**ChBE 4830 – Assignment 3**

**Lennard-Jones simulations using HOOMD-Blue**

1. Download and install the Anaconda Python package manager and the HOOMD blue simulation engine (NOTE: All steps prefaced by “>>” indicate commands that should be executed from the command line.)
   1. Download Anaconda from <https://www.anaconda.com/download/>
      1. Choose the Python 3.6 version
      2. If you have a Windows machine…
      3. If you have MacOS or Linux, we recommend choosing the command line installer
         1. After the download has completed open up a Terminal
         2. Navigate to the Downloads folder
            1. >> cd ~/Downloads
         3. Execute the installer
            1. >> bash Anaconda3-4.4.0-MacOSX-x86\_64.sh

Note: Your script may have a slightly different name

* + - 1. Follow the prompts to complete the installation
  1. Install HOOMD and dependencies
     1. >> conda install –c glotzer hoomd fresnel gsd
        1. Note: If you receive a “-bash: conda: command not found” error message you may need to source your bash profile
           1. >> source ~/.bash\_profile
  2. Download the ChBE4830 repository from Github
     1. >> git clone https://github.com/summeraz/chbe4830.git
  3. Navigate to and launch the Lennard Jones tutorial in a Jupyter notebook
     1. >> cd chbe4830/Assignment3
     2. >> jupyter notebook
        1. Note: If you receive an error message about jupyter not being found, you can download the package with conda
           1. >> conda install jupyter
     3. Select LJ-NVE.ipynb
  4. Work through the Lennard-Jones tutorial, paying close attention to the description for each block of code. (Note: To execute a code block use SHIFT+ENTER) If you are unsure of the purpose of a particular command, refer to the documentation at the link provided at the beginning of the notebook.

1. Determine the optimum timestep for the simulation in the above tutorial (Hint: think energy). Provide plot(s) to support your answer.
2. Optimize neighborlist settings in the above tutorial (using a reduced timestep of 0.005).
   1. What is the optimal value of `r\_buff` when `check\_period` is 1? Provide plots to support your answer.
   2. What is the optimal value of `check\_period` when `r\_buff` is 0.6?

Provide a description of how optimal values were determined. (Hint: When running a simulation we want to use the neighborlist settings that yield the fastest simulation time without missing interactions.)