
The Shell

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COURSE

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INTRODUCTION

Welcome to our introduction to using the Bash shell. This session is composed of two three-hour sessions

- June 4 from 9:00-12:00 and 13:30-16:30 (Eastern Daylight Time)

and each session is a series of short live demos and exercises.

Each part builds on the previous parts, so it is best to attend the entire thing from start to end and to do the complete the exercises. While we are starting assuming no prior knowledge of the command line, we will go quite far, so do not be off put if things seem pretty basic at the start.

Our training website <https://training.computeontario.ca> has links to a readable version of today's presentation in web, pdf, and epub format. You do not have to worry about taking notes or falling behind.

If you don't have a Digital Research Alliance of Canada account to access the nimbi cluster, you can use our summer school Magic Castle training cluster. Get your username and password under the *Magic Castle Username and Password* link in the morning session, and substitute `nibi.alliancecan.ca` with `cos2026a.c3.ca` in what follows.

1.1 BigBlueButton and Etiquette

Before getting started, we would like to introduce you to the online platform BigBlueButton and discuss the online etiquette that we expect throughout the workshop.

First I would like to ask everyone to mute their microphone. You can do this by click the *microphone icon*. The *microphone icon* is in the far left of the menu bar on the bottom of the BigBlueButton window. You know your microphone is muted when you see a slash through the *microphone icon*.



It is good etiquette to leave your microphone off unless you are speaking as otherwise everyone will hear the background noise from your space, and we will be forced to mute you, which is something you cannot undo. If you want, you can also turn off your video by clicking the *video camera icon* to the immediate right of the microphone icon. A slash through indicates it is off too.

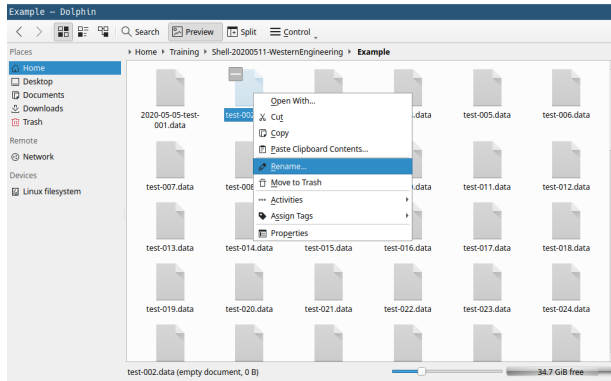
There is a public chat messaging system in the upper left. Feel free to use this to ask any questions you may have during the presentation. Our staff members are monitoring this and will respond. Also note that there is a maximize button in the upper right of the main window that will expand the content to fit the main window.

On the subject of etiquette, we want to maximize learning in these sessions by creating a welcoming and supportive environment for everyone regardless of background, identity, or knowledge level. Please be mindful to not engage in any behavior that is going to diminish the experience for any of the participants or the instructors.

1.2 Motivation

We are going to teach you the old school way of running your programs and processing your data with your keyboard and commands and not your mouse and menus. In the process, we hope that you will discover that the keyboard and commands, far from being archaic, are actually very well suited for automation and keep track of what you have done to repeat it or communicate it to others in the future.

As a small example, say we had collected 100 *.data* files in the *Example* folder and wanted to prefix them with today's date. This would be a long tedious point and click session using a GUI



Using the command line though, it would only be four simple lines and complete in less than a second

```
today=$(date +%Y-%M-%d)
for file in *.data; do
    mv $file $today-$file
done
```

It would also be trivial to save these lines in a file for future reference, share with a colleague, or incorporate them into a bigger set of commands to do more complex operations on the files. This last point is key. The command line composes. You can combine small bits into big bits, and big bits into bigger bits. This is extremely powerful. GUIs do not compose.

COMMAND LINE

The command line is a text interface on a computing system into which we type commands to tell the computer what to do. In times past this would be done via a dedicated monitor and keyboard combination called a terminal. This has been replaced with a program that emulates these old system and provides us a window into which we can type.

The command line program that we will be learning is the Bash shell. It is the descendant of a long line of shell programs, and it is specialized to help us manipulate our file, start programs, and automate tasks involving these things. It is also the only way to run jobs on the Canadian supercomputers.

I will be demonstrating everything on the supercomputers in order to help you become more familiar with them. Almost everything in this course does not require the supercomputers though, so there is no need for you to use them unless you would like the practice.

Under both Linux and Mac OS X, you can start up a Bash command line session by starting a terminal program (search for terminal in your applications menu). The default command line interface in Windows is the older Command Prompt or the newer Power Shell. To use Bash you need either install the Windows Subsystem for Linux (a full Linux installation) or Cygwin (a collection of UNIX programs, including Bash, compiled for Windows).

For this course, it is sufficient to install the free version of MobaXterm (a popular with our Windows users). It includes a basic Cygwin installation along with a graphical file transfer program that lets you click-to-edit and drag-and-drop to transfer files when connected to the supercomputers. An even lighter option is to install the *secure shell installable component* (this requires Windows 10 or later, for earlier versions you can use the standalone PuTTY program). Then you can secure shell from the Windows Command Shell to the supercomputers and use Bash there.

- MobaXterm - <https://mobaxterm.mobatek.net/>
- Secure Shell - https://docs.microsoft.com/en-us/windows-server/administration/openssh/openssh_install_firstuse
- PuTTY - <https://www.chiark.greenend.org.uk/~sgtatham/putty/latest.html>

2.1 Secure Shell

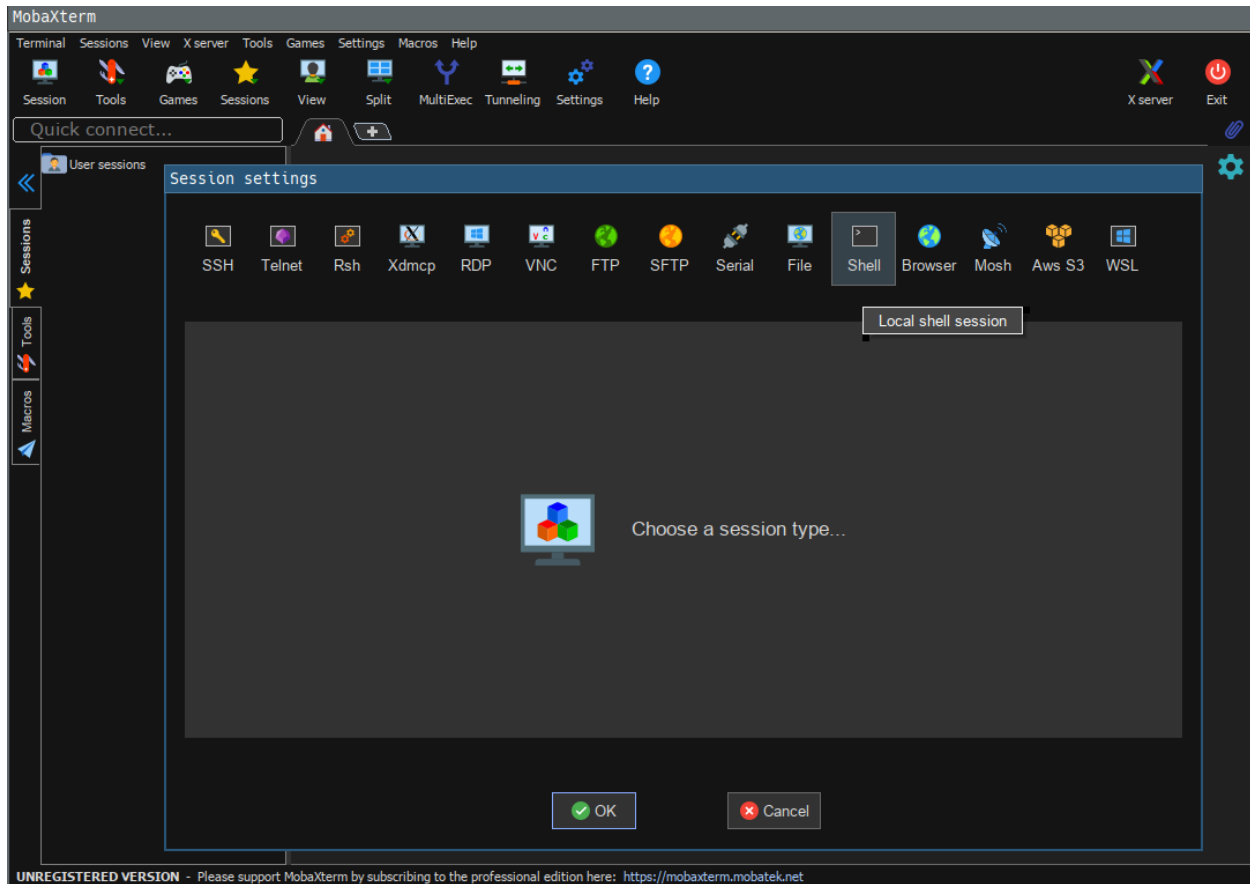
The Canadian supercomputers can be access from anywhere there is internet access using the address *<supercomputer>.alliancecan.ca* and the *secure shell* client suite of commands

- `ssh` - used to run commands (secure shell)
- `scp` - used to copy files (secure copy)
- `sftp` - alternative to copy files (secure file transfer protocol)

As a demonstration of our first command, I am now going to show how to connect to the SHARCNET supercomputern ibi from a local shell session on your computer using the `ssh` command. Connecting to the supercomputer is not required for this course (unless you are using Windows and haven't installed MobaXterm), but it is required to use the supercomputer, so it is good practice.

The Shell

First we need to open our terminal program. For Linux and Mac OS X, the terminal program can be found by searching for *terminal* under the applications menu. For Windows, if you installed MobaXterm, click the *Sessions icon* in the upper-left, and then click the *Shell icon* the middle-right. If you installed the *secure shell installable component*, start the *Command Shell* under the applications menu. If you have installed PuTTY, start it.



To connect with PuTTY, we type `nibi.alliancecan.ca` into the *Host Name* box and then press *Open*. It will then prompt for my username and password and then give us a terminal that is connected to *nibi* and running the *bash* (the default *nibi* shell). For all other methods we start with a terminal on our local computer running our local shell (generally *bash* or a *bash* based derivative). The shell, which is also referred to as the *command line* or the *terminal*, does what is known as a *read-evaluate-print-loop (REPL)*. That is, it interacts with us by

- (R)eading a command from me,
- (E)valuating the command,
- (P)rinting the results of the command, and
- (L)oooping (reads the next command, etc.)

