

## Odyssey Setup

**Convention:** commands will be written in typewriter font (e.g. type `ls`). Italics such as *ESC* denote the corresponding special key.

## Odyssey Account

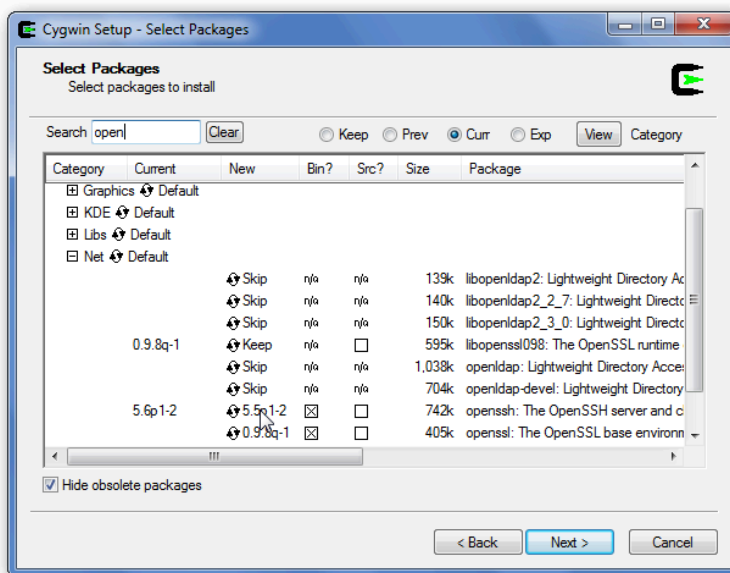
Odyssey is Harvard's high-performance computing network. Calculations require an Odyssey account (<https://rc.fas.harvard.edu/account-access-request-forms/>). Please tell them you require access to *Gaussian*, a standard program for performing electronic structure calculations.

## PC Setup

You will require PuTTY to access Odyssey by SSH (secure shell). You can download it here at <http://www.putty.org/>.

I recommend downloading Cygwin (<https://cygwin.com/install.html>). Cygwin gives you the ability to run Linux commands in Windows. Install the 64-bit version and install the *coreutils*, *awk*, *vim*, *git*, and *openssh* packages.

When this dialog pops up, type the names of the above packages:



Ensure that the “bin” column is marked with an x. This will download the binaries for the particular package (you don’t need “src,” the source code). You can select multiple packages before proceeding. Clicking “next” will install all the packages.

Check that Cygwin is working by opening a terminal. This is a Linux prompt that will run commands on your local computer. At the Cygwin prompt:

```
git clone https://github.com/ekwan/chem106_calculations.git
cp chem106 calculations/config/.vimrc .
```

This downloads some Chem 106 files we will need and sets up *vim*, a text editor. (Note: if you are already using *vim* and have your own configuration file, do not follow this step.)

## Mac Setup

Download iTerm (<https://www.iterm2.com/downloads.html>), which will let you run Linux commands on your local computer. (iTerm is an improved version of Terminal.) iTerm will also let us use SSH to access Odyssey.

Install Homebrew, a package manager for macOS. A “package manager” is a program that downloads and installs programs for you. If the program you want requires other programs (“dependencies”), the package manager will download and install those too. Run this command at the iTerm prompt:

```
/usr/bin/ruby -e "$(curl -fsSL https://raw.githubusercontent.com/Homebrew/install/master/install)"
```

You can also copy and paste this command from <https://brew.sh/>. You may be prompted to install Xcode. Install that too.

You will need a few standard packages. At the iTerm prompt:

```
brew install coreutils git gnu-sed
```

Then, download the Chem 106 files we will need and set up *vim*, a text editor (note: if you are already using *vim* and have your own configuration file, do not follow this step):

```
cd ~
git clone https://github.com/ekwan/chem106_calculations.git
cp chem106_calculations/config/.vimrc .
```

If you already have the repository, type:

```
cd ~/chem106_calculations
git pull
cp ~/chem106_calculations/config/.vimrc ~
```

This will download the latest version of the files.

