsb.org;
- Eglin xtal and NMR papers:
    - Bode, W., Papamokos, E., Musil, D. The high-resolution X-ray crystal structure of the complex formed between subtilisin Carlsberg and eglin c, an elastase inhibitor from the leech Hirudo medicinalis. Structural analysis, subtilisin structure and interface geometry. Eur.J.Biochem. v166 pp.673-692, 1987.
    - Hyberts, S.G., Goldberg, M.S., Havel, T.F., Wagner, G. The solution structure of eglin c based on measurements of many NOEs and coupling constants and its comparison with X-ray structures. Protein Sci. v1 pp.736-751, 1992.
- Eglin research paper: Reich L, Weikl TR. Substructural cooperativity and parallel versus sequential events during protein unfolding. Proteins. 2006 Jun 1;63(4):1052-8.
- DEAC cluster web pages: http://www.deac.wfu.edu/index.php?title=WFU_DEAC_Cluster
- NAMD web pages: http://www.ks.uiuc.edu/Research/namd/
- MD introduction paper: Hansson T, Oostenbrink C, van Gunsteren WF. Molecular dynamics simulations. Current Opinion In Structural Biology 12 (2): 190-196 APR 2002
- Free energy calculation paper: Kollman PA, Massova I, Reyes C, et al. Calculating structures and free energies of complex molecules: Combining molecular mechanics and continuum models Accounts of Chemical Research 33 (12): 889-897 Dec 2000