A *Bash* command is generally the name of the program to run followed by any information that program needs to be told in order to do its thing. Assuming we aren't running PuTTY and already connected to *nibi*, we need to run *ssh* and tell *ssh* to connect to *nibi.alliancecan.ca* with our *nibi* username. So I type

```
[tyson@tux:~]$ ssh tyson@nibi.alliancecan.ca
```

(*tyson* is my *nibi* username) and press enter. This brings us to the second step. The computer runs the *ssh* command. The *ssh* command prompts for a password (note there are no stars when typing it in), logs into the *nibi* supercomputer, and starts a new *command line* session inside my existing one.

When we are done running commands on nibi, type

```
[tyson@l1.nibi ~]$ exit
```

This causes the command line session on nibi to complete, and, in turn, the ssh command ran on our local computer to also complete. This brings the local computer to the loop phase, and it will then prompt for our next command. We can enter another command for the local computer or type `exit`, which will cause the the local session to also end and close the terminal application.

2.2 Data storage

Now we are going to review the basics of data storage on computers. Data is stored in a hierarchical tree structure. For this course we will be working with some data we can download using the `wget` (web get) command

```
[tyson@l1.nibi ~]$ wget https://staff.sharcnet.ca/tyson/flights.zip
```

You don't need to exit from nibi at the end as I did as will continue using it with our next exercise. Note also that the alliance wiki page contains details pages on using ssh, PuTTY, and MobaXterm. or the `curl` command (in the event your system doesn't have `wget`)

```
[tyson@l1.nibi ~]$ curl -LO https://staff.sharcnet.ca/tyson/flights.zip
```

We can then unpack this file using the `unzip` command

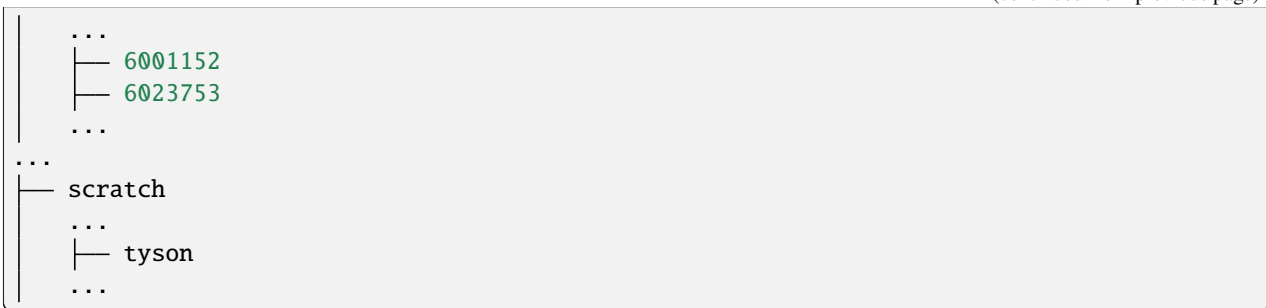
```
[tyson@l1.nibi ~]$ unzip flights.zip
```

which leaves me with this tree of files and folders (much of the details outside of the unpacked flights folder are specific to Linux and our supercomputer storage layout and will be different for your personal computer)

```
/
├── home
│   ├── ...
│   └── tyson
│       ├── flights.zip
│       ├── flights
│       │   ├── 0144f5b1.igc
│       │   ├── 2191bc99.igc
│       │   └── ...
│       ├── nearline
│       │   ├── def-tyson -> /nearline/6001152
│       │   └── def-tyson-ab -> /nearline/6023753
│       ├── projects
│       │   ├── def-tyson -> /project/6001152
│       │   └── def-tyson-ab -> /project/6023753
│       └── scratch -> /scratch/tyson
│   └── ...
├── ...
├── nearline
│   ├── ...
│   ├── 6001152
│   └── 6023753
│   └── ...
├── ...
└── project
```

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- file - named piece of data
- folder - container holding files and further folders
- link - a reference to another file or folder

Before the graphical analogy to a filing system, folders were called directories, and this is reflected in the names of command line commands (e.g., change directory, print working directory, etc.), so we will use that.

To specify a piece of data, we need to specify both the file name the data is stored under and the series of directories (folders) that that filename is stored under. It isn't sufficient to tell someone (or the computer) just the filename as they would then have to look through all the folders to find it, and they very well might find another file with the same name in a different directory (folder).

To uniquely specify a piece of data we, therefore, have to specify all the parts from the start. For example

- start at the start
- under the *home* directory
- under the *tyson* directory
- under the *flights* directory
- the data is in the *0144f5b1.igc* file

When writing this down, we separate all the components with a / and call it a path because it gives the path to follow through the directories to locate the file. A leading / says the path is absolute as it starts at the very start. The above example would be */home/tyson/flights/0144f5b1.igc*.

Frequently we are only referring to files relative to some common starting point, such as the location of my person storage */home/tyson*, in which case we call it a relative path and do not include the leading /. The above example would be *flights/0144f5b1.igc*.

When working with data on another computer, we need to specify not only the full file path to the data, but also computer it is on, and the username to use to login to that computer to get it. An example might be *tyson@nibi.alliancecan.ca:/home/tyson/flights/0144f5b1.igc*

You may be more familiar with a Windows file specifications, which would look something more like *C:\Users\Tyson\Desktop\flights\0144f5b1.igc*. The key difference here is that in Windows uses \ instead of / to separate the components and explicitly specifies the physical location of the storage at the start of the path with a drive letter like *C:*.

There are also no drive letters with Linux. The physical storage is implicit in the path. When I plugin a USB stick, for example, a new path like */media/tyson/80BC-6336* shows up under which I can access all the files and directories on that USB stick. The *mount* command can be used to view what storage is under what paths, but we won't be plugging any USB sticks into the supercomputers, so we will leave it at that.

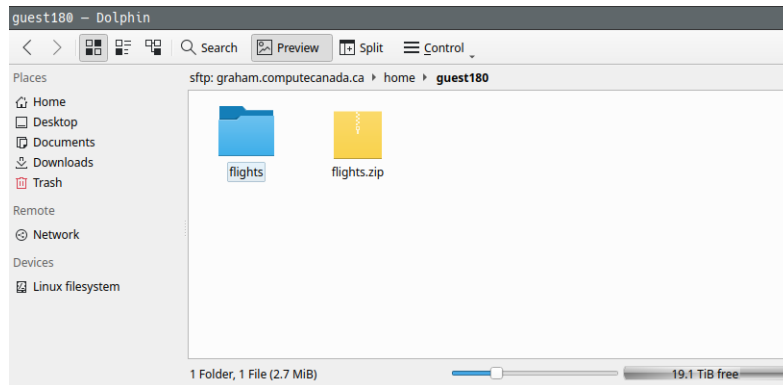
2.2.1 Exercises

Doing the following exercises help ensure you understand the course material. The results of some of the later ones are needed to answer the course completion quizzes.

1. The `tree` command displays a tree view of your directories and files. Run it and see if the results are what you expect (note this command may not be available on your personal computer).

2.3 Getting around

Under a GUI we navigate our folders (directories) and files with a file manager. A typical graphical file manager shows us the path of the folder we are viewing and its contents as a series of icons



Like a file manager, the command line has a directory (folder) that it is currently in. We call this the working directory, and the `pwd` (print working directory) command will tell us what it is

```
[tyson@l1.nibi ~]$ pwd
/home/tyson
```

We so frequently want to refer to files relative to our home directory, that the command line provides `~` as shortcut to means `/home/tyson`. With this information, you can see that the command line is actually configured to tell us exactly where we are every time we enter a command. That is, `[tyson@l1.nibi ~]$` is saying the command you enter is going to run

- under the user *tyson*
- on the computer *l1.nibi*
- in the directory */home/tyson*

If you become a power user with many terminals open at once, you will appreciate this information in your face every time you enter a command.

The file manager also shows us each of the files and folders (directories) in its working directory. The `ls` (list) command does the same in the command line

```
[tyson@l1.nibi ~]$ ls
flights  flights.zip  nearline      projects  scratch
```

If we hover our mouse over a file or folder or right click and picking *properties*, we can get extra details about a file or folder, such as the day it was created, its size, and the access permissions. The `ls` command will also provide this information to us if we ask it to with the `-l` (long) switch

```
[tyson@l1.nibi ~]$ ls -l
total 2804
drwxr-xr-x 2 tyson tyson    141 Mar  1 2018 flights
-rw-r----- 1 tyson tyson 2794605 Mar  2 2018 flights.zip
drwxr-xr-x 2 root  tyson     4 May 24 23:47 nearline
drwxr-xr-x 2 root  tyson     4 May 24 23:47 projects
lrwxrwxrwx 1 tyson tyson    14 May 24 23:47 scratch -> /scratch/tyson
```

The file manager lets us open the file by double clicking on it, or right clicking and picking *open with*. For example, double clicking on the *flights.zip* will likely open it in the zip extractor program and let us unpack it. We have already seen how to do this with the command line when we ran the command `unzip flights.zip`.

The file manager also lets us go into the other folders (directories) in the current folder (working directory) by single or double clicking on them. The command line provides a `cd` (change directory) command to do this. For example, the equivalent of going into the *flights* folder and looking around would be

```
[tyson@l1.nibi ~]$ cd flights
[tyson@l1.nibi flights]$ pwd
/home/tyson/flights
[tyson@l1.nibi flights]$ ls
0144f5b1.igc 2191bc99.igc 4620f232.igc ...
```

You will note that when we moved into the *flights* directory, the prompt changed from `~` (the abbreviation for */home/tyson*) to *flights* to reflect the fact that we are now in the *flights* folder. In the file manager, we can click a prior part of the path (or the back arrow) to return to where we were. The command line provides a special folder called `..` that refers to the parent folder to allow you to go back

```
[tyson@l1.nibi flights]$ cd ..
[tyson@l1.nibi ~]$ pwd
/home/tyson
```

This is actually baked right into the operating system, it just isn't normally shown as files and folders that begin with a period are not shown unless the `-a` (all) flag is used

```
[tyson@l1.nibi ~]$ ls -a
.  ..  .bash_history  .bash_logout  ...
```

It is good to know this as many time special things like configurations are stored under files or folders with a leading dot in order to not cluttering up your regular listing. You can also see there is a `.` in addition to the `..` directory. The `.` directory is the directory itself. This is convenient as we frequently want to tell a command to do something to this directory (i.e., copy the files from some place to this directory).

