CHEM5302 Fall 2017: Introduction to Maestro and the command line

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1 Introduction

As this course has evolved through the years, the landscape of computational hardware and software has evolved as well. Computational Chemsitry, as with other computational sciences, has rapidly grown and taken advantage of the exponential growth in computational resource and tool development over the past few decades. The remaining classes in this course will consist of computational laboratory experiments (and accompanying lectures) in which you will get a flavor for both the technical details that go into computational experiments, and the type of questions one can attempt to answer using computational experiments.

The labs are built on the conceptual and theoretical foundation you have gained so far in this course, but the labs will also require you to delve into using modern computers in ways that you may be unfamiliar with, such as using a terminal and commandline interfaces and using technical scientific software. This lab will briefly introduce you to common commandline usage and the graphical interface of the main software tool we will use, Maestro.

The Command Line

Most computational science is done on Unix-based operating systems, and a large portion of this work is done using a command line interface. This semester, we will be using MacOS, and you should be able to access the commandline by either:

- using Finder to navigate to `/Applications/Utilities` and double clicking the `Terminal` application, or

- using Launcher and typing `Terminal<Enter>`.

A new window should open, and should have the following prompt:

`mac-ip-addr:~ username$`

From here, any commands you type will appear after the `$`.

We have designed a small scavenger hunt based around the command line. The commands you need to complete it (along with some other helpful commands) are described below. Read through the commands below, or skip the next section to start the scavenger hunt right away.

Basic Commands

Type single terminal commands with spaces separating a command and its arguments and use `Enter` to execute the command. Multiple commands can be entered on the same line when separated by `;` (semicolon).

Some common commands are listed below, grouped by category.

Navigation

`pwd` Displays your current location. Directory levels are separated by `/` (forward slash)

`cd <dir>` Changes your directory. For example, `cd newdir` will change your directory to `newdir` if it exists in your current directory.

  The root, or top-most, directory is denoted by `/`. All other directories can be specified using their path relative to `/`, such as `/home/yourname/chem5302/`, which is called the absolute path of that directory.

  Alternatively, you can move around quickly relative to where you currently are by using the two aliases: `.` represents the current directory, and `..` represents the current parent directory. Thus, `cd ..` and `../../..` move you up a single directory and 3 directories, respectively. Another helpful alias is   which represents your home directory. If you ever get lost, `cd`   will take you to your home.

`mkdir <dir>`

  Makes a new directory relative to the current directory. For example, `cd /home/yourname; mkdir newfiles`   will   create   the   directory `/home/yourname/newfiles`.

`ls <dir>` Lists the contents (files and directories) of the current or specified directory. Use `ls -l` to get more detailed information, such as time last modified.

File manipulation

`cp <src> <dst>`

  Copies files at `<src>` to `<dst>`.

`mv <srv> <dst>`

  Moves files from `<src>` to `<dst>`.

`cat <file>` Output all contents of a file to the terminal.

`less <file>`

  Open a file for viewing. Allows searching and more controlled viewing when compared with `cat`.

`vi <file>` Open a file for editing. `vi` is just one of several editors. Others in Mac OS X include `pico`, `open -e`, `nano`, `vim`, `emacs`, and `/Applications/TextEdit.app`.

`rm <file>` Deletes a file. Be careful, as unlike with some other operating systems, `rm` does not place the deleted file in a trashcan incase you want to recover it later.

`rmdir <dir>`
>
> Deletes an empty directory.

`*,?` Not commands, but wildcard characters. Used to specify patterns of filenames and other text strings in use with other commands. `?` represents any one character, and `*` represents any string of characters. For example, `rm *.txt` will delete all files in the current directory that end in `.txt`. Similarly, `cp ../q??.maegz .` will copy all `.maegz` files that are three characters long starting with q located in the parent directory to the current directory.

(Un)Compression

`zip <dst.zip> <things to be zipped>`
>
> Zip files into `dst.zip`. Add the recursive option `zip -r` to zip entire directories.

`unzip <src.zip>`
>
> Unzip a zip archive.

`tar -cf <dst.tar> <things to be tarred>`
>
> Create a tar archive `dst.zip`. Add the gzip option `tar -czf` to create a tar.gz (tgz) archive.

`tar -xf <src.tar>`
>
> Untar a tar archive. Just as above, add `-z` to extract a tgz archive.

Other

`man <cmd>` Displays the manual or help page for a command.

`ssh <username@remote-host>`
>
> Log into a remote machine using your username and password. Note that if you want to use gui-applications, use the optional flag `ssh -X`.

`scp <src-host:src-files> <dst-host:dst-files>`
>
> Copy files between different computers (hosts).
>
> The two common usages are copying files to a remote machine: `scp local-files username@remote.host.temple.edu:/home/username/dst`, and copying files from a remote machine: `scp username@remove.host.temple.edu:src-files .`
>
> If you want to include directories as well as files, add the recursive optional flag: `scp -R <src-host:src-files> <dst-host:dst-files>`

`curl -O <URL>`
>
> Retrieve a file from a web URL.

