Problem 1: Molecular Graphics Program Download and Tutorial

d (10 points). Render the figure on page 28.

![Figure 1: Question 1d, protein colored by time step](image1)

Figure 1: Question 1d, protein colored by time step

e (10). Render the plot on page 37.

![Figure 2: Question 1e, VDW representation colored by hydrophobicity](image2)

Figure 2: Question 1e, VDW representation colored by hydrophobicity
Problem 2: Jupyter Notebooks and VPython

d (10). Reproduce the plot from the VMD tutorial.

Figure 3: Graphing example.

e (10). Make an image of one sphere orbiting another.

Figure 4: vPython example.

Problem 3: Case Study Water and Ice

This case study introduces the properties of water and ice that are essential for living systems. You will be introduced to the pure solvent (water or ice), but also to the behavior of the solvent near proteins and so-called hydrophilic and hydrophobic surfaces. Please work through the case study and then do the exercises stated below, answering in scholarly English (full, grammatically correct sentences).

a (5 points). Do Exercise 1.

- (1) One might think there should be more hydrogen bonding in liquid water because the density of liquid water is higher than that of ice. While the molecules will be in closer proximity to one another on average, it does not mean there are more hydrogen bonds. In fact, the script yields approximately 2.15 hydrogen bonds per molecule, noticeably less than the average number of bonds in ice.

- (2) The green molecule makes 2 hydrogen bonds, the orange makes 4, and the yellow makes 2.
b (5). Do Exercise 2.

Figure 6: This is my best attempt. I even moved the hydrogens on the OH group to better display the hydrogen bonds that could form. I’m still not that happy with it, but I couldn’t find any better solution.
c (5). Do Exercise 3.

- (1) The distance between the oxygen and hydrogen atoms is 0.98 Å. This is the equilibrium distance utilized in the TIP3P model of water molecules.

- (2) The angle formed by hydrogens and the oxygen atom is 104.5 degrees. Again, this is the equilibrium value utilized in the TIP3P model of water molecules.

- (3) The file `par_all27_prot_lipid.inp` contains the parameters used by the CHARMM force field for simulating proteins and lipids. The parameters of the TIP3P model of water stated there are:
  
  - For the bond energy term \( V_{\text{bond}} = K_b(b - b_0)^2 \) between water hydrogen and oxygen atoms we have \( K_b = 450 \text{ kcal/mol/Å}^2 \) and \( b_0 = 0.9572 \text{ Å} \).
  
  - For the angle energy term \( V_{\text{angle}} = K_\theta(\theta - \theta_0)^2 \) of a water molecule we have \( K_\theta = 55 \text{ kcal/mol/Å}^2 \) and \( \theta_0 = 104.52 \text{ degrees} \).
  
  - For the Lennard-Jones potential

\[
V_{\text{LJ}} = \epsilon_{i,j} \left( \left( \frac{R_{\text{min},i,j}}{r_{i,j}} \right)^{12} - 2 \left( \frac{R_{\text{min},i,j}}{r_{i,j}} \right)^6 \right)
\]

where \( \epsilon_{i,j} = \sqrt{\epsilon_i \epsilon_j} \) and \( R_{\text{min},i,j} = R_{\text{min},i}/2 + R_{\text{min},j}/2 \), we have \( \epsilon_H = -0.046 \text{ kcal/mol} \); \( R_{\text{min},H}/2 = 0.2245 \text{ Å} \); \( \epsilon_O = -0.1521 \text{ kcal/mol} \); \( R_{\text{min},O}/2 = 1.7682 \text{ Å} \).

d (5). Do Exercise 4.

Due to the ordered structure of ice, a higher spring constant would make the individual molecules less flexible and thus the lattice more stable with a higher melting temperature. A lower spring constant would allow the molecules to break the lattice more easily and thus give a lower melting temperature. However, one could potentially rationalize the opposite, e.g., that a higher spring constant makes the lattice more brittle. To test it, I re-ran the melting simulations with angle spring constants of \( k = 20 \text{ kcal/mol-rad}^2 \), 55 kcal/mol-rad\(^2 \) (the default one), and 550 kcal/mol-rad\(^2 \). I then plotted the pair distribution function for OH2 after 300 ps, i.e., where the ice is starting to melt in the original simulation.

We can see that while the reference and larger force constants still have some order beyond 2.5 Å, the smaller force constant simulation is already disordered by this time.
e (5). Do Exercise 5.

- (1) The pair distribution function for hydrogen atoms of liquid water is shown in Fig. 5. The first maximum is located at 1.5 Å, which matches the distance between two hydrogen atoms in a single water molecule. Clearly, the distance between hydrogen atoms is shorter than the distance between oxygen atoms, as one would expect due to the geometry and arrangement of water molecules.

- (2) The pair distribution function for oxygen atoms of ice is shown in Fig. 6. The crystalline order of ice is reflected in the sharp peaks of the pair distribution function.
Figure 9: Question 3e, Pair Distribution Function for oxygen in water at 10 K