gilgamesh-setup

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1 Login

To login to gilgamesh, you must use ssh and either be on campus, or use the VPN/Library resources with ssh. Remember to start your x-server (XMing) before you connect to gilgamesh.cheme.cmu.edu, and to enable X11-forwarding in your ssh client.

Your login id is your andrew id. I will give you the password in class. The first thing you should do is change your password by running this command:

```
1  passwd
```

Next run this command:

```
1  emacs .bashrc
```

You want to make your .bashrc file look like this:

```
1  # .bashrc
2
3  # Source global definitions
4  if [ -f /etc/bashrc ]; then
5      . /etc/bashrc
6  fi
7
```

```
 8    # User specific aliases and functions
 9    source /etc/profile.d/modules.sh
10    module load molsim-06640-f12
11    # end
```

After you modify the .bashrc file, save it and exit emacs. Then run this command:

```
 1    source ~/.bashrc
```

That will update your session with the new commands. You only need to do this once. From now on, the .bashrc file will be loaded when you login. Next we need to clone the dft-course repository.

```
 1    git clone git://github.com/jkitchin/dft-course.git
```

You should now be setup to run DFT calculations on gilgamesh.