CLI Scavenger Hunt

To have you gain some experience with the command line, we have designed a short scavenger hunt using the command line. **Your goal is to download an archive and follow the instructions it contains. All commands that you need to complete this task**

are described above. Further, because you likely won't read everything above, the really important commands are underlined.

Use `curl -O` (capital O as in Orange) on the following URL to download the tgz archive `intro.tgz` into your current directory.

`https://ronlevygroup.cst.temple.edu/courses/2017_fall/chem5302/intro.tgz`

Extract its contents, locate the file `README`, and display its contents for future instructions.

2 Maestro

In your working directory, open Maestro by supplying the command line with its entire path:

`/opt/schrodinger/suites2015-2/maestro &`

Running commands with an ampersand (`&`) after them will run them in the background. This is optional.

Using Maestro

In the main window, you should see both a row of drop-down menus (`File`, `Edit`, etc.) and row of buttons. First, let's set up the main window. Enable toolbars by selecting from the top drop-down menus: `Window → Toolbars`. Enable the following toolbars:

- `View`

- `Edit`

Let's start with a molecule that we can manipulate with Maestro. Under `Edit`, go to `Build` and select `Fragments....` A new window will appear titled `Build`. Currently this window will show `Organic` fragments, but in the `Fragments:` window, you can select other options such as `Amino acids`. Under `Amino acids`, you will see the three letter abbreviation. Click on "ARG" for now. Move the pointer to the view window and left-click. An arginine will appear. Close the `Build` window.

Move and rotate the arginine around with the different mouse buttons. **Note:** When using Mac OSX, you may need to adjust the machine's mouse settings for 2 or 3 button mouse controls to function. To do this, open `System Preferences → Mouse` and change the middle button to `Button 3` and the right button to `Secondary`.

- While pressing the center mouse button, you can rotate the arginine around.

- By pressing the right mouse button, you can translate the molecule.

- By clicking the left mouse button while pointing at an atom, that atom will be selected.

- To unselect that atom, you can click the left mouse button in any blank space.

Furthermore, we can manipulate the view and which atoms are selected and deleted by using the bottons on the `View` and `Edit` toolbars we enabled earlier.

- To recenter the atom, press the button with four arrows pointing to the corners (Fig 2.1a). If you select an atom on the arginine and press the recenter button, Maestro will center about that atom and zoom into it. To unzoom, unselect the atom and press the recenter button.

- You can use the delete button (Fig 2.1b) to delete atoms, molecules, etc. While holding the mouse button down on the X, a drop-down menu will appear letting you delete atoms, bonds, residues, etc. with one click of the mouse in the main viewing window. Select `Atoms` first. By left clicking on an atom, the atom will be erased. Now select `Molecules`. Left click on any atom and the entire arginine will disappear. When finished deleting, press the delete button to turn this feature off.

- You can also use the select button (Fig 2.1c) to turn the delete button off.

Feel free to build many molecules.

One last notable feature is the Project Table. Open the Project Table using the `Table` button on the main menu bar (or keyboard shortcut `CMD + t`. There should be a single entry listed in the Project Table labeled "Structure 1". This entry contains all the molecules that you placed in the workspace. You can display separate entries for each molecule by right clicking on "Structure 1" and selecting `Split → By molecule`. By clicking the square in the "In" column, you can toggle which molecules are displayed in the workspace (hold shift or individually include/exclude by right clicking an entry and selecting `Include` or `Exclude`). When done, select all molecules in the project table so that all entries are highlighted in yellow and press the delete key.

With the window cleared, you are ready to start the first lab. Before you do, make sure you can locate the `Applications` menu at the top of the window. If you do not see the `Applications` menu, enable it by selecting: `Tasks → Application View`.
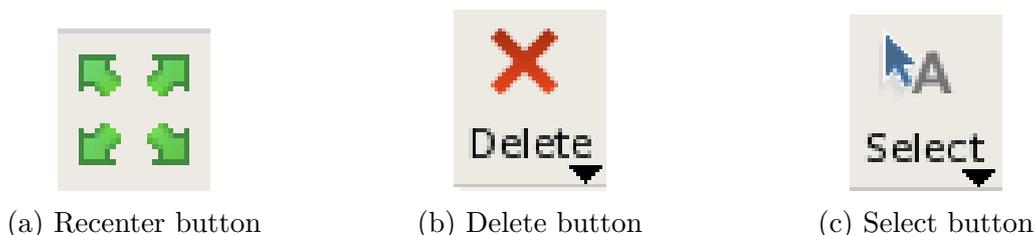

(a) Recenter button   (b) Delete button   (c) Select button

Figure 2.1: View Toolbar buttons