**Software installation**

**Note:** All lines prefaced by `>>` indicate commands to be entered in the command line.

**Installing Anaconda**

**Note:** These instructions should work without issue if using a Mac or Linux machine. For Windows users you may need to set up a virtual box that runs Linux.

* Download Anaconda (Python package manager) from <https://www.anaconda.com/download/>
  + Choose the Python 3.6 version
  + You can choose either the graphical or command-line installer; however, the following directions assume that the **command-line** installer has been chosen
    - After the download is completed open up a Terminal
    - Navigate to the Downloads folder
      * >> cd ~/Downloads
    - Execute the installer
      * >> bash Anaconda3-4.4.0-MacOSX-x86\_64.sh
        + Note: Your script may have a slightly different name
    - Follow the prompts to complete the Anaconda installation
* Create a new Anaconda environment (we’ll name is mosdef35) to use for this class
  + >> conda config --add channels glotzer
    - Note: If you receive a “-bash: conda: command not found” error message you may need to source your bash profile
      * >> source ~/.bash\_profile
  + >> conda config --add channels omnia
  + >> conda config --add channels mosdef
  + >> conda create -y --name mosdef35 python=3.5 mdtraj mbuild foyer jupyter pytest hoomd fresnel gsd matplotlib
* Activate the environment (note, you will want to have this environment active when running the Jupyter notebooks used for the next couple of assignments)
  + >> source activate mosdef35
* Test to make sure your environment is working properly by launching an interactive Python session
  + >> python
  + Within the interactive Python session, try importing the packages you will need
    - >> import hoomd
    - >> import mbuild
    - >> import foyer

**Downloading the ChBE 4830 git repository**

* Several homework assignments will be available within a git repository created for this class
  + <https://github.com/summeraz/chbe4830>
  + To access the git repository, you will need to create an account on Github
    - <https://github.com/>
  + After creating an account you will need to clone the ChBE 4830 repository to your local machine
    - >> git clone <https://github.com/summeraz/chbe4830.git>
      * This will create a new subdirectory with the name `chbe4830`.
  + If at any time you need to update your local git repository to grab changes from the remote you can use the `git pull` command
    - >> git pull

**Accessing Assignment 3**

* In the command line, navigate to the class git repository
  + >> cd chbe4830
* Navigate to the `Assignment3` directory
  + >> cd Assignment3
* Start a Jupyter notebook server
  + >> jupyter notebook
    - This will open the notebook dashboard in a new window of your default browser.
    - If you’re having issues, more information is located at <http://jupyter.readthedocs.io/en/latest/running.html>
* Select the notebook titled `LJ-NVE.ipynb`
  + This will launch a Jupyter notebook that contains a tutorial of a Lennard-Jones molecular dynamics simulation performed using the HOOMD simulation engine.
    - To execute a block of code within the notebook you can use SHIFT+ENTER
* Instructions for your homework assignment are located in a Word document within the same `Assignment3` directory you launched the notebook from.
* **Note:** It is recommended you make a copy of the tutorial notebook, as you will need to make changes to complete your homework and will want the original for reference
  + >> cp LJ-NVE.ipynb LJ-NVE-copy.ipynb
  + The original notebook will also always be available on the class github repository.
* **Note:** If you run into problems and need to restart the notebook, you can select `Restart and Clear Output` from the `Kernel` menu at the top of the notebook