Exam Practice Questions

CS 279, BIOE 279, BMDS 245, BIOPHYS 279, and CME 279

Fall 2026

Exam Details

The exam will be held on Thursday, December 10, 2026 from 12:15-3:15 PM (Location TBA). The exam will be closed-book, but you may consult one double-sided 8.5x11 page (or two single-sided pages) of notes.

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, you're not required to provide a great deal of detail). Depending on when you're reviewing this, some questions may be about topics to be covered in a future lecture.

Question 1: Why can template-based modeling often make reasonable predictions of protein structure even when the query protein and the template protein have significantly different sequences? (e.g. only 20% sequence identity)

Question 2: How do the energy functions used for molecular dynamics simulations differ from those used for ab initio protein structure prediction?

Question 3: 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 4: X-ray crystallography and cryo-electron microscopy are both techniques for determining the structure of a molecule or molecular complex. Why is cryo-electron microscopy typically used for larger molecules or complexes than x-ray crystallography?

Question 5: Discuss the trade-offs between 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 6: 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.