With the file manager we could create a new folder called *downloads* by right clicking and picking *create new -> folder* and then copy the *flights.zip* file to it by dragging it over and dropping it on the new *downloads* folder icon. With the command line we can make a new folder with the `mkdir` (make directory) command and copy the *flights.zip* file to it with the `cp` (copy) command

```
[tyson@l1.nibi ~]$ mkdir downloads
[tyson@l1.nibi ~]$ cp flights.zip downloads/
```

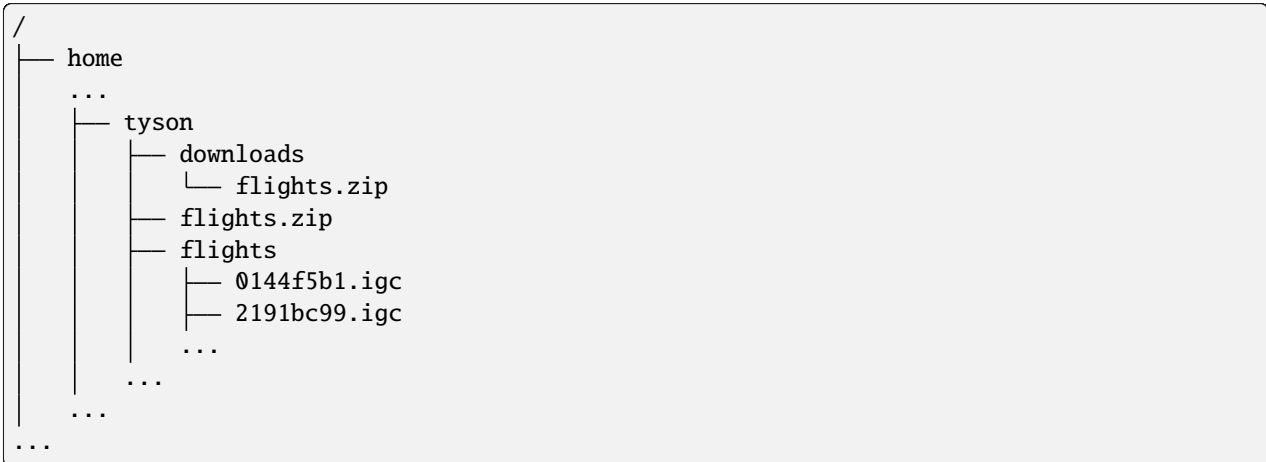
where for copy like commands you generally specify one or more source followed by a destination separated by spaces. The trailing `/` on the destination is optional, but it makes it unambiguous that *downloads* is suppose to be a directory to a copy of the *flights.zip* file in. Without the trailing `/` the `cp` command determines whether *downloads* is a folder to put it based on checking to see if *downloads* is an existing directory or not.

We have put together a quick reference guide to many of the common (and not so common) commands and options for you to refer to (see the reference link in the course index) as the goal of this course it not to put you to work memorizing a bunch of commands. The commands you frequently use will commit to your memory soon enough through regular usage without any effort on your part. You can look up the others when you need to.

2.3.1 Exercises

Doing the following exercises help ensure you understand the course material. The results of some of the later ones are needed to answer the course completion quizzes.

These exercises assume the following file and directory layout that exists after the previous demonstration (adjusting *tyson* to your username)



Discuss your answers and test them out to verify if you are correct or not.

1. The full set of options for a command can be found in the manual page. The command `man <command>` (e.g., `man ls`, `man cp`, etc.) will bring up the manual page for a command. Use the arrows and page up/down keys to scroll around, `q` to quit, and `/<text>` to search for `.`. Using the `ls` manual page, answer the following questions
 - a. What does the command `ls -lh` do?
 - b. What does the command `ls -R` do?
 - c. How do you sort by last modified date?
2. Starting from `/home/tyson/flights` directory, which of the following commands can be used to switch to the home folder (remember `..` goes the parent directory and `.` stays in the same place)?
 - a. `cd .`
 - b. `cd /`
 - c. `cd /home/tyson`
 - d. `cd ..`
 - e. `cd ~`
 - f. `cd home`
 - g. `cd ~/flights`
 - h. `cd`
 - i. `cd ../../tyson`

3. If `pwd` displays `/home/tyson/flights`, what does `ls ../downloads` display?
 - a. `ls: cannot access './downloads': No such file or directory`
 - b. `downloads flights flights.zip`
 - c. `0144f5b1.igc 2191bc99.igc ...`
 - d. `flights.zip`
4. The `rmdir` (remove directory) command removes a directory. Trying to remove the `downloads` directory gives

```
[tyson@l1.nibi ~]$ rmdir downloads
rmdir: failed to remove 'downloads': Directory not empty
```

This implies we have to empty the directory first with the `rm` (remove) command. Fortunately `rm` has an option that will remove everything in one go. Use the manual page to figure out the required command.

5. How can the `mv` command be used to rename `flights.zip` in `/home/tyson` to `flights-downloaded.zip`?

2.4 Technicalities

Now that we have run some commands, and had a look at some of the manual pages, we are going to take a moment to step back discuss some of the technicalities and syntax. The command line we are using is called *bash*. This is an acronym for Bourne-again shell, which is a word play on the original Bourne shell from which it descended. There are many shells, including the original *sh*, *ksh*, *csh*, their decedents *ash*, *bash*, *dash*, *tcsh*, and the even newer *zsh* and *fish*.

The subject of what shell to use can be somewhat of an almost religious issue for some. We are learning *bash* as it is the most widely used and the default on most system. It is bit crufty due to its extended history, but works well. The biggest gotchas with *bash* is that variable expansion also undergoes word splitting and pathname expansion unless quoted. This means many people's scripts do not properly handle filenames with spaces in them. Neither *zsh*, which is very compatible with *bash*, nor *fish*, which is not, have this issue.

In the command line quick reference we have stated that programs are run by specifying the command followed by the arguments separated by spaces. That is

```
[tyson@l1.nibi ~] <program> [argument] ...
```

When we write something this way, it is not something you are suppose to type in literally. Rather it is a syntax specification that tells you how to put together the required components when specifying your command. You need to replace the items in the angle and square brackets with what they describe.

That is, `<program>` should be replaced by the *the name of the program you wish to run* (e.g., `ls`), and `[argument]` should be replaced by the *argument you wish to provide to the program* (e.g., `-l`). The difference between the `<>`s and `[]`s is that the former has to be present while the later is optional. That is, a command must included a program to run, it does not need to include an argument. The full syntax is

- `<xyz>` - *xyz* is required
- `[xyz]` - *xyz* is optional
- `<xyz> ...` - *xyz* is optionally repeated (more of the same)
- `<xyz> | <uvw>` - either *xyz* or *uvw* but not both

With this in mind, we can now see that saying the syntax for a command line is `<program> [arguments] ...` means a command is a required program name followed by any number of optional arguments (including none) separated by spaces.

Sometimes type faces or capitalization are also used to indicate what parts of a statement are suppose to be typed exactly as is and what parts are suppose to be substituted. Running `man cp` to bring up the manual page for the `cp` command gives the following three ways the `cp` command can be used

```
cp [OPTION]... [-T] SOURCE DEST
cp [OPTION]... SOURCE... DIRECTORY
cp [OPTION]... -t DIRECTORY SOURCE
```

We can see that this manual page is using capitalization instead of angle brackets to specify what parts are suppose to be substituted with what they describe. From this we see there are actually three distinct modes in which `cp` can run, and all three allow any number of the options (e.g., `-a`, `-b`, `-d`, `-f`, etc.) to be specified. The first is when you specify only a source and destination file name, as in

```
[tyson@l1.nibi ~] mkdir example
[tyson@l1.nibi ~] cp -T flights-downloaded.zip example/flights.zip
```

This make a copy of the *SOURCE* file called *DEST*. We have provided the optional `-T` parameter in this example. This doesn't do anything unless *DEST* happens to exist as a directory. In this case `cp` will provide an error instead of assuming you are invoking the second variant of the command.

```
[tyson@l1.nibi ~] cp -T flights-downloaded.zip example
cp: cannot overwrite directory 'example' with non-directory
```

Without this option, we would inadvertently invoke the second form of the `cp` command which copies one or more files into a destination directory, as in

```
[tyson@l1.nibi ~] cp flights/0144f5b1.igc flights/2191bc99.igc example
```

The final is the same as the second except you specify the destination directory first

```
[tyson@l1.nibi ~] cp -t example flights/0144f5b1.igc flights/2191bc99.igc
```

again this is provided only to ensure you don't accidentally invoke the first form when you really wanted the second form.

```
[tyson@l1.nibi ~] cp -t examplee flights/0144f5b1.igc flights/2191bc99.igc
cp: failed to access 'examplee': No such file or directory
```

One final nice feature of `bash` is that it has a history of prior run commands and does completion of commands and filenames. Pressing the up and down arrow keys will scroll through your previously run commands so you can edit and rerun them without having to type them all back in. Pressing the `tab` key partway through a filename or command will complete it up to the first ambiguity. Pressing `tab` key again will display all possibilities. For example

```
[tyson@l1.nibi ~] r<PRESS TAB TWICE>
Display all 158 possibilities? (y or n) y
ranlib reduce_test ...
[tyson@l1.nibi ~] rm -fr exa<PRESS TAB ONCE>
[tyson@l1.nibi ~] rm -fr example/
```

where we are abusing our angle bracket and capital notation to tell you to press the `tab` key. I would strongly recommend forcing yourself to use *tab competition* throughout this workshop as, once it becomes second nature, it will vastly improve the speed with which you can run commands.