Next, we will setup your Odyssey connection. You can find more detailed instructions here: <https://rc.fas.harvard.edu/resources/documentation/linux/using-ssh-controlmaster-for-single-sign-on/>.

```
ssh-keygen (skip if you already have an SSH key, use ls -al and see if you have a .ssh directory)
cd .ssh
vim config
```

Press *i* and type in the following:

```
Host ody
User myusername
HostName login.rc.fas.harvard.edu
ControlMaster auto
ControlPath ~/.ssh/%r@%h:%p
```

You will need to replace *myusername* with your Odyssey user name. Press *ESC* :wq and enter to save your changes. (See below for details on how to use *vim*.)

This will prevent you from having to type in your password many times a day.

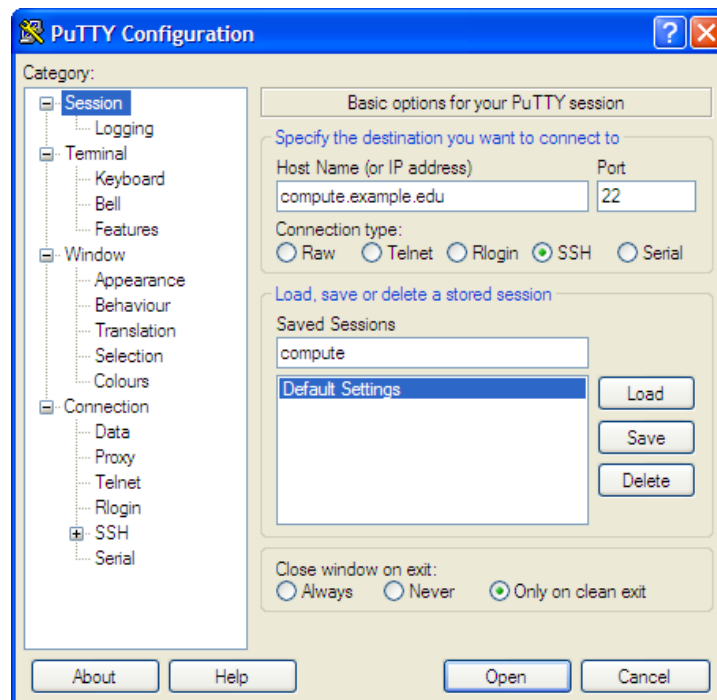
## Logging In (PC Instructions)

Open PuTTY and type in `login.rc.fas.harvard.edu` where it says “Host Name”. To avoid having to type this in every time, type `odyssey` in the box under “Saved Sessions” and press “save.” Next time, click on Odyssey in the list and press “open.”

Note: in the image below, `compute.example.edu` and `compute` with the locations given above. PuTTY stores configuration files in files that may clutter up your desktop. You can hide them by right-clicking on them and giving them the “hidden” attribute.

**Alert!** Don’t confuse the Cygwin and PuTTY prompts. Typing in the Cygwin prompt tells *your local computer* to run commands. Typing in the PuTTY SSH prompt tells *the Odyssey computer* to run commands. Both prompts are Linux-based and look similar.

You will be prompted for your username and password. Your password is your Odyssey password, not your HUID password. You will also be prompted for a passcode, which is the code on your Odyssey token, not your HUID token. You can get your token at <https://rc.fas.harvard.edu/resources/faq/how-to-install-openauth/>. You can either put your token on your computer as Java app or download the token onto your phone. If you login incorrectly, you must use a fresh passcode on your next attempt.



## Logging In (Mac Instructions)

Open iTerm and type:

```
ssh -Y -C -o ServerAliveInterval=30 -fN ody
```

Enter in your username, password, and passcode. You will return to the prompt on your local computer instead of getting an Odyssey prompt. This means that you have established a “background” connection to Odyssey. Type `ssh ody` to login. You should not need to type in your password again until the background connection is severed (by closing your laptop, for example).

