Final Exam Practice Questions

CS/BIOE/CME/BIOPHYS/BIOMEDIN 279

Fall 2016

Test Details

The final exam will be held on Tuesday, December 13, 2016 from 3:30 PM - 6:30 PM in 200-002 (history corner of the quad, room 002). The exam will be closed-book, but you may consult one double-sided 8.5x11 page (or two single-sided pages)..

Instructions

These are practice questions in the style of questions you might expect on the exam. Each question should be answerable in a few sentences (that is, youre not required to provide a great deal of detail).

Question 1: Compare and contrast the energy functions used for molecular dynamics simulations and those used for ab initio protein structure prediction.

Question 2: Describe, at a high level, how Rosetta predicts protein structure (in particular, for ab initio modeling).

Question 3: How would you go about estimating how long it would take to run an MD simulation? What information would you need to consider?

Question 4: We would like to estimate how tightly a particular drug candidate binds to a particular target protein.

(a) Provide a quantitative definition of binding affinity (i.e., binding strength). That is, what does it mean for one ligand to bind more tightly than another?

(b) Suppose we have a single molecular dynamics simulation in which the drug candidate binds to the target and stays bound for the remainder of the simulation. Can we accurately estimate the binding affinity from that simulation? Why or why not?

Question 5: Describe one common approximation made by ligand docking methods, and explain why it helps simplify the problem to be solved.

Question 6: X-ray crystallography and single-particle electron microscopy are both techniques for determining the structure of a molecule or molecular complex. Why is single-particle electron

microscopy typically used for larger molecules or complexes than x-ray crystallography?

Question 7: Discuss the trade offs of a stochastic particle-based reaction-diffusion simulation versus a continuum approach (in which concentrations of each type of molecule are represented in each voxel).

Question 8: There is a very efficient algorithm for computing the Fourier Transform known as the Fast Fourier Transform (FFT). Describe how this algorithm is useful for one of the methods covered in this course.