### Linux Bootcamp

An introduction to the Linux environment

v2018-11





#### Programme

- Linux Basics
  - What is Linux
  - Using the BASH shell to run and automate programs
- Installing and managing software
  - Understanding the file system
  - Installing operating system packages
  - Installing external software
  - Installing packages for other languages (R, Python, Perl)
- Other Useful Stuff
  - Using containers
  - Remote connections through SSH
  - Installing operating systems on hardware or virtual machines
  - Using Linux in a cloud environment

#### Learning Outcomes

- By the end of the course you should be able to:
  - 1. Install a Linux operating system on your machine, either directly or through a virtual machine
  - 2. Be able to run and customise installed applications using the BASH shell
  - 3. Be able to perform simple automation, linking programs together and iterating the processing of large numbers of files.
  - 4. Be able to install and configure new software packages
  - 5. Understand how to use Linux in a variety of environments from personal computers to cloud infrastructure.

### Linux Basics

Understanding Linux and the BASH shell

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#### What (exactly) is Linux?















#### Unix, Posix and Linux

- Unix was a set of concepts which defined a number of early operating systems developed in the 1970s.
- These concepts allowed for interoperability of software written based on them.
- The original Unix concepts developed into POSIX, a more formal standard defining
  - The way that devices, configuration, memory and libraries are handled
  - A standardised development environment based on C and make
  - A core set of commands and a command interpreter (shell) in which to run them
  - A standard set of documentation



#### Linux - what most people now use (apart from OSX!)

- Linux is more correctly called GNU/Linux
  - Linux is the kernel
  - GNU is a collection of applications and libraries
- POSIX
  - The way that devices, configuration, memory and libraries are handled
  - A standardised development environment based on C and make
  - A core set of commands and a shell in which to run them
  - A standard set of documentation





#### Linux comes in different distributions

#### • They vary in

- Their choice of (non-core) software
- Their support packages (the way software is installed for example)
- How much non-core software they provide
- Their frequency of update and length of support



### Most Popular Distributions

- Ubuntu
  - Mostly aimed at desktop users
  - Friendly and well supported
  - Regular updates (some with long term support)
  - Based on Debian
  - Other offshoots such as Mint
- CentOS
  - Free version of the RedHat commercial distro
  - Mostly aimed at servers
  - Stable software and long term support
  - Used in many large environments

# ubuntu®



### Specialised Distributions

- Bio Linux
  - Many pre-built scientific programs
  - Based on Ubuntu





- ROCKS
  - Linux distribution to run on clusters
  - Includes automated building and management
  - Based on CentOS

## Running programs in the BASH shell

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#### Running programs in Linux

- Two major methods
  - Graphical
  - Command line
- Graphical launches only work for graphical programs accessed through a graphical environment
- Most data processing will be command line based, as will most remote access
  - Graphical programs can still be launched from the command line

#### Shells

- A shell is a command line interpreter, used to launch software in Linux
- There are many different shells available:
  - BASH
  - CSH
  - ZSH etc.
- Most software will work the same in all shells
- Some functions and automation are different between shells
- We will use the most popular shell, BASH

#### What does a shell provide

- Command line editing and construction tools (eg auto complete)
- History
- Job control
- Configuration management (startup scripts)
- Aliases
- Automation
  - Scripting language
  - Variables, functions etc

#### Running programs in BASH

- We will be using a graphical terminal running BASH
- Right click and select "Open terminal"
- ...or, from Applications menu find Terminal
- Once running, right click on icon and select "Add to favourites"

Activities	🔄 Ter	minal 🔻
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#### Running programs

- Type the name of the program you want to run
- Add on any options the program needs
- Press return the program will run
- When the program ends control will return to the shell
- Run the next program!

#### Running programs

babraham@babraham-VirtualBox:~\$ ls
Desktop Documents Downloads examples.desktop Music
Pictures Public Templates Videos

babraham@babraham-VirtualBox:~\$

Command prompt - you can't enter a command unless you can see this

- The command we're going to run (1s in this case, to list files)
- The output of the command just text in this case

### Running graphical programs

babraham@babraham-VirtualBox:~\$ xeyes



babraham@babraham-VirtualBox:~\$

Note that you can't enter another command until you close the program you launched



Each option or section is separated by spaces. Options or files with spaces in must be put in quotes.