## Odyssey Setup

We will also need the Chem 106 calculation files on Odyssey.

```
git clone https://github.com/ekwan/chem106_calculations.git
```

If you already have the repository, type:

```
cd ~/chem106_calculations
git pull
```

To setup your account:

```
cp ~/chem106_calculations/config/.vimrc ~
cp ~/chem106_calculations/config/.bashrc ~
```

Logout by typing `exit` and log back in. Type `g09` to see if Gaussian is installed. If Gaussian is working, you should see:

*Entering Gaussian System, Link 0=g09*

If you see *permission denied*, you must email [rchelp@fas.harvard.edu](mailto:rchelp@fas.harvard.edu) and request access to Gaussian.

To check that you have the correct version of Gaussian loaded, press `CONTROL D` and ensure that *Gaussian 09, Revision D.01* is shown.

## Basic Shell Commands

Congratulations! You are now setup to use Odyssey. You will need some basic Linux skills to get around. An excellent tutorial can be found at <http://www.ee.surrey.ac.uk/Teaching/Unix/>. Tutorials 1-4 would be a good start. Here are some basic shell commands to get you started:

`ls` : lists files (use `ls -alht` to list all files, represent things in a list, give sizes in human readable format, and sort by time)

`cd directory_name` : change directory

`pwd` : print working directory (shows you which directory you are in now)

Here's how to work with files:

`rm filename` : deletes a file (use `rm -rf directory_name` to delete a directory)

`cp source destination` : copies a file from *source* to *destination* (use `cp -r source destination` for directories)

`mv source destination` : moves a file from *source* to *destination* (this is the same as renaming a file)

**Alert! Deleting, moving, copying, etc. is forever. There is no undo function.**

A few special filenames:

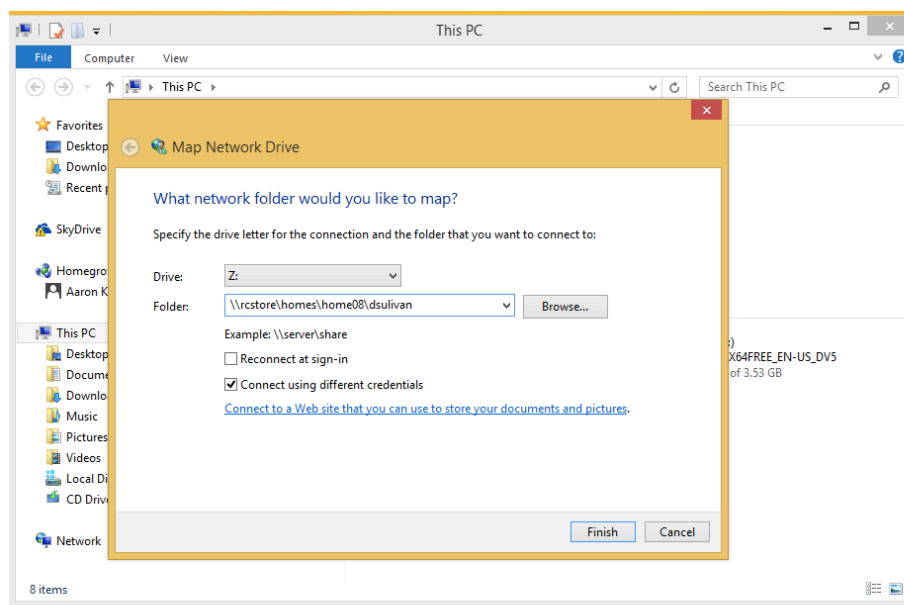
- . : (i.e., one period) your current directory
- .. : (i.e. two periods) one directory up from where you are now
- ~ : (tilde) your home directory
- \* : (asterisk) a wildcard that represents any text (for example, \*.out would include 1.out, 2.out, etc.)