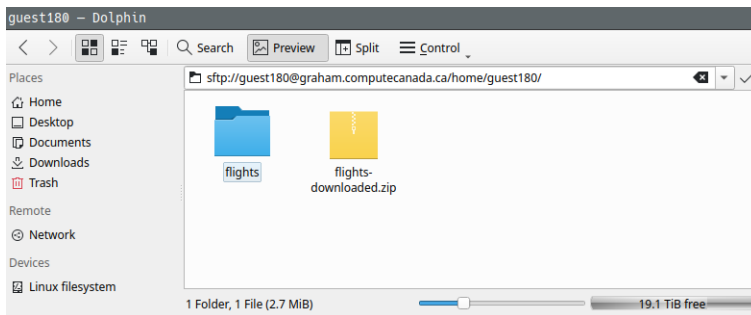
2.5 Transferring files

The other use of the *secure shell* client programs is for transfer files. The `scp` (secure copy) command is basically a version of the `cp` command where you can specify a remote computer as the source or destination. As an example of this command, I will end my session on `nibi`, which returns me to the command line on my local Linux computer, and use the `scp` command to copy the `/home/tyson/flights/0144f5b1.igc` file from `nibi`

```
[tyson@l1.nibi ~] exit
[tyson@tux:~]$ scp tyson@nibi.alliancecan.ca:~/flights/0144f5b1.igc .
```

Note that I've used `.` as the location to copy the file to, which means the working directory.

There are also many graphical applications, such as MobaXterm and WinSCP under Windows, that use the *secure file transfer protocol* (`sftp`) in the background to let you simply drag and drop files between your computer. Most Linux file managers also have this ability built into them and you simply needs to specify the remote path to accessing using the special `sftp://<user>@<computer>/<path>` URL



You may need to setup your *secure shell* client with a secure shell key so it can login to `nibi` without using a password for this work. See the alliance documentation wiki for details on how to do this.

Linux and Mac OS X (if you install `FUSE for macOS`) also have the the ability to splice a remote file system into your local file system using the `sshfs` command. For example,

```
[tyson@tux:~]$ mkdir nibi
[tyson@tux:~]$ ls nibi
[tyson@tux:~]$ sshfs tyson@nibi.alliancecan.ca:/home/tyson nibi
[tyson@tux:~]$ ls nibi
flights flights-downloaded.zip
```

This is quite powerful as you can then do anything you can do with local files on the remote files. Examples include simply using the standard `cp` (copy) command to copy them to a local path

```
[tyson@tux:~]$ cp nibi/flights-downloaded.zip .
```

or even directly edit them in your standard editor. Of course they will take longer to access though as they are actually being transferred back and forth under the hood using the *secure shell* system. The `fusermount` command with the `-u` option un-splices the remote file system

```
[tyson@tux:~]$ fusermount -u nibi
[tyson@tux:~]$ ls nibi
```

2.5.1 Exercises

Doing the following exercises help ensure you understand the course material. The results of some of the later ones are needed to answer the course completion quizzes.

1. Transfer some of the *.igc* files in the *flights* directory to your computer. Have a look at them in your text editor and view them in the [online IGC file viewer](#). We will be using command line tools to automate processing of these files shortly.
2. The `rsync` command is very useful when working on multiple computers. An example of typical usage might be

```
[tyson@tux:~]$ rsync -e ssh -auvP tyson@nibi.alliancecan.ca:/home/tyson/flights .
```

Use the `rsync` manual page to describe what this command does.

3. What advantage does `rsync` have over using `-r` with `scp` to recursively copy all files and directories?
4. Would it be easier to automate dragging and dropping new files or running an `rsync` command for weekly updates?

COMPOSITION

As has already been hinted at, the power of the command line system is not so much how amazing (or not) the individual commands are, but how well those commands can be easily combined together to give new desired behavior. The reason for this is, in any graph, the number of edges can grow much faster than the number of nodes.

That is, consider a system with just 10 programs. If these programs can only be used independently of each other, as is often the case with GUI programs, then we have 10 programs that we can run. If each of these programs can be combined with one of the others though, then we also have $10 \times 9 = 90$ compositions we can run. Further, when we get another program, if it only stands on its own, then we have increase our options by 1 (from 10 to 11). If it can be combined with the others though, then our combinations increases by 20 (from $10 \times 9 = 90$ to $11 \times 10 = 110$).

In order for programs to compose, they need to talk a common language. In Linux, with its Unix heritage, this is text. As Doug McIlrory, who invented Unix pipes said,

This is the Unix philosophy: Write programs that do one thing and do it well. Write programs to work together. Write programs to handle text streams, because that is a universal interface

The other universality you will find in Linux is a huge amount of information about the operating system itself is exposed as text files. This allows all programs to consume and manipulate this information. To quote the Unix Architecture page on Wikipedia

With few exceptions, devices and some types of communications between processes are managed and visible as files or pseudo-files within the file system hierarchy. This is known as *everything's a file*.

As a simple example of this lets look at the `/proc/cpuinfo` and `/proc/meminfo` files using the `cat` command which prints all the files it is given to the screen one after another (concatenates them together)

```
[tyson@l1.nibi ~] cat /proc/cpuinfo
processor       : 0
vendor_id     : GenuineIntel
cpu family    : 6
model        : 79
model name    : Intel(R) Xeon(R) CPU E5-2667 v4 @ 3.20GHz
...
[tyson@l1.nibi ~] cat /proc/meminfo
MemTotal:    131624960 kB
MemFree:     27484820 kB
MemAvailable: 53464260 kB
SwapCached:  42912 kB
...
```

Having all this information available to us as simple text files gives us a lot of power in our shell. Things that would be only available by writing a program to make a special operating system (OS) call in another OS, can be retrieved and manipulated with our basic file commands like `cat` in our shell.

3.1 Viewing and editing

One of the challenges in preparing a course is to come up with interesting examples. Several years ago, my wife's cousin took her flying in a glider. She really enjoyed the experience, and a couple of years ago we joined the London Soaring Club to learn how to fly gliders too. This has proven to be a lot of fun. To give you a better visual, here is a random picture from the internet of a trainee in a two-seater trainer (the instructor sit in the seat behind you).



The gliders all have GPS trackers in them, and the club has a variety of awards that are awarded each year based on the traces (e.g., who gained the most altitude, who flew the furthest, etc.). Going through these files by hand is a tedious chore, but it is easy to automate with the command line, and is typical of the sort of data and log file real-world pre- and post-processing we frequently have to do as researchers.

The `flights.zip` file we have downloaded and unpacked contains a variety of glider flight traces and we are going to use them for our exercises now. We have already introduced the `cat` command to display the entire contents of a file (or multiple files). Often we are only interested in the start or end of a file though. The `head` and `tail` commands allow us to extract just the start or end of a file. Both show ten lines by default, but can be told to show an arbitrary number with the `-n <number>` option. Using this to look at one of the `igc` files

```
[tyson@l1.nibi ~]$ head flights/0144f5b1.igc
AXCSAAA
HFDTE030816
HFFXA050
HFPLTPILOTINCHARGE:Lena
HFGTYGLIDERTYPE:L23 Super Blanik
...
[tyson@l1.nibi ~]$ tail flights/0144f5b1.igc
B2116474309137N08057022WA002870042000309
B2116524309138N08057024WA002870041800309
B2116574309138N08057024WA002870041800309
B2117024309138N08057024WA002870041800309
B2117074309138N08057024WA002870041800309
...
```

We see the files are composed of a series of records. Googling will give the full `igc` file specification, but, for our purposes, the records of interest are the date record, the pilot record, the plane record, and GPS position record

```
HFDTE<DD><MM><YY>           (date: day, month, year)
```

```
HFPLTPILOTINCHARGE:<NAME> (pilot: name)
```

```
HFGIDGLIDERID:<CALLSIGN> (plane: call sign)
```

B<HH><MM><SS>	(time: hour, minute, second,
<DD><MM><mmmm>N	(latitude: degrees, minute, decimal minutes)
<DDD><MM><mmmm>W	(longitude: degrees, minutes, decimal minutes)
A<PPPPP><GGGGG>	(altitude: pressure, gps)
<AAA><SS>	(gps: accuracy, satellites)

Linux also comes with a variety of text editors. The two most common ones are `emacs` and `vi`, both of which were created in 1976, have an almost cult-like following, and will seem quite strange to the uninitiated. The quick reference guide contains the basic key strokes/commands to use these editors. For a new user, the most important thing to know is how to exit these editors if you accidentally get into them

- `emacs` - press `CTRL+x CTRL+c`
- `vi`- type `:q!`

where `CTRL+<key>` means to press `<key>` while holding down the *control key*. Other ways you will see `CTRL+c` written is `^c` and `C-c`.

For a first time user, `nano` is likely a good choice for making simple edits. It is a basic no-frills editor that lets you move around with the cursor keys and make edits as most people expect. The key sequences to exit, save (write out) the file, and so on are printed at the bottom of the screen using the `^<key>` format (e.g., press `^o` while holding down the *control key* to exit), so you won't forget them.

Sometimes, when you run a command, it will start an editor for you to edit something. Chances are this editor will be `vi` and you will need to know the `:q!` sequence to get out. You can set a person default editor by setting `EDITOR` environment variable to the editor you want

```
export EDITOR=nano
```

There are actually many such settings that programs inherit from your command line session, and even more that are just specific to `bash` and not inherited by other programs. They are documented in the various commands manual pages. The commands in `~/.bash_profile` (`~` mean `/home/tyson`) are always run at each login, so it is a good place put such setting that you always want set.

We will do this now to demonstrate editing a file.

```
[tyson@l1.nibi ~]$ nano .bash_profile
```

```

tyson@manny: ~
nano 2.6.3      File: .bash_profile      Modified
# .bash_profile
# Get the aliases and functions
if [ -f ~/.bashrc ]; then
    . ~/.bashrc
fi

# User specific environment and startup programs
PATH=$PATH:$HOME/.local/bin:$HOME/bin
export PATH
export EDITOR=nano[]

Get Help  Write Out  Where Is  Cut Text  Justify   Cur Pos
Exit      Read File  Replace   Uncut Text To Spell  Go To Line

```

After editing `~/.bash_profile` (runs every login) or `~/.bashrc` (runs every time `bash` runs), always test you can still login with a new `ssh` session in a new terminal. These are startup files, and some errors can leave you unable to login, which will be impossible to fix unless you still have an active sessions running to fix things.

3.1.1 Exercises

Doing the following exercises help ensure you understand the course material. The results of some of the later ones are needed to answer the course completion quizzes.

An example of something we may want to do with these files is determine which pilot each file belongs to in order to give each member a copy of their file. In this exercise we are just going to use our new commands to look at the files a do a few operations by hand to get an idea of the sort of things we will be automating.

