**Physics 4251 / Fall 2017**
**Problem Set 1, August 22**
**Due: Thursday, August 31 before class**

**Policy on emailed homework:** If you want to move into an all-digital age, you may email your homework to me (gumbart@physics.gatech.edu) provided that you do it **BEFORE** class on the due date. Begin the subject with **[PHYS 4251]** for easy identification.

This assignment will help you to become familiar with VMD (Visual Molecular Dynamics) and running Python code, both of which will be used for some assignments in the future. If there is any trouble finding a computer or printer to use for this exercise, please let me know.

### 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 6 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 print it out.** (See page 18 for how to render a figure. NOTE: please change the background color in VMD to white to avoid wasting printer ink).

(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. **Print it out.**

(f) On page 67 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 3.6.

(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.**