Final Exam Practice Questions

CS/BIOE/CME/BIOPHYS/BIOMEDIN 279

Fall 2020

Final Assessment Logistics

The final assessment will be released on Thursday November 19, 2020. It is an 80-minute timed assessment. You will be able to start and finish the assessment at any time on Nov. 19, provided you finish within 80 minutes of when you start. The final will be open-book and open-internet, but we stress the importance of answers being written in your own words.

Instructions

These are practice questions in the style of questions you might expect on the final assessment. Each question should be answerable in a few sentences (that is, you're 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: How would you go about estimating how long it would take to run an MD simulation? What information would you need to consider?

Question 3: We would like to estimate how tightly a particular drug candidate binds to a particular target protein.

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

Question 5: 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 6: 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 7: 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.