1. Using `head` to look at a few (say 3-5) of the `igc` files (refer to the `igc` file specification given earlier) and answer the following questions
 - a. who the pilot is, and
 - b. what the year was.
2. For each of these files, use the `mkdir` and `cp` commands to
 - a. make a directory for that pilot (if required),
 - b. make a directory in the pilot's directory for that year (if required), and
 - c. copy the file into the pilot/year directory.
3. What happens if you run `cat`, `head`, and `tail` without any filename argument? In trying this, be aware that `CTRL+c` can be used to abort most command and `CTRL+d` signals the end of keyboard input.

3.2 Regular expressions and globbing

The `grep` (global regular expression search) command searches through files for regular expressions. Regular expressions are a sequence of characters that define a search pattern. Variants of them are supported by a wide range of applications, including google sheets, and are well worth learning. A very simple usage would be to use `grep` to extract all the line that starts with `HFPLT` from an `igc` file

```
[tyson@l1.nibi ~]$ grep ^HFPLT flights/0144f5b1.igc
HFPLTPILOTINCHARGE:Lena
```

As can be seen in the above example, a regular expression is simply a sequence of regular characters that match themselves plus some special characters like `^` that match things like the start of the line. The most basic matches supported by almost all regular expressions are (these are covered in our quick reference guide and the `grep` manual page too)

- `^` - match start of line
- `$` - match end of line
- *character* - match the indicated character
- `.` - match any character
- `[...]` - match any character in the list or range (`^` inverts)
- `(...)` - group
- `... | ...` - match either or
- `?` - match previous item zero or one times
- `*` - match previous item zero or more times
- `+` - match previous item one or more times
- `{...}` - match previous item a range of times

Regular expression implementations frequently differ in what special characters have to be escaped (preceded with a `\`) to have the above special meaning or not. For example, `grep` supports both basic and extended regular expressions where the former requires several of the special characters to be escaped to have their special meaning and the latter does not.

A more complex example would

```
[tyson@l1.nibi ~]$ grep '^B.*A.....5..' flights/0144f5b1.igc
B1837024309903N08053926WA009230050102706
B1837074309873N08053817WA009200051002706
...
```

which gives all GPS trace lines with a GPS altitude recording of 500-599 meters.

In this example we have enclosed the regular expression in single quotes. This is because `bash` also has sequences that it treats special, and this includes `*` which, without the single quotes, indicates a glob pattern for pathname expansion. Glob patterns allow us to specify pathnames with the following wildcards

- `*` - match any number of characters (include none)
- `?` - match any single character
- `[...]` - match any character in this list

When `bash` sees unquoted versions of these in a command line, it replaces the pattern with all pathnames that match the pattern. This allows us to easily run commands like extract the pilot line from all the `igc` files

```
[tyson@l1.nibi ~]$ grep ^HFPLT flights/*.igc
0144f5b1.igc:HFPLTPILOTINCHARGE:Lena
04616075.igc:HFPLTPILOTINCHARGE:Bill
...
```

It is important to realize is that it is `bash` that literally replaces the pattern with all the matching pathnames. The command that is being run never sees the patterns. It just gets the list of files, exactly as if we had typed in all the filenames ourselves.

There are actually many such expansions that can occur, and sometimes it is useful to know what the command really being run is. The `set -x` command tells `bash` to print out each command it runs, and `set +x` tells `bash` to stop printing them out. We can use this to see exactly how our pattern gets expanded into the command that is run

```
[tyson@l1.nibi ~]$ set -x
[tyson@l1.nibi ~]$ grep ^HFPLT flights/*.igc
+ grep --color=auto '^HFPLT' flights/0144f5b1.igc flights/04616075.igc ...
0144f5b1.igc:HFPLTPILOTINCHARGE:Lena
04616075.igc:HFPLTPILOTINCHARGE:Bill
...
[tyson@l1.nibi ~]$ set +x
```

This also shows something I hadn't intended to talk about. The `grep` command is automatically being provided an `--color=auto` option. This is done with the `bash` aliases feature which can provide default arguments and short forms for various commands. It is also commonly used to make `-i` (verify) a default for many commands like `rm`. You can view the current set of alias with the `alias` command and read more about them in the `bash` manual page.

3.3 Redirection and pipes

Now that we have a simple way of extracting all the pilot and date fields from all the `igc` files, we need to use a redirection to save it in a file so we can process it further. Redirections are specified at the end of the command line with the `<` and `>` characters. A simple mnemonic is that they are like arrows re-directing the input and output, receptively from and to a file. An example redirection to save out list of pilots to `pilots` would be

```
[tyson@l1.nibi ~]$ grep ^HFPLT flights/*.igc > pilots-extracted
```

Running this command produces no output as all the output has been redirected from the screen to the `pilots` file, as we can easily verify by loading `pilots` in our editor or printing it out using `cat`

```
[tyson@l1.nibi ~]$ cat pilots-extracted
flights/0144f5b1.igc:HFPLTPILOTINCHARGE:Lena
flights/04616075.igc:HFPLTPILOTINCHARGE:Bill
flights/054b9ff8.igc:HFPLTPILOTINCHARGE:Lena
...
```

We only want the pilot names though, not the filename and the `HFPLTPILOTINCHARGE:` field identifier. To remove these we can use the `cut` command which lets us cut out bits from a line. The pilot names always start at the 41st character in this output, so one way to do this would be to specify `-c 41-`, which means give me from character 41 to the end of the line. A simpler way though is to note the line is broken in parts with the `:` character. With this observation, we can use `-d :` to break it up into three pieces as `-f 3` to select the third

```
[tyson@l1.nibi ~]$ cut -d : -f 3 pilots-extracted
Lena
Bill
Lena
...
[tyson@l1.nibi ~]$ cut -d : -f 3 pilots-extracted > pilots-names
```

The only issue we have now is we have each pilot listed for each flight they took. We would like to have each pilot listed only once. As it happens, there is `uniq` command that removes duplicate lines. On closer reading of the manual page though, it becomes apparent that `uniq` only removes duplicate lines if they are adjacent, and states that you have to run your file through the `sort` command first. Doing this we get

```
[tyson@l1.nibi ~]$ sort pilots-names > pilots-sorted
[tyson@l1.nibi ~]$ uniq pilots-sorted
Aasia
Bill
Fred
...
```

Creating a bunch of intermediate files simply to feed the output from one command into the input of the next command is tedious though, so `bash` provides a `|` (pipe) syntax to do this for us. With this syntax we can eliminate all the temporary files in

```
[tyson@l1.nibi ~]$ grep ^HFPLT flights/*.igc > pilots-extracted
[tyson@l1.nibi ~]$ cut -d : -f 3 pilots-extracted > pilots-names
[tyson@l1.nibi ~]$ sort pilots-names > pilots-sorted
[tyson@l1.nibi ~]$ uniq pilots-sorted
```

and collapse it down to just

```
[tyson@l1.nibi ~]$ grep ^HFPLT flights/*.igc | cut -d : -f 3 | sort | uniq
Aasia
Bill
Fred
...
```

As a small point of clarification, this pipe command is not creating temporary files and providing them to the commands. Rather it redirecting the (screen) output of each program into the (keyboard) input of the next one. This works as all the above commands (and most others) get their input from the keyboard if a filename is not specified (this came up in an earlier exercise). The above is then technically equivalent to

```
[tyson@l1.nibi ~]$ grep ^HFPLT    flights/*.igc    > pilots-extracted
[tyson@l1.nibi ~]$ cut -d : -f 3 < pilots-extracted > pilots-names
[tyson@l1.nibi ~]$ sort          < pilots-names    > pilots-sorted
[tyson@l1.nibi ~]$ uniq          < pilots-sorted
```

3.3.1 Exercises

Doing the following exercises help ensure you understand the course material. The results of some of the later ones are needed to answer the course completion quizzes.

In these exercises we are going to create a series of pipelines for extracting key bits of information from our igc files. In the next section we will be converting these pipeline commands into shell scripts.

The key to building a successful pipeline is to build it up slowly and test each addition. Instead of typing in an entire pipeline, running it, and then not knowing where it went wrong, test each stage and get it correct before adding the next. This is very easy to do as the up arrow brings up the previous commands run for further editing and re-running. For example

```
[tyson@l1.nibi ~]$ grep ^HFPLT flights/*.igc | head
[tyson@l1.nibi ~]$ grep ^HFPLT flights/*.igc | cut -d : -f 3 | head
[tyson@l1.nibi ~]$ grep ^HFPLT flights/*.igc | cut -d : -f 3 | sort | head
[tyson@l1.nibi ~]$ grep ^HFPLT flights/*.igc | cut -d : -f 3 | sort | uniq
```

First an output redirection question though.

1. What is the difference between redirecting output with `>` and `>>` (hint, try running the same redirected command twice and see what happens to the output file in each case).
2. Create pipelines to extract
 - a. the flight date from a single igc file,
 - b. all flight years from all igc files,
 - c. all GPS time records from a single igc file, and
 - d. all GPS altitude records from a single igc file.
3. Extend the GPS time record extraction pipeline
 - a. to give the starting (first) time, and
 - b. to give the finishing (last) time.
4. Extend the GPS altitude record extraction pipeline to give the highest altitude.

AUTOMATION

The command line keeps track of prior commands that have been run. These include both interactively selecting prior commands to re-run

- *up* and *down* arrow keys to bring back up prior commands
- *CTRL+r* to interactively search through prior commands

and the `history` command to display the last commands. This lets us process our history of commands with our commands.

