

Assignment 2 Setup

Assignment 2 involves using two software packages, PyMOL and PyRosetta. Both packages, as well as Python, are already installed on the FarmShare **rye** machines. Below we give instructions on how to access these packages remotely and also give some instructions on how to install the packages on your own machine. Both packages are available on Mac, Linux, and Windows.

Suggested workflow

Students may either work with PyMol and PyRosetta remotely on the **rye** machines, or they may install the software on their own machines. We recommend that OS X and Linux users try installing the software on their own machine (to avoid overloading the **rye** machines), and work remotely on the **rye** machines if they run into problems. Installing PyRosetta on Windows may be trickier, so we recommend that Windows users work on the **rye** machines. If you're having trouble setting up, do not hesitate to post to Piazza or come to the TAs' office hours.

Working remotely (FarmVNC)

We have several **rye** machines! You will need to use FarmVNC to set up an ssh tunnel to access the machines. Before beginning, follow the directions listed under [FarmVNC'S "First Steps"](#) to ensure that you have AFS tokens and a VNC password set up on Farmshare. You only have to set the VNC password once. Before beginning, you will also need a VNC client. Mac and Linux users should download and install [TurboVNC](#). Windows users should download and install [SS-VNC](#).

Establishing an SSH tunnel with FarmVNC

Now you need to `ssh` into one of the **rye** machines. You must choose one of **rye01**, **rye02**, **rye03**, **rye04**, **rye05**, **rye06**. Load the `farmvnc` module and run it. It will output a lot of initialization jargon – the important steps and information are highlighted.

```
$ ssh your-sunid@rye01.stanford.edu
# PuTTY users would use rye01.stanford.edu for the hostname (or any of the other rye's)
rye01:~> module load farmvnc
rye01:~> farmvnc 1024x768 # choose appropriate resolution for your screen
checking for current vnc sessions on this host

checking port 5901
using display 1
searching for available GPU
GPU 0 available
using GPU 0

Initializing built-in extension Generic Event Extension
** Other initializations omitted **
Initializing built-in extension DRI2
```

```
Loading extension GLX
Loading extension NV-GLX
Loading extension NV-CONTROL
```

```
###
##
# Mac and Linux users
# run this command in another window to setup the SSH tunnel
#
# ssh -L 5901:localhost:5901 osamae@rye01.stanford.edu
#
# Windows users
# use these values in SS-VNC
#
# VNC Host Display: localhost:1
# Proxy/Gateway: osamae@rye01.stanford.edu
##
###
```

For Mac and Linux users, copy the instructed ssh **command**, open up a new terminal window, and paste the command. After logging in, open up TurboVNC Viewer, and enter `localhost:5901` into the VNC Server box. The next screen will ask you for your VNC password that you set earlier (different from your SUNET password).

For Windows users, open up SS-VNC and enter the highlighted **credentials**.

Using the VNC Client and Loading PyRosetta

A window should have popped which gives you remote access to the rye machine. Open up the terminal. If you are just starting the assignment, you can copy the assignment files hosted on the website into your local space. The following will copy the zip file into a `cs279/` directory in your home directory. You can use the `unzip` command to unzip compressed files.

```
rye01:~> cp /afs/ir/class/cs279/www/assignments/assn2.zip ~/cs279/
rye01:~> cd cs279/
rye01:~> unzip assn2.zip
```

To begin working on assignment 2, it is imperative that you load the `pyrosetta` module in the VNC Client's Terminal every time. `PyMOL`, on the other hand, can be launched by just typing `PyMOL` in the terminal.

```
rye01:~> module load pyrosetta
```

The last and most important step: **PLEASE log out of the VNC client by clicking on the gear icon at the top right corner of the virtual desktop and clicking log-out.** For good measure, kill all the processes under your SUNetID on the rye machine you using to ensure that you do not leave behind "zombie" processes:

```
rye03:~> pkill -u your-sunetid
Connection to rye03.stanford.edu closed by remote host.
Connection to rye03.stanford.edu closed.
```

You should be good to go for assignment 2!

