# CS612 Homework Assignment 4

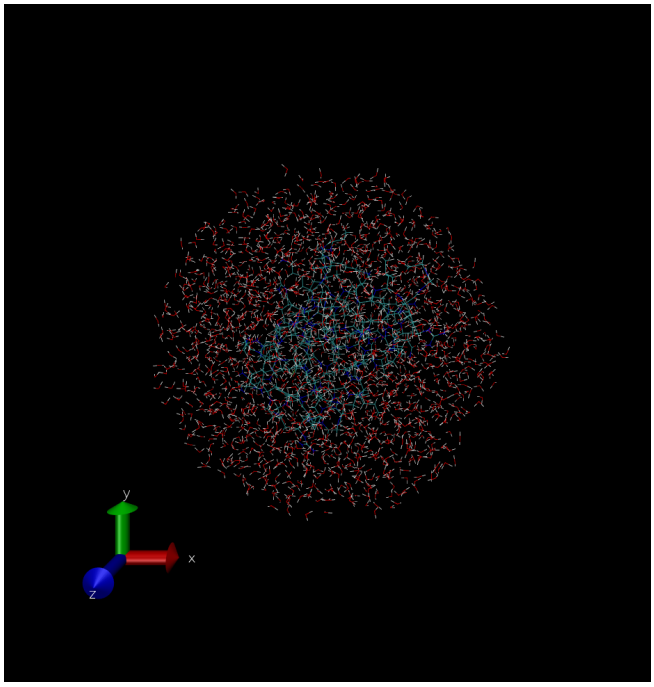
Solutions

1. **Molecular Dynamic simulations hands-on exercise:** In this assignment you will perform a simple MD simulation of Ubiquitin. You will have to download the NAMD software and you will use VMD for visualizing and processing the results. Download NAMD at http://www.ks.uiuc.edu/Development/Download/download.cgi.

   a. Do the NAMD tutorial at http://www.ks.uiuc.edu/Training/Tutorials/#namd . Do only the part that refers to ubiquitin in a water sphere. Attach a screenshot of the final trajectory, and e-mail me your output (it's quite a large set of files, don't try to print it).
   b. The log files contain a lot of information about the run of the simulation. Look at the log file and see how the information is output to the file (quite self-explanatory). What is the final potential energy of the system? What is the final bond energy? VdW energy?

   Solutions:

   (a) Here is the screenshot. Please notice that I asked to do the sphere, not box.




   (b) The log file is enclosed separately. The energy can be read from the end of the file. The values I got on my PC are the following:

   | | |
   |---|---|
   | Potential | -19925.6054 |
   | Bond | 234.3510 |
   | VdW | 1564.0266 |

   I accepted a wide variety of results because different computers, NAMD versions, as well as different runs, may give slightly different results, but they should be in this ballpark.

2. **Transformations on Molecules:**

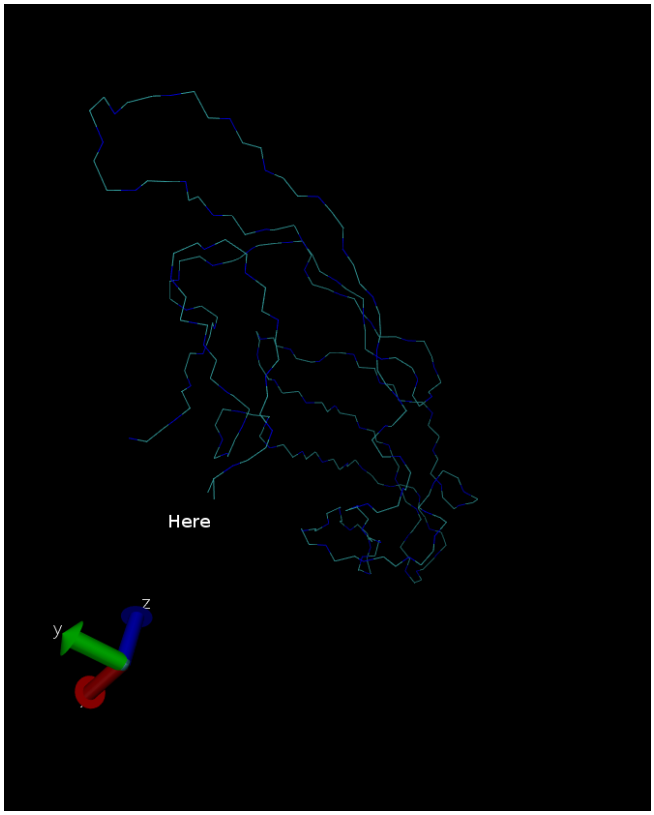
a. Read the PDB file 2EZM from the PDB website. Leave only the C,N and CA atoms (you can either edit the file or use the VMD selection option). These are only the main backbone atoms (except the carboxyl O but it's not important for the dihedral calculations below). Calculate the backbone dihedral angles ($\phi$ and $\psi$) for amino acid 10.
**Answer:** $\psi = 35.70$ and $\phi = 56.20$ . See solution code.

b. Calculate the energy for the structure above with only the backbone atoms. Use a simplified energy function that counts only steric clashes between atoms. The energy is the sum over all the pairs of atoms that are at least 4 atoms apart on the peptide chain (that is – do not share a covalent bond, a planar angle or a dihedral angle). The energy for each pair of atoms is:

$$Eij = \begin{cases} 100/r_{ij}^2 & \text{if } r_{ij} < 3.4 \\ 0 & \text{Otherwise} \end{cases}$$

Where $r_{ij}$ is the distance between two atoms. In this (simplied) function we model each atom as a hard sphere with a radius of 1.7Å, hence the 3.4 - two atoms collide only if their distance is smaller than the sum of their radii. Output the total energy and also report the pairs of severely clashing atoms, whose contribution to the energy is at least 20, and their distances.
**Answer:** E=255.96 and there were no severely clashing atoms this time. See code.

c. Rotate the dihedral bond between the N and CA of the last amino acid by $30^\circ$. You can perform the rotation using quaternions or matrices as taught in class. If using quaternion, use the N-CA vector as the rotation axis and don't forget to translate the molecule such that N is at the origin. The rotation is equivalent to transforming all the atoms **after** the axis by $30^\circ$. Does the structure change much? What atoms move in space as the result of this rotation? What is the RMSD between the original and the modified structure? You can measure the RMSD using VMD or the code you wrote for HW3.
**Answer:** The structure changes very little. Only one atom moves (the last one). The energy is the same and the RMSD is very small – $0.043\mathring{A}$ or so. See two structures superimposed. Notice the only differece is the last atom.




d. Now rotate the dihedral bond between CA and C of amino acid 40 by 20°. What is the RMSD between the original and the modied structure now? Upload the three structures to vmd or chimera and attach an image of the superimposed structures as part of your homework.
**Answer:** This time the change is much bigger, because we rotate more than half the atoms. There are several severe clashes (see below). The energy is

e. Calculate the energy for the two structures you created in c and d above.
**Answer:** See above.