As an example, we created a variety of pipelines for extracting information from the `igc` files, such as

```
[tyson@l1.nibi ~]$ grep '^B' flights/0144f5b1.igc | cut -c 31-35 | sort | tail -n 1
```

which gives the highest GPS altitude recorded in the given `igc` file. After such a session we can use the `history` command along with output redirection to save the commands we came up with to a file for future reference or sharing with a colleague

```
[tyson@l1.nibi ~]$ history 20 > flight-commands
```

where the `20` specifies that we want the last twenty commands run. From this it is trivial to open our file up in a text editor like `nano` and clean it up a bit to get a nice reference

```
[tyson@l1.nibi ~]$ nano flight-commands
...
[tyson@l1.nibi ~]$ cat flight-commands
Reference of useful pipes for working with igc files extracted from history

Date
  grep '^HFDTE' flights/0144f5b1.igc | cut -c 6-
Pilot
  grep '^HFPLT' flights/0144f5b1.igc | cut -d : -f 2
Plane
  grep '^HFGIDGLIDERID' flights/0144f5b1.igc | cut -d : -f 2

Start time
  grep '^B' flights/0144f5b1.igc | cut -c 2-7 | head -n 1
End time
  grep '^B' flights/0144f5b1.igc | cut -c 2-7 | tail -n 1

Highest GPS altitude
  grep '^B' flights/0144f5b1.igc | cut -c 31-35 | sort | tail -n 1
```

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```
All pilots
grep ^HFPLT flights/*.igc | cut -d : -f 3 | sort | uniq
```

Once we have our commands in a file, it is pretty natural to wonder if we can get bash to just run our commands from the file instead of us having to type them back in each time.

4.1 Scripting

This is precisely what a shell script is: a file with a list of commands in it that we get our shell (bash) to run. Our *flights-command* is almost a shell script as we have written it above. The only issue is that bash doesn't know what to make of the comments as they aren't proper commands. We can fix this by prefixing them with # to mark them as comments

```
[tyson@l1.nibi ~]$ nano flight-commands
...
[tyson@l1.nibi ~]$ cat flight-commands
# Reference of useful pipes for working with igc files extracted from history

# Date
grep '^HFDTE' flights/0144f5b1.igc | cut -c 6-
...
```

Now we can tell bash to run our commands directly for us from our file

```
[tyson@l1.nibi ~]$ source flight-commands
```

There are actually several ways this last step can be done

- . <filename> or source <filename> - run commands in current session
- (source <filename>) - run commands in a sub shell (current directory and such will be restored)
- bash <filename> - start a new shell, run the commands, and exit back to current shell

Earlier we had mentioned that Linux doesn't use a .exe extension to identify executable files. Instead executable files have the executable mode set on them. We can set this with the command `chmod +x <file>` and we can see it as the x when we run look at the `ls -l` long listing. Because our program is a script, we also have to tell Linux what program to use to run it by adding a special `#!<interpreter>` comment to start of it

```
[tyson@l1.nibi ~]$ ls -l flights-commands
-rw-r----- 1 tyson tyson 630 May 11 22:32 flights-commands
[tyson@l1.nibi ~]$ chmod +x flight-commands
-rwxr-x--- 1 tyson tyson 630 May 11 22:32 flights-commands
[tyson@l1.nibi ~]$ nano flight-commands
...
[tyson@l1.nibi ~]$ cat flight-commands
#!/bin/bash

# Reference of useful pipes for working with igc files extracted from history
...
```

With all this in place (the executable mode set and the special interpret comment as the first line) we can now directly run our file as if it was just another command

```
[tyson@l1.nibi ~]$ flight-commands
-bash: flight-commands: command not found
[tyson@l1.nibi ~]$ ./flight-commands
030816
Lena
...
```

The first run attempt failed because the current directory is not somewhere bash look for a command unless we explicitly tell it to as we did in the second command. The locations bash looks are those specified in the `PATH` environment variable in a `:` delimited format. We can see the setting of this variable by either using variable substitution with the `echo` command or using the `declare` command to print it

```
[tyson@l1.nibi ~]$ echo $PATH
/opt/software/slurm/current/bin:...:/home/tyson/bin
[tyson@l1.nibi ~]$ declare -p PATH
declare -x PATH="/opt/software/slurm/current/bin:...:/home/tyson/bin"
```

The `declare` version is interesting as it actually prints the `declare` command we would have to run to set it to its current value. This shows us additional information such as the `-x` which means that it is to be also made available (exported) to commands that bash runs as well.

You might be tempted to add `.` (the current directory) to this list. This will work, but don't do it. If someone puts a `ls` command in a directory you go into and run `ls` in, it will then run their `ls` command and not the system one you are expecting. Their `ls` command could do anything, including deleting all your files or giving them access to your account in the background. The last element of `PATH` is a `bin` directory under your home directory. Create this directory instead and put your scripts there

```
[tyson@l1.nibi ~]$ mkdir bin
[tyson@l1.nibi ~]$ mv flight-commands bin
[tyson@l1.nibi ~]$ flight-commands
030816
Lena
GBJY
...
```

Our command isn't as useful as the other commands though as we can tell them what files to operate on. Our command just ignores everything we tell it and always does the same operations on the same files

```
[tyson@l1.nibi ~]$ flight-commands --you-are-just-going-to-ignore-this--
030816
Lena
GBJY
...
```

To make our command more useful, we can use variables to change it from a specific command to run to a template command to run. We do this by replacing the fixed filenames with special symbols (variables) that get replaced with the arguments provided on the command line

- `$(n)` - the `n`th argument provided on the command line
- `$@` - all the arguments provided on the command line separated by spaces
- `$#` - the number of arguments provided on the command line

With this we can make a copy of our example commands file and edit it into a command that takes an `igc` filename and prints the date of the flight

```
[tyson@l1.nibi ~]$ cp bin/flights-commands bin/igc-date
[tyson@l1.nibi ~]$ nano bin/igc-date
...
[tyson@l1.nibi ~]$ cat bin/igc-date
#!/bin/bash

# Run the date extraction pipeline using the first argument as the source filename
grep '^HFDTE' $1 | cut -c 6-
[tyson@l1.nibi ~]$ igc-date flights/fffdcaad.igc
250616
```

All we have done is put a name to pipeline template. This isn't trivial though. Our minds can only deal with so much information at any one point. Switching from thinking about a complex pipeline to a simple, appropriate-named command, frees up the brain power required to successfully integrate that command into its some other complex operation. Repeating this process lets us build up from small blocks to mansions.

4.1.1 Exercises

Doing the following exercises help ensure you understand the course material. The results of some of the later ones are needed to answer the course completion quizzes.

In these exercises, you will see the `;` character. In bash the `;` is equivalent to a *newline* (pressing *enter* on your keyboard). This lets us write multiline commands on a single line. You will see when you scroll back through your history (the *up* key), that bash will replace you *newlines* with `;`s.

1. In the live session, we converted our example date extension pipeline into an new `igc-date` command

- `igc-date <filename> - date field from the igc-file`

Do this for the other pipelines to create the following commands

- a. `igc-pilot <filename> - pilot field from the igc-file`
 - b. `igc-plane <filename> - plane call sign from the igc-file`
 - c. `igc-start <filename> - starting (first) time for the igc-file`
 - d. `igc-end <filename> - ending (last) time for the igc-file`
 - e. `igc-maxalt <filename> - maximum altitude recorded in the igc-file`
2. The `[[<test>]]` command lets us perform a variety of test (see `help [[` and `help test`). Combined with the `if <command>; then <command>; else <command>; fi` command (see `help if`), this lets us write a further improved `igc-date` command that provide feedback to the user if it was invoked incorrectly.

```
[tyson@l1.nibi ~]$ cat bin/igc-date
#!/bin/bash
if [[ $# -eq 1 ]]; then
    grep '^HFDTE' $1 | cut -c 6-
else
    echo "Proper usage is igc-date [igc file]"
fi
```

Give this a try and update the other commands to also do this.

3. Add an `elif [[$# -eq 0]]; then <command>` branch to make the command also support reading the `igc` file directly from the keyboard when not given any filenames as most other commands do (remember `CTRL+c` aborts and `CTRL+d` signals the end of the input when testing this out).

4.2 Submitting jobs

Earlier we discussed how the nibi supercomputer is actually a large number very beefy standard computers, and that you ran programs on these computers by telling the system

- what commands you want to run, and
- what resources those commands require to run.

Now that we know how to create scripts, we know how to do this first of these. The second is a simply a matter of looking through the command options for `sbatch` (slurm batch) command. The alliance [documentation wiki](#) has pretty extensive coverage of most circumstances and what options should be specified. At a minimum we need

- `--time` `[[dd-]hh:]<mm>` - amount of time required
- `--mem-per-cpu` `[megabytes]` - amount of memory required
- `--account` `<account>` - sponsor account to record usage against
- `--output` `<file>` - file to record output in

The script will be killed if it exceeds the resources specified, so we want to give ourselves a bit of room when specifying our limits. We don't want to be excessive though, as our script will not run until the system has secured all the specified resources for us, so the more we specify, the longer we wait before running.

For most people there is only one account to submit the script under (their sponsor's default account), so it does not need to be specified. If there are multiple accounts, then it has to be specified. Not doing so will give an error listing all the available accounts. A sample submission might then be

```
[tyson@l1.nibi ~]$ sbatch --time 5 --mem-per-cpu 500 --account def-tyson --output_
↪example.log igc-date flights/0144f5b1.igc
Submitted batch job 31352623
```

To avoid having to specify all these options every time, the `sbatch` command also lets us put them in the comments at the top of our script file after the `#!/bin/bash` line but before any commands by prefixing them with `SBATCH`.

```
#SBATCH --mem-per-cpu 500
#SBATCH --account def-tyson
```

If an option is specified on both the command line and the script file, the command line will take precedence. In this sense, putting options in our script files gives us a powerful way to specify our defaults.

The returned number is the job identifier. Make sure to provide this to us if you ever request support for an issue regarding your job so we can look it up. It can also be used to cancel a job with the `scancel` (slurm cancel) command. The `squeue` (slurm queue) command shows you the status of queued jobs

```
[tyson@l1.nibi ~]$ squeue -u tyson
      JOBID USER   ACCOUNT           NAME  ST  TIME_LEFT  NODES  CPUS      GRES  MIN_
↪MEM  NODELIST (REASON)
      31352623 tyson def-tyson   igc-date  R    4:50      1     1     (null)  ↪
↪500M c71 (None)
```

The `-u <username>` option limits the output to just the jobs queued for the specified user. From this we see that our job is running (ST is R) on the node (computer) c71. Once a job has completed running, it is removed from the queue and no longer shows up in the output of `squeue`. Information about it can still be retrieved using the `sacct` (slurm accounting) command

```
[tyson@l1.nibi ~]$ sacct -S 2020-05-01 -u tyson
...
```

The Shell

where the `-S <date>` option specifies how far back in the job records to report on (the default is just the current day). We can also look in the specified output file to get any messages that may have been printed by the job (the extracted flight date in our case)

```
[tyson@l1.nibi ~]$ cat example.log
030816
```

The supercomputers have a lot of standard software already installed on them. It is not possible to enable all these software packages at the same time though, as many provide the same commands, so you need to use the `module` command to tell the system what software you want enabled. The `module avail` command lists what software is available. For example

```
[tyson@l1.nibi ~]$ module avail python
...
  ipython-kernel/3.10      ipython-kernel/3.12      python-build-bundle/2024a (D)
↪      python/3.11.5 (t,D:3.11)
  ipython-kernel/3.11 (D)  python-build-bundle/2023b  python/3.10.13      (t,
↪3.10)      python/3.12.4 (t)
...

```

and the `module load` command enables the chosen software

```
[tyson@l1.nibi ~]$ python --version
Python 3.11.4
[tyson@l1.nibi ~]$ module load python/3.12.4
[tyson@l1.nibi ~]$ python --version
Python 3.12.4
```

The `module avail` command only shows software that is compatible with the current core packages that loaded. To see all available software you need to use the `module spider` command. It will also tell you what other packages you need to load in order to make your desired package available. For example

```
[tyson@l1.nibi ~]$ module avail intelmpi
No module(s) or extension(s) found!
...
Use "module spider" to find all possible modules and extensions.
...
[tyson@l1.nibi ~]$ module spider intelmpi
...
  Versions:
    intelmpi/2019.7.217
    intelmpi/2021.2.0
    intelmpi/2021.6.0
    intelmpi/2021.9.0
...
  For detailed information about a specific "intelmpi" package (including how to load
↪the modules) use the module's full name.
...
[tyson@l1.nibi ~]$ module spider intelmpi/2021.9.0
...
  You will need to load all module(s) on any one of the lines below before the
↪"intelmpi/2021.9.0" module is available to load.

