BMB 173 – Winter 2017

Homework Set 9.2 (80 points) – Assigned 3/9/17. Due 3/14/17

TA: Emily Wyatt, ewyatt@caltech.edu

Office Hours:

Friday 3/10/17 from 2-3pm in Spalding B123 or by appointment
Monday 3/13/17 from 3-4pm in Spalding B123 or by appointment

1. **Course-grained Molecular Dynamics** (30 points)
   a. (5 points) In your current research, what might be a potential use of MD simulation?
   b. (10 points) Estimate the number of atoms in your system.
   c. (5 points) Is this system size tractable, or would you need to perform course-grained molecular dynamics? What length of time is needed to answer your question?
   d. (10 points) Describe one potential strategy for course graining your system if you wanted to expand your system size or simulation time. For example, how might you cluster your atoms?

2. **Structural Genomics** (20 points)
   a. (10 points) One challenge in structural genomics is developing technology to automate the process. Thinking about the structural genomics pipeline, what steps do you think were the most difficult to automate? Why?
   b. (10 points) If you were to write a grant, how would you pick the targets for a structural genomics project?

3. **The Future of Structural Biology** (30 points)
   a. (15 points) Please read the following review on X-ray Free-Electron Lasers (XFELs):
      http://www.ncbi.nlm.nih.gov/pubmed/24914150
      i. (5 points) Briefly explain how XFELs work.
      ii. (10 points) Describe two advantages to XFELs in comparison to traditional x-ray crystallography.
   b. (15 points) Of the ~125,000 structures in the PDB, 90% have been solved by traditional x-ray crystallography, another 9% by NMR, and the last 1% have been determined using other strategies.
      Explain the relative advantages and disadvantages of three up and coming techniques to solve structures of proteins in the future – cryo-EM, XFELs, and MicroED.