## Transferring Files (PC)

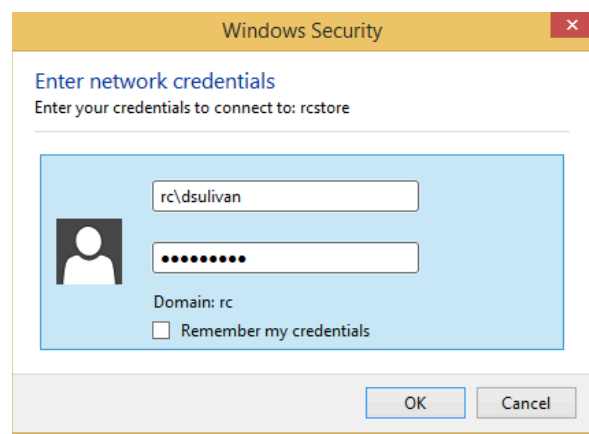
The best solution is to “mount” Odyssey directories on your computer. “Mounting” means that you will see the remote directory on your computer as if it were actually stored on your own hard drive. Detailed instructions are available at <https://rc.fas.harvard.edu/resources/access-and-login/>.

Connect to the RC VPN (not the regular Harvard VPN!). Instructions are given here: <https://rc.fas.harvard.edu/resources/vpn-setup/>.

Open up a Windows Explorer window. Press the “Map Network Drive” button in the toolbar at the top:



Replace the address shown with your home directory (use pwd when you are in ~ on Odyssey). Make sure that “Connect using different credentials” is checked. Press finish.



You will need to add `rc\` to your username. The requested directory will appear as a drive on your computer. You can get to these files in Cygwin in `/cygdrive/z/`. (Actual path may vary.) Your home directory (`~`) is in `/cygwin64/home/yourusername`.

## Transferring Files (Mac)

*Copying files from your local computer to Odyssey:* In iTerm, at a local prompt (*not* an Odyssey prompt!), type: `scp filename yourusername@ody:/path/to/destination`

*Copying files from Odyssey to your local computer:* In iTerm, at a local prompt (*not* an Odyssey prompt!), type: `scp -C yourusername@ody:/path/to/filename_to_get .`

The `.` will place the remote file in your current directory on your local computer.

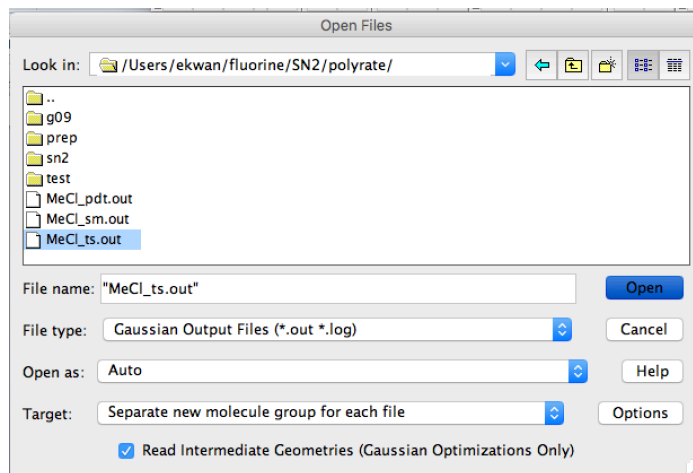
The `-C` flag turns on compression, which helps when moving around big text files.

## GaussView

*GaussView* is the program we will use to create input files and examine output files. (In contrast, *Gaussian* is the program that runs the calculations. *GaussView* runs on your computer; *Gaussian* runs on Odyssey.) You can download *GaussView* from Research Computing here:

<https://downloads.rc.fas.harvard.edu/>

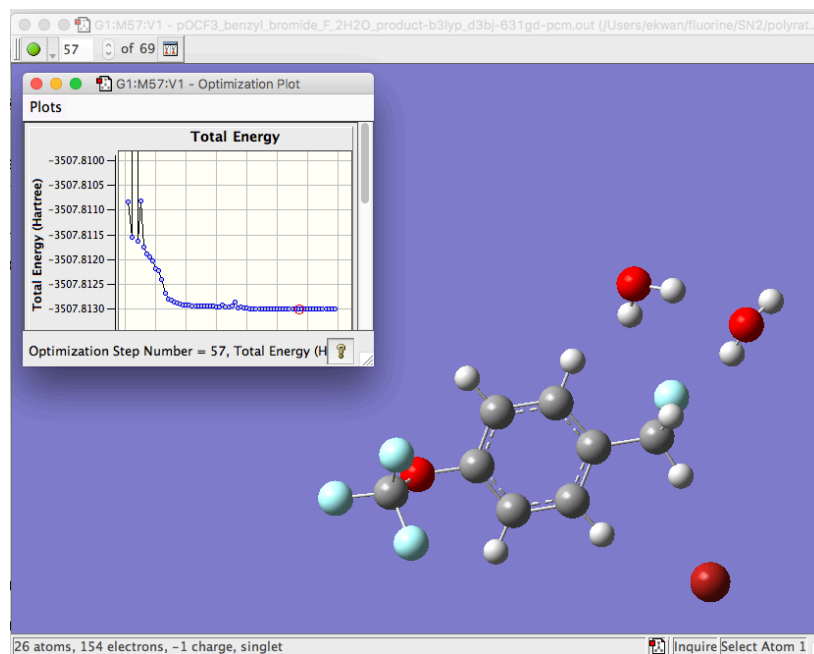
To open a file, select File...Open. You will see a dialog box like this:



Ensure that “File type:” is set to Gaussian Output Files.

Ensure that the “Read intermediate Geometries) box is checked and press open.

Click on Results...Optimization. You will see something like this:



This plots the energy as a function of optimization step. You can click through the different geometries to see how Gaussian minimized the energy of the molecule.

If you performed a frequency calculation, click on the last geometry and go to Results...Vibrations:

Mode #	Freq	Infrared
18	316.23	66.9725
19	339.24	52.9054
20	365.77	43.5371
21	371.62	51.4556
22	407.16	22.3362
23	422.96	39.0303

Animate Vibration:

Start Animation Save Movie...

Animation Frequency: \_\_\_\_\_

Displacement Amplitude: \_\_\_\_\_

☐ Show Displacement Vectors Scale: \_\_\_\_\_

☐ Show Dipole Derivative Unit Vector Scale: \_\_\_\_\_

☐ Manual Displacement: 0.00 Save Structure...

Close Cancel Spectrum Help

Normal modes and frequencies (in  $\text{cm}^{-1}$ ) are listed. You can animate the normal mode displacements by clicking on "Start Animation." This can be helpful for visualizing transition states.

Try transferring the .out files from `~/chem106_calculations/test_job/` to your computer and visualizing them. We will learn how to create and submit calculations in the next tutorial.

## The vi Editor

*vi* is a standard text editor that can be found on any Linux system. It is very fast, ideally suited for terminals and large files, and used by computational chemists and programmers everywhere. Here is a good tutorial: <http://ryanstutorials.net/linuxtutorial/vi.php>

**Alert!** On some systems, there are two related programs, *vi* and *vim*. You want *vim*. You can type `alias vi='vim'` to call *vim* whenever you type *vi*. Add this command to your `~/.bashrc` file to make it a permanent change.

*Open file in vi:*

`vi filename` (if the file does not exist, it will be created)

*To start typing:*

press `i` (enters insert mode)

*To save:*

press `ESC` (enters *vi* mode) : (enters command mode) `w ENTER`

*To quit:*

press `ESC : q ENTER`

*To quit without saving changes:*

press `ESC : q! ENTER`

*To save and quit:*

press `ESC : wq ENTER`

A few other useful commands:

go to beginning of file: `ESC : 1 ENTER`

go to end of file: `ESC : $ ENTER`

delete current line: `ESC dd`

To paste text, press `i F2`. Paste and then press `F2` again. This prevents *vi* from adding tabs to your pasted text.

*Eugene Kwan  
March 2017*