  StdEnv/2023  intel/2023.2.1
```

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...

4.3 Loops

At the very start, we demoed how easy it was to add the date to the name of a large number of files with the command line instead of a graphical user interface. We did this using a for loop. For loops let us create a template command (such as one to renaming a file to include the date), and then apply it to a large number of cases.

Lets consider the case of getting all our pilot names. We have our `igc-pilot` command that gives us the pilot field from a single `igc` file. If we wanted to retrieve all our pilot, we would have to run this command once for each file. That is

```
[tyson@l1.nibi ~]$ igc-pilot flights/0144f5b1.igc
[tyson@l1.nibi ~]$ igc-pilot flights/04616075.igc
[tyson@l1.nibi ~]$ igc-pilot flights/054b9ff8.igc
...
```

Comparing these first few cases, it is pretty clear that the only thing changing between each of these commands is the name of the `igc` file. That is, we have a common command template that we are running

```
igc-pilot $file
```

where `$file` is placeholder for the filename that changes with each command. Our initial commands could then equally well be written as

```
[tyson@l1.nibi ~]$ file=flights/0144f5b1.igc; igc-pilot $file
[tyson@l1.nibi ~]$ file=flights/04616075.igc; igc-pilot $file
[tyson@l1.nibi ~]$ file=flights/054b9ff8.igc; igc-pilot $file
...
```

where we are simply setting the value `file` each time and then doing our template that runs `igc-file` on our file.

A for loop is nothing more than special syntax for doing that only requires us to have to specify the template once, which makes sense as the template is the same every time. In bash the syntax looks like this

```
for file in flights/0144f5b1.igc flights/04616075.igc flights/054b9ff8.igc ...; do
    igc-pilot $file
done
```

By bringing the list of file we run our template for into one place, we have also now made it possible for us to specify our file list using a *glob pattern*. That is, we can say

```
[tyson@l1.nibi ~]$ for file in flights/*.igc; do
    igc-pilot $file
done

Lena
Bill
Lena
...
```

A `for` statement is also a command, and can be used as any other commands. For example, its output can be piped through `sort` and `uniq` in order to obtain a compact list of our pilots

```
[tyson@l1.nibi ~]$ for file in flights/*.igc; do igc-pilot $file; done | sort | uniq
Asia
Bill
Fred
Lena
Mary
Mo
```

When we say `$(<command>)` in bash, it gets replaced with the output `<command>`. We can use this to write a powerful for loop to (finally!) rename all our files to something more useful than their current names

```
[tyson@l1.nibi ~]$ cd flights
[tyson@l1.nibi ~]$ for file in *.igc; do
    pilot=$(igc-pilot $file)
    date=$(igc-date $file)
    mv $file $date-$pilot-$file
done
[tyson@l1.nibi ~]$ ls
000000-Lena-551a9c25.igc  010815-Aasia-7cded70f.igc  010815-Mary-4bf15e07.igc ...
```

Having the pilot name and date in each of the files allows us to easily do things like select all the files for a specific pilot or year using *glob patterns* (e.g., `*-Lena-*` will select all of Lena's flights).

4.3.1 Exercises

Doing the following exercises help ensure you understand the course material. The results of some of the later ones are needed to answer the course completion quizzes.

In this exercise we are going to create a triple loop to print out the highest altitude obtained by each pilot for each year by filling in the missing command in the following double loop

```
for year in 15 16 17; do
    for pilot in Aasia Bill Fred Lena Mary Mo; do
        maxalt=$(<command to retrieve greatest altitude for $pilot in $year>)
        echo "$year - $pilot: $maxalt"
    done
done
```

Past experience has shown this is a very tough problem for people to solve outright. When you get stuck like this, the key is to switch from trying to find an outright solution, and instead focus on trying to break the problem down into a series of smaller problems that you can produce outright solutions to. Often the steps become obvious if you do a few cases by hand. You just need to take note of what you did and get the computer to do the same.

For this problem, we can break it down into the following sub-problems (which are the exercise)

1. Extract the highest altitude for a single flight (we made a command for this).
2. Come up with a *glob pattern* to select all the flights in a given year for a given pilot.
3. Use both of these to extract the highest altitudes for a given pilot in a given year (put the highest altitude command in a *for loop* over the files that match the *glob pattern*).
4. Extract the highest of the highest flight altitudes (pipe the output of the for loop into a pipeline that extracts the largest value).
5. Insert the command you built up in 1-4 into the loop above and run that to see which pilot achieved the highest altitude each year.

QUICK REFERENCE

5.1 Key Features

Unix Architecture page on Wikipedia

Files are stored on disk in a hierarchical file system, with a single top location throughout the system (root, or “/”), with both files and directories, subdirectories, sub-subdirectories, and so on below it.

With few exceptions, devices and some types of communications between processes are managed and visible as files or pseudo-files within the file system hierarchy. This is known as *everything's a file*.

Doug McIlroy (inventor of Unix pipes)

This is the Unix philosophy: Write programs that do one thing and do it well. Write programs to work together. Write programs to handle text streams, because that is a universal interface

5.2 File system

Key differences from Windows

- there are mount points instead of A:, C:, etc.,
- directories and files are case sensitive, and
- the separation character is / instead of \

What would appear as a separate media hierarchy in Windows (e.g., A:\MyDir\MyCode.c) simply appears under a separate directory (known as a mount point) in Unix (e.g., /media/disk/MyDir/MyCode.c).

5.2.1 Root (/)

- /boot - boot loader files
- /etc- configuration files
- /dev - device files
- /bin - user programs required for booting
- /sbin - system programs required for booting
- /lib{,32,64} - libraries required for booting
- /usr - programs, libraries, and such not required for booting
- /root - superuser directory
- /home - users directories (shared by all nodes)
- /tmp - temporary files

- /var - variable data (spool files, log files, etc.)
- /opt - add on package directory
- /media - mount point for removable media
- /proc - process information pseudo-file system
- /sys - system information pseudo-file system

5.2.2 User (/usr)

The /usr directory is split off from the / directory mostly because disk space used to be precious.

- /usr/bin - user programs not required for booting
- /usr/sbin - system programs not required for booting
- /usr/lib{,32,64} - libraries not required for booting
- /usr/games - game programs
- /usr/share - architecture independent data
- /usr/man - on-line manuals
- /usr/src - source code
- /usr/include - header files

5.2.3 User Local (/usr/local)

The /usr/local directory is a place to locally install programs without messing up /usr.

- /usr/bin - user programs not required for booting
- /usr/sbin - system programs not required for booting
- /usr/lib{,32,64} - libraries not required for booting
- /usr/games - game programs
- /usr/share - architecture independent data
- /usr/man - on-line manuals
- /usr/src - source code
- /usr/include - header files

5.2.4 Alliance supercomputers

- /project - group data files (shared by all nodes and all group members)
- /scratch - user temporary data files (local to each cluster)

5.3 Devices

Some of the special /dev files are

- /dev/null - discards all data written and provides no data
- /dev/zero - provides a constant stream of *NULL* characters
- /dev/random - provides a stream of random characters

- `/dev/urandom` - provides a constant stream of pseudo-random characters

5.4 Commands

Programs are run by specifying the command followed by the arguments separated by spaces.

program [*argument...*]

By convention, arguments are switches followed by strings (e.g., regexps, paths, file names, etc.). Switches are usually single dashes followed by letter for each switch or a double dash followed by a descriptive string (e.g., `rm -fr mydir` or `rm --force --recurse mydir`). Most commands also understand

- `-` - as a file name means read or write to the terminal
- `--` - the end of switches and the start of the strings (in case the string needs to start with `-` or `--`).

5.4.1 Help

Traditionally man pages (a single help page) have been the de facto documentation source, however, some software suites have been switching to info pages (a collection of hyperlinked pages). Help for the shell built in commands is available by the built in `help`.

- `man command` - on-line reference manuals
- `apropos [-a] keyword ...` - search on-line reference manuals (same as `man -k`)
- `info item` - info documents

5.4.2 Directories

The current directory is `.` and the parent directory is `..`

- `pwd` - current directory
- `cd directory` - change directory
- `mkdir directory` - make directory
- `rmdir directory` - remove directory

5.4.3 Files

Files beginning with `.` are considered hidden and not normally shown.

- `ls [-a] [-l] destination` - list files
- `cp [-a|-p] [-r] [-s] source ... destination` - copy files
- `ln [-s] target name` - link to file
- `mv source ... destination` - move files
- `rm [-r] [-f] destination ...` - remove files

5.4.4 Permissions

Standard permissions are read, write, and execute for user, group, and other. They are frequently abbreviated as three octal numbers (0=000, 1=001, 2=010, 3=011, 4=100, 5=101, 6=110, 7=111) corresponding to user read, write, and execute; group read, write, and execute; other read, write, and execute.

For directories, read allows the contents to be listed, write allows files to be added or removed, and execute allows the directory to be traversed.

- `chmod [u|g|o|a]... [+|-|=] [r|w|x|X]... [-R] destination ...` - change mode (user/group/other permissions)
- `chown [-R] user destination ...` - change owner
- `chgrp [-R] group destination ...` - change group
- `setfacl [-m|-x] [-R] [[u|g|o|m]...:user:[r|w|x|X]...] destination* ...` - set file access control list *(individual users)
- `getfacl destination ...` - get file access control list (individual users)

5.4.5 View Files

The space key will advance a page and the q key will quit in `more` and `less`. In addition, the arrow keys will move in the appropriate direction in `less`.

- `more file` - view one page at a time
- `less file` - view forward and backwards
- `cat [file ...]` - concatenate files in sequence
- `head [-n lines] [file ...]` - first part of files
- `tail [-n lines] [-f] [file ...]` - last part of files
- `paste [-d delimiter] [file ...]` - concatenate files in parallel
- `cut [-d delimiter] [-f range] [file ...]` - extract columns
- `sort [-g] [-f] [-u] [file ...]` - sort lines

5.4.6 Comparison

Digests are numbers computed from the content of files such that it is extremely difficult to come up with two different files with the same number.

- `diff [-w] [-i] [-u number|-y] file1 file2` - compare files line by line
- `sdiff [-W] file1 file2` - compare files side by side (similar to `diff -y`)
- `md5sum [file ...]` - compute MD5 digest
- `sha256sum [file ...]` - compute SHA256 digest

5.4.7 Searching

- `egrep [-i] [-v] regexp [file ...]` - find lines matching regexp in files (same as `grep -E`)
- `fgrep [-i] [-v] strings [file ...]` - find lines matching strings in files (same as `grep -F`)
- `find directory ... predicates` - find files satisfying predicates in directories

5.4.8 Process

Each process (a running programs) is identified by a unique number.

- `ps [-A|-U user] [-H] [-f]` - process list
- `kill [-s signal] process ...` - signal process
- `nohup command` - disconnect command
- `nice command` - low priority command

5.4.9 Remote

- `ssh [user@]host [command]` - login to remote system
- `scp [[user@]host:] source ... [[user@]host:]destination` - copy remote files
- `unix2dos file ...` - convert to DOS line breaks
- `dos2unix file ...` - convert to Unix line breaks

5.4.10 Other

- `sleep seconds` - waits given number of seconds
- `echo [-n] [-e] strings` - prints strings
- `test tests` - perform various string (e.g., equality) of file (e.g., existence) tests

5.5 Editors

The two most popular Unix editors are `vi` and `emacs`. Both are extremely powerful and very complex. A simpler editor is `nano`.

- `vi [file ...]` - common Unix editor
- `emacs [-nw] [file ...]` - common Unix editor
- `nano [file ...]` - simple Unix editor

5.5.1 Vi

Vi distinguishes between command and insert mode. Command mode allows you to move around and enter commands. Insert mode allows you to edit text.

- `:h` - help
- `:w[!] [file]` - write file (exclamation forces it)
- `:e file` - edit file
- `:q[!]` - quit Vi (exclamation forces it)
- `:n[!]` - next file (exclamation forces it)
- `[a|A]` - append after cursor or at end of line
- `[i|I]` - insert (capital for beginning of line)
- `[v|V]` - select to cursor or to end of line
- `[c[w|c]|C]` - change selection/word/line or to end of line
- `[d[w|d]|D]` - delete selection/word/line or to end of line
- `[y[w|y]|Y]` - copy selection/word/line or to end of line
- `[p|P]` - paste before or after cursor/line
- `J` - join lines
- `[u|U]` - undo (capital for current line)
- `ESC` - revert to command mode

5.5.2 Emacs

Emacs is a more traditional single mode editor. Partially typed entries can be completed by pressing *TAB* (twice to list).

- CTRL+h - help (b list keys and k describes keys)
- CTRL+g - abort current operation
- CTRL+[1 | 2 | 3] - single window or split vertical/horizontal window
- CTRL+x CTRL+s - save current buffer
- CTRL+x CTRL+b - switch current buffer
- CTRL+x CTRL+k - quit current buffer
- CTRL+x CTRL+c - quit Emacs
- CTRL+SPACE - mark start of region
- CTRL+w - copy from start of region to cursor
- CTRL+y - past copied region
- CTRL+k - delete to end of line or line if start of line
- CTRL+s - search for text
- CTRL+_ - undo
- ALT+x - enter command (*TAB* twice to list)

5.6 Command Line

The shell is a command line interpreter that lets users run programs. It provides ways to start programs and to manipulate/setup the context in which they run. The main parts of this are

- arguments,
- environment,
- standard input (stdin),
- standard output (stdout),
- standard error (stderr), and
- return value

A standard command looks like so