Rye Machine Overloaded Troubleshooting

It is possible, and at times, very likely that you will experience problems with the **rye** machines due to them being overloaded with “zombie” processes. Often times, these errors are cryptic and confusing. Here are the two most common errors you may encounter:

1. When you load the farmvnc module and execute the farmvnc command with specified screen resolution, you may get an error that the machine has no available GPUs.
2. When you launch the VNC client and enter the host credentials, you may get a weird abort message indicating the connection was refused (i.e. “channel 3: open failed: connect failed: Connection refused.”)

If you get either of these errors, or are consistently running into odd connection refused error messages, this is a good indication that the rye machine you are using is overloaded with other students’ processes. Your options here are somewhat limited:

1. Try using the other **rye** machines (**rye01** through **rye06**). If you have no luck with one machine, be sure to kill the processes under your SUNetID before trying another (i.e. execute `pkill -u your-sunetid`)
2. Try installing and developing locally on your own machine
3. Wait a few hours. There is a script that runs in the middle of the night that cleans zombie processes

All that being said, it is imperative that you begin this assignment early to ensure that you can deal with any technical difficulties before the deadline!

Working on your own OS X/Linux machine

The installation of PyMOL should be straightforward. If you are having trouble installing PyRosetta, refer to the section below:

Detailed notes on PyRosetta installation from <http://www.pyrosetta.org/dow>

1. Obtain a **Rosetta license** from to receive a username and password.
2. Download **PyRosetta 3** (PyRosetta 4 has issues with a toolbox import). Link here: <http://www.pyrosetta.org/dow/pyrosetta3-download>. Make sure to download **release.monolith**
3. Unpack the downloaded file to the location of your choice to create the PyRosetta directory.

4. (From a terminal/console window, you can unpack the archive using the command: `tar -vjxf PyRosetta-<version>.tar.bz2`. Please note, there is no special install procedure required; after unpacking, PyRosetta is ready to use. So unpack it to the location from where you want to execute it.)

```
$ cd ~/Downloads # navigate to the directory which you've downloaded the tar.bz2
$ tar -vjxf PyRosetta-<version>.tar.bz2 # Unpack the tar.bz2
$ cd PyRosetta-<version> # navigate to the unpacked pyrosetta directory
```

5. From within the new PyRosetta directory, type into the command line: `source SetPyRosettaEnvironment.sh` to set up the PyRosetta library file paths.

```
# Method 1
# You will have to do this every time you start up Pyrosetta
$ source SetPyRosettaEnvironment.sh

# Method 2
$ vim ~/.bash profile # It's ~/.bash.profile for Mac users and ~/.bashrc for linux
users
# press 'i'
$ source SetPyRosettaEnvironment.sh
# press 'esc', ':wq', then 'Enter'
$ source ~/.bash profile # applied every time you open a new terminal
```

6. Start Python.

```
$ python
```

7. In Python, you should be able to import the PyRosetta library with the command `import rosetta; rosetta.init()`.
8. (If this step does not produce a complaint or error, your installation has been successful.)

Working with PyRosetta and PyMol on your local machine (for OS X and Linux users)

After implementing the required methods in the MonteCarloPredictor, open PyMol and type the following:

```
PyMOL> run PyMOLPyRosettaServer.py
```

In a separate terminal window:

```
$ cd ~/Downloads/assn2 # navigate to your a2 dir
$ mkdir out # make a directory for your outputted pdb files to be stored
# If you've installed Pyrosetta using bash.rc/bash.profile (Method 2 in the previous section),
skip this
$ source ~/Downloads/PyRosetta-<version>/SetPyRosettaEnvironment.sh
```

```
# After running the command below, you should see the protein change conformation in Pymol
```

Your pdb files should now be in your out directory

\$ python predict.py pdbs/sequence.pdb dihedral1000.pdb -dihedral -pymol -1000