Computational Biology

Jenkins Department of Biophysics
Fall Semester, 2018

Course Instructor: Dr. Patrick Fleming
Class Times: Tuesday and Thursday, 10:30 - 11:45 am
Room: UTL G98

Sept 4 Lecture 1 – Introduction
Sept 6 Lab 1a - UNIX, Editing files, plotting data, VIM, XMGRACE
Sept 11 Lab 1b – Python Tutorial
Sept 13 Lab 1c - Python Examples – Data Manipulation, Local Code
Sept 18 Lab 1d - Python Examples – PDB files, LOCAL CODE (Hmwk1 Due)
Sept 20 Lecture 2 – Molecular Simulations
Sept 25 Lab 2 - Molecular graphics, VMD, PYMOL (Hmwk2 Due)
Sept 27 Lab 3a - LJ Particle Simulation, MC, Local Code
Oct 2 Lecture 3 - Boltzmann Distribution (Hmwk3 Due)
Oct 4 Lab 3b - LJ Particle Simulation, MD, LOCAL CODE (Hmwk4 Due)
Oct 9 Review
Oct 11 Mid-term Exam (Covering Lectures 1-3 and Labs 1-3)
Oct 16 Lecture 4 – Protein Dynamics – Exp. Evidence
Oct 18 Lab 4a – Peptide MC1 – RIBOSOME, TORSION, LINUS (Hmwk5 Due)
Oct 23 Lab 4b – Peptide MC2 Simulation/Force Fields
Oct 25 Lab 4c – Peptide MC3 Simulation/Sterics & Entropy (Hmwk6 Due)
Oct 30 Lab 5a - Prot MD1 Simulation – NAMD
Nov 1 Lecture 5 - Force Fields
Nov 6 Lab 5b - Prot MD2 Simulation – Trajectory Analysis, VMD
Nov 8 Lab 5c - Prot MD3 Simulation - Probability Density Maps, VMD
Nov 13 Lecture 6 – Allostery/Intro to Final Project (Hmwk7 Due)
Nov 15 Lect 7/Lab 6 – Prot. Collective Motions, VMD

Nov 19-23 Thanksgiving Break, No Class

Nov 27 Lecture 8 - Information Theory and Protein Function (Hmwk8 Due)
Nov 29 Lab 7 - Deterministic and Stochastic Modeling
Dec 4 Lab 8 – Ligand Docking AutoDock (Hmwk 9 Due)
Dec 6 Research Project Consultations (In class)

Dec 18 Final Exam Time (Research Report Due, 5 pm)