Physics 4251/6250 – Fall 2019
Problem Set 1, August 20
Due: Thursday, August 29 by 5 PM

This assignment will help you to become familiar with VMD (Visual Molecular Dynamics) and running Python code, both of which will be used here and for some assignments in the future. Please turn in your assignment on Canvas.

I emphasize again that we (Zijian and myself) will help you get through any difficulties you have *but you have to ask.*

Problem 1: Molecular Graphics Program Download and Tutorial

(a) Download and install the molecular visualization program VMD from http://www.ks.uiuc.edu/Research/vmd/ (see "Download VMD" on the left side of the page).

(b) Download the tutorial "Using VMD" from http://www.ks.uiuc.edu/Training/Tutorials/.

(c) Work through sections 1, 3, 4, and 5 of the tutorial. You will need to read some of section 2 in order to make figures, but for now there is no need to work through every aspect.

(d) On page 28 of the tutorial, you will color a protein according to its time step during the simulation. **Render a snapshot of this figure and insert it into your assignment.** (See page 22 for how to render a figure.)

(e) There is a picture on page 37 of the tutorial of ubiquitin. Please try to duplicate this figure to the best of your ability. **Render a snapshot and insert it into your assignment.**

(f) Starting at the bottom of page 47 of the tutorial, you will produce two files containing distances between residues 10 and 76 with the center of ubiquitin, respectively. **You will need these files in Prob. 2d below.**

Problem 2: Jupyter Notebooks and VPython

You are free to use the Python interpreter of your choice provided it uses Python 3 and supports VPython.

(a) Install Anaconda following the instructions here: http://jupyter.readthedocs.io/en/latest/install.html. Make sure to select Python 3.5 or later.

(b) At the command line, type `conda install -c vpython vpython` and hit enter. Make sure there are no errors.

(c) At the command line, type `pip install ivisual` and hit enter. Make sure there are no errors.

(d) Start Jupyter by typing `jupyter notebook` at the command line. Create a New "Python 3"

notebook. In a separate tab, navigate to https://github.gatech.edu/jcgumbart/Biophysics and click **HW1**. Click on `graphing-1.ipynb`. Run the individual commands one-by-one in your own notebook ("shift-enter" runs a command). Note that you need to either start Jupyter in the same directory as the dat files from Prob. 1f above **or** move them to the appropriate directory **or** call them using the full path. **Choose your favorite two colors and reproduce the plot, including the image in your assignment.**

(e) Now create a new "VPython" notebook. Cut and paste the command from `vpython-2.ipynb` into your new notebook and run it. Change the colors of the two spheres and run it again (Note: to re-run a VPython notebook, you have to first restart the kernel using the circular arrow at the top and wait a few seconds). Rotate and/or zoom to a view you like and use "print screen" function of your computer to save an image of the orbits. **Include this image in your assignment.**

Problem 3: Case Study Water and Ice

We'll continue to get our feet "wet" with VMD by working through the water case study. This study examines 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). The case study can be downloaded from http://www.ks.uiuc.edu/Training/CaseStudies/ (see "Water").

(a) Do Exercise 1.

(b) Do Exercise 2. Note that you may find it easier to use mouse commands (e.g., "move fragment") to adjust the protein's position.

(c) Do Exercise 3.

(d) Do Exercise 4.

(e) Do Exercise 5.