non HiPerGator.md 1/28/2021

An Introduction to the Linux Command Line



Non-HiPerGator version

Last updated: January 28, 2021

This version of the handout is for users who do not have a HiPerGator account. It uses the free repl.it service to run the examples. These instructions *should* work in most Bash environments, so you do not need to use repl.it, it is offered as a suggestion.

Getting Around in Linux

• File paths (directories or folders): /, /home/runner/, /home/runner/crazy_name/

In this documentation, we will use the convention of putting text that needs to be substituted for your specific case in *italic font*.

- pwd, cd, ls (Where am I, change directory, list directory)
- cp, mv, rm (copy, move (also used for rename), delete)
- more, less, head, tail, cat (examine files)
- nano, vim (text editors in Linux)

Note that most things in Linux are case-sensitive. This applies to commands and file names. e.g. CD test will not work to change directories to the "test" folder, while cd test will work (assuming there is a folder named "test" in the current folder). Similarly, Test and test are different folders or files.

Making Things Easier

- **Tab completion** type part of a path or file name and hit tab-key, the shell will auto-complete for you.
- history: redo something that you did before without retyping (use arrow key)
- man: getting help. Many built-in Linux applications have manual pages that document their use and options that they have. e.g. man ls will bring up the page for the ls command, documenting the many options that change how the ls command functions.
 - Another way to get help information about applications is using the name of the application followed by either the -h or --help flags. Many applications use this convention to provide documentation to users.

Learning by Doing

(Note: some of the data and examples are taken from software-carpentry.org):

- 1. Connect to a repl.it Bash server:
 - 1. Navigate to https://repl.it/
 - 2. Click on the <> Start coding button

non HiPerGator.md 1/28/2021

3. In the Create new repl Language selection window, type "Bash", select that, and click Create repl.

- 4. When the repl opens, for the most part we will focus on the command prompt on the right-hand side. You can resize that pane to get some more room to work.
- 5. Copy and paste (you will probably need to use right-click to paste) this command to get a copy of these notes and the data for the exercise: git clone

```
https://github.com/UFResearchComputing/Linux_training.git
```

- 2. Where are you when you login? pwd
- 3. What files are there? 1s
- 4. Let's make a directory to put some data in: mkdir cli demo
- 5. Now what's there? 1s -1
 - 1. Linux commands usually have flags to change how they work
 - 2. man, -h or --help often give you help
- 6. Change into cli_demo directory: cd cli_demo or cd cl-Tab-key
- 7. Copy some demo data here (.):

```
cp -r ../Linux_training/data/molecules .
```

- 1. Note the -r to recursively copy, since cp won't copy directories by default
- 2. Also note the "." at the end to copy the molecules directory to your current location.

You could use the copy in the repository you cloned, but this keeps the directions in parallel with the directions for users on HiPerGator and practices the mkdir and cp commands. This folder originated from the software-carpentry Shell Training materials.

- 8. Check that the copy worked: 1s
- 9. Change directories into the molecules directory: cd molecules
- 10. Look at these files with more, cat, head, tail:

```
1. more propane.pdb and cat propane.pdb
```

- 2. head propane.pdb or head -n2 propane.pdb
- 3. tail propane.pdb or tail -n2 propane.pdb
- 11. **Redirects**: You can redirect the output of a command to a file with the > character (see below for more information about STDIN, STDOUT and STDERR). *Caution: This erases the file you are redirecting to first if it exists, replacing it with the new contents.* **You can** *append* **to a file with >>**.
 - 1. As an example, we can get the lengths, in number of lines, of all the files ending in .pdb using the wildcard * and redirect the output to a file: wc -1 *.pdb > lengths.txt
 - 2. Let's see what this file looks like: cat lengths.txt

Wildcard expansion (e.g. *.pdb) is a convenient way to operate on a list of files matching some characteristic: e.g. having the .pdb ending, starting with "p" (p*), etc. The wildcard is evaluated and the list of matching files is passed into the command.

non HiPerGator.md 1/28/2021

- 12. **Sorting**: We might want the lengths sorted: sort -n lengths.txt
 - 1. What happens without the -n?
- 13. Pipes: We can connect commands together by piping the output from one command into the input for the next command using the vertical bar character " | ":

The pipe character, "|", is typically located above the Enter-key on your keyboard with the "\" and is accessed with the Shift-key

```
1. wc -1 *.pdb | sort -n > lengths.txt
2. Or if we only want to know the shortest file: wc -1 *.pdb | sort -n | head -n1
```

Why this works: Most Linux programs can take input from what is called "standard in", often abbreviated as "STDIN". In addition, they typically have *two* output streams, "standard out", "STDOUT", and "standard error", "STDERR"--both of which print to the screen by default, but can be redirected as we saw above (in fact we only redirect STDOUT with the >; any STDERR would still print to the screen).

So, while you can run a command like wc -1 propane.pdb, you can also get the same result by running the cat command and "piping" the STDOUT of that to the STDIN of wc: cat propane.pdb | wc -1. Similarly, you can keep piping commands connecting the output of one command to the input for the next command.

14. grep: We can search for text using grep:

```
1. grep ATOM propane.pdb
```

15. awk: awk can do a lot, but one thing it's good it is pulling out columns from files, in this case the 3rd column:

```
1. grep ATOM propane.pdb | awk '{print $3}'
```

- 16. *uniq*: uniq is a command to find unique entries in a **sorted** list: grep ATOM propane.pdb | awk '{print \$3}' | sort | uniq
- 17. **Loops**: One of the great things about the command line is the ability to automate repetitive tasks. Let's say we want to verify that all our molecules are hydrocarbons (made up of only C and H atoms). Below is what the loop looks like neatly spaced out as if it were in a script:

```
for molecule in *.pdb
do
  echo $molecule
  grep ATOM $molecule | awk '{print $3}' | sort | uniq
done
```

As we type this in on the command line, once you hit the Enter-key at the end of the first line, Bash gives you the continuation prompt, ">", essentially telling you that you have started a command (a for loop), but not finished it:

non_HiPerGator.md 1/28/2021

```
[user@login1 molecules]$ for molecule in *.pdb
>
```

You can keep typing the rest of the lines, so that it looks like this:

```
[user@login1 molecules]$ for molecule in *.pdb
> do
> echo $molecule
> grep ATOM $molecule | awk '{print $3}' | sort | uniq
> done
```

Once you hit the Enter-key after the "done", that completes the for loop and Bash executes it, showing the output.

If you find yourself stuck in the continuation prompt mode, you can use the key combination Ctrl-C to cancel and exit back to the main command prompt. Ctrl-C will usually cancel execution of a program in Bash and is a handy key-combination to know!

- 18. **Deleting files**: Let's get rid of the lengths.txt file: rm lengths.txt
 - 1. That file is now gone!! There is no undo, no recycle bin or trash can. As soon as you type the command and hit return, the file is gone!
 - 2. Be careful... but don't keep everything forever either!

Additional exercises

- Which molecule has the most H atoms?
- Make a directory in your cli_demo folder and copy the methane.pdb file there (preferably without moving from the molecules directory)
- From the molecules directory, get the head of the methane.pdb file in the directory you created above
- Change directories to the directory you made above, rename the methane.pdb file to my_methane.pdb.
- Edit the my_methane.pdb file and put your name as the AUTHOR. I typically recommend the nano text editor on the command line for new users: nano my_methane.pdb and use the arrow keys to move around. The commands at the bottom of the screen use the Ctrl-key in combination with another key, so ^X means hold down the Ctrl-key and the X-key at the same time to exit.
- How many ATOMS does methane have?
- Use an SFTP program to download the molecules folder to your computer