```
command [<stdinfile] [>[>]stdoutfile] [2>[>]stderrfile] [&]
```

5.6.1 Arguments

Options passed to the program to tweak its behaviour. Traditionally switches (e.g., *-xzf* or *--extract --gzip --file*) followed by strings (e.g., *regexp*, *paths*, *file names*, etc.). Partially typed file names and directories can be completed by pressing *TAB* (twice to list).

- *...{...}...* (brace expansion) - if not quoted, expands once for each comma separated list or once for each number in *..* separated range
- *~...* (tilde expansion) - if not quoted, expands to home directory of user following the tilde or the current user if no user specified

- `${...}` (parameter and variable expansion) - if not single quoted, expands to environment variable specified or the corresponding parameter if number specified (`{` and `}` are not always required)
- `$(...)` (command substitution) - if not single quoted, expands to output for command (``...`` is an alternative syntax)
- `$(...)` (arithmetic substitution) - if not single quoted, expands to evaluated result of the expression
- `...` (word splitting) - if not quoted, splits into separate arguments anywhere an IFS character (by default space, tab, and newline) occurs
- `...[*|?|[...]]...` (path name expansion) - if not quoted, is considered a pattern and replaced with matching file names (`*` matches any string, `?` matches any character, and `[...]` matches all the enclosed characters)

5.6.2 Quoting

Special characters can be escaped with `\` to remove their special meaning. Single and double quoting strings affect escaping as well as which expansions and substitutions are preformed.

- `'...'` - no expansion or substitutions is preformed
- `"..."` - only escaping, parameter and variable expansion, command substitutions, and arithmetic substitutions occur

5.6.3 Environment

A set of key value pairs (e.g., `USER=root`) that programs can look up and use. Each program gets a fresh copy (i.e., changing it will not change the original) of all environment variables marked for export.

- `key=value` - make a local environment variable
- `export key[=value]` - mark an environment variable for export
- `unset key` - delete an environment variable

Two important environment variables are

- `PATH` - list of `:` separated directories to look for programs in
- `LD_LIBRARY_PATH` - list of `:` separated directories to look for libraries in (ahead of the system defaults specified in `/etc/ld.so.conf`)

5.6.4 Input and Output

Programs are run with a standard place to read input from, a standard place to write output to, and a standard place to write error messages to. By default these are all the terminal window in which the program is run. This can be changed via

- `<file` - read standard input from file
- `[>|>>] file` - write standard output to file (overwriting or appending)
- `[2>|2>>] file` - write standard error to file (overwriting or appending)
- `[&>|&>>] file` - write standard output and error to file (overwriting or appending)

5.6.5 Status

Programs return an integer exit status. The status of the most recent executed foreground command is available as `$?`.

- 0 - program completed successfully
- 1...127 - program specific error code

- 128...255 - program terminated by signal 127+*signal*

5.6.6 Job Control

Programs run in the foreground by default. Background jobs will be suspended if they require input. Existing jobs will be sent SIGHUP when the shell exits.

- `jobs` - list jobs
- `fg id` - switch job to foreground
- `bg id ...` - switch jobs to background
- `disown id ...` - release jobs from job control

Foreground jobs usually respond to the following key combinations

- `CTRL+Z` - suspend program
- `CTRL+C` - abort program
- `CTRL+D` - end of input

5.6.7 Multiple Commands

Commands can be combined in several ways.

- `... ; ...` - run first command and then second (same as pressing *ENTER*)
- `... & ...` - run first command in background at the same time as second
- `... | ...` - run first command in background with its output going to the second as input
- `... && ...` - run first command and then second only if first returns success
- `... || ...` - run first command and then second only if first returns failure

Commands can be combined in several ways.

- `{...}` - group command in current shell – has to end with `;` or newline
- `(...)` - group command in sub shell – does not have to end with `;` or newline

5.7 Scripting

Executable text files that start with `#!/command` (`#!/bin/bash` for shell scripts) are run as *command file*.

5.7.1 Parameters

- `$#` - number of parameters
- `$0` - name of shell or shell script
- `$number` - positional parameter
- `$*` - all positional parameters (in double quotes expands as one argument)
- `$@` - all positional parameters (in double quotes expands as separate arguments)

The following functions manipulate parameters

- `shift [number]` - drop specified number of parameters (one if unspecified)
- `set parameter ...` - set parameters to given parameters

5.7.2 Programming

- `if command ...; then command ...; [elif command ...; then command ...;] ... [else command ...;] fi` - conditionally run commands depending on success if and elif commands
- `for key in value ...; do command ...; done` - for each value, set key to value and run commands
- `while command ...; do command ...; done` - repeatedly run commands until while commands fail
- `case value in [pattern [| pattern]...) command ...;;] ... esac` - run commands where first pattern matches (same as path name expansion)
- `continue [number]` - next iteration of enclosed loop (last if not specified)
- `break [number]` - exit enclosed loop (last if not specified)
- `function name { command; } ...` - create a command that runs the commands with passed parameters
- `return [number]` - return from function with given exit status (last command if not specified)
- `exit [number]` - quit shell with given exit status (last command if not specified)

5.8 Regular Expressions

Regular expressions are strings where several of the non-alphanumeric characters have special meaning. They provide a concise and flexible means for string searching and replacing and are used by several Unix programs.

5.8.1 Anchoring

- `^` - match start of line
- `$` - match end of line

5.8.2 Characters

- `character` - the indicated character
- `.` - any character
- `[...]` - any character in the list or range (^ inverts)

5.8.3 Combining

- `(...)` - group
- `...|...` - match either or

5.8.4 Repetition

- `?` - match zero or one times
- `*` - match zero or more times
- `+` - match one or more times
- `{...}` - match a range of times

5.8.5 Replacement

- `\digit` - substitute text matched by corresponding group

SEARCH

- search