#### Command line switches

- Change the behaviour of the program
- Come in two flavours (each option usually has both types available)
  - Minus plus single letter (eg -x -c -z)
    - Can be combined (eg -xcz)
  - Two minuses plus a word (eg --extract --gzip)
    - Can't be combined
- Some take an additional value, this can be an additional option, or use an = to separate (it's up to the program)
  - -f somfile.txt (specify a filename)
  - --width=30 (specify a value)

#### Manual pages

- All core programs will have a manual page to document the options for the command
- Manual pages are accessible using the man program followed by the program name you want to look up.
- All manual pages have a common structure

#### Manual Pages (man cat)

CAT (1)

User Commands

#### NAME

cat - concatenate files and print on the standard output

#### SYNOPSIS

cat [OPTION]... [FILE]...

#### DESCRIPTION

Concatenate FILE(s) to standard output.

With no FILE, or when FILE is -, read standard input.

```
-A, --show-all
equivalent to -vET
```

```
-n, --number
number all output lines
```

```
-T, --show-tabs
display TAB characters as ^I
```

```
--help display this help and exit
```

#### EXAMPLES

```
cat f - g
```

Output f's contents, then standard input, then g's contents.

cat Copy standard input to standard output.

CAT(1)

### Exercise 1

Understanding Unix File Systems

#### Unix File Systems

- Consists of a hierarchical set of directories (folders)
- Each directory can contain files
- No drive letters (drives can appear at arbitrary points in the file system)
- No file extensions (you can add them, but they're not required)

#### A simple unix filesystem

(Always the top of the file system) home / (Directory containing all home directories) anne/ simon/ DOCUMENTS / (All names are case sensitive) test.txt (A file we want to work with) /home/simon/Documents/test.txt media/ MVUSb/ (A USB stick added to the system)

#### Drives in a Linux file system

\$ mount /dev/sda1 on / type ext4 (rw) /dev/sda5 on /state/partition1 type ext4 (rw) /dev/sda2 on /var type ext4 (rw) Private-Cluster.local:/ifs/homes on /bi/home type nfs (rw,addr=10.99.101.5) Private-Cluster.local:/ifs/Scratch/Scratch on /bi/scratch type nfs (rw, addr=10.99.101.5) Private-Cluster.local:/ifs/Group on /bi/group type nfs (rw, addr=10.99.101.4) Private-Cluster.local:/ifs/apps-nfs on /bi/apps type nfs (rw, addr=10.99.101.5) central-cluster.local:/ifs/bioinformatics/pubcache on /bi/pubcache type nfs (rw, addr=10.99.102.7) central-cluster.local:/ifs/bioinformatics/seqfac on /bi/seqfac/seqfac type nfs (ro, addr=10.99.102.6) /dev/fuse on /bi/sequencing type fuse (ro,nosuid,nodev,allow\_other)

### Specifying file paths

- Some shortcuts
  - ~ (tilde, just left of the return key) the current user's home directory
  - . (single dot) the current directory
  - .. (double dot) the directory immediately above the current directory



### Specifying file paths

- Absolute paths from the top of the file system
  - /home/simon/Documents/Course/some\_file.txt
- Relative paths from whichever directory you are currently in
  - If I'm in /home/simon/Documents/Course/
  - ../../Data/big\_data.csv
    - is the same as /home/simon/Data/big\_data.csv
- Paths using the home shortcut
  - ~/Documents/Course/some\_file.txt will work for user simon anywhere on the system

#### Command line completion

- Most errors in commands are typing errors in either program names or file paths
- Shells (ie BASH) can help with this by offering to complete path names for you
- Command line completion is achieved by typing a partial path and then pressing the TAB key (to the left of Q)

#### Command line completion

Actual files in a folder:

Desktop Documents Downloads examples.desktop Music Pictures Public Templates Videos If I type the following and press tab:

De [TAB] will complete to Desktop as it is the only option

T [TAB] will complete to Templates as it is the only option

Do [TAB] will no nothing (just beep) as it is ambiguous

Do [TAB] [TAB] will show Documents and Downloads since those are the only options

Do [TAB] [TAB] c [TAB] will complete to Documents

You should ALWAYS use TAB completion to fill in paths for locations which exist so you can't make typing mistakes (it obviously won't work for output files though)

#### Wildcards

- Another function provided by your shell (not your application)
- A quick way to be able to specify multiple related file paths in a single operation
- There are two main wildcards
  - \* = Any number of any characters
  - ? = One of any character
- You can include them at any point in a file path and the shell will expand them before passing them on to the program
- Multiple wildcards can be in the same path.
- Command line completion won't work after the first wildcard
#### Wildcard examples

#### \$ ls Monday/\*txt

Monday/mon\_1.txt Monday/mon\_2.txt Monday/mon\_3.txt Monday/mon\_500.txt

#### \$ ls Monday/mon\_?.txt

Monday/mon\_1.txt Monday/mon\_2.txt Monday/mon\_3.txt

#### \$ ls \*/\*txt

Friday/fri\_1.txt Monday/mon\_1.txt Monday/mon\_3.txt Tuesday/tue\_1.txt
Friday/fri 2.txt Monday/mon 2.txt Monday/mon 500.txt Tuesday/tue 2.txt

#### \$ ls \*/\*1.txt

Friday/fri\_1.txt Monday/mon\_1.txt Tuesday/tue\_1.txt

#### The structure of a Unix command



Each option or section is separated by spaces. Options or files with spaces in must be put in quotes.

# Programs for manipulating files

# Manipulating files

- You will spend a lot of time managing files on a Linux system.
  - Viewing files (normally text files)
  - Editing text files
  - Moving or renaming files
  - Copying files
  - Deleting files
  - Finding files

# Viewing Files

- Simplest solution
  - cat Sends the entire contents of a file (or multiple files) to the screen.
- Quick look
  - head or tail will look at the start/end of a file
    - head -10 [file]
    - tail -20 [file]
- More scalable solution
  - less is a 'pager' program, sends output to the screen one page at a time

• Return / j	=	move down one line	less -S (no wrapping)
• k	=	move up one line	
<ul> <li>Space</li> </ul>	=	move down one page	
• b	=	go back one page	
• /[term]	=	search for [term] in the file	
• q	=	quit back to the command prompt	

# Editing files

- Lots of text editors exist, both graphical and command line
- Many have special functionality for specific content (C, HTML etc)
- Technically, only the  $v \mbox{i}$  editor is required to be present in POSIX
- nano is a simple command line editor which is nearly always present
- You can try several until you find one you like

## Using nano to edit text files

#### • nano [filename] (edits if file exists, creates if it doesn't)

GNU nano 2.9.3	test.txt	Modified			
This is the nano tex	t editor.				
You can type stuff i	n here				
The options at the bottom are commands, the ^ means the control key					
eg: Control+K cuts the current line of text and Control+U will paste it.					
Control+O will write out the current contents of the editor, and Control+X will exit back to the shell.					
^G Get Help ^O W ^X Exit ^R F	Nrite Out <b>^W</b> Where Is <mark>^K</mark> Cut Text <b>^J</b> Jus Read File <b>^\</b> Replace <b>^U</b> Uncut Text <b>^T</b> To	stify ^C Cur Pos Spell ^ Go To Line			

# Moving / Renaming files

- Uses the  $\mathrm{mv}$  command for both (renaming is just moving from one name to another)
- mv [file or directory] [new name/location]
- If new name is a directory then the file is moved there with its existing name
- Moving a directory moves all of its contents as well
- Examples
  - mv old.txt new.txt
  - mv old.txt ../Saved/
  - mv old.txt ../Saved/new.txt
  - mv ../Saved/old.txt .

# Copying files

- $\bullet$  Uses the  ${\tt cp}$  command
- cp [file] [new file]
- Operates on a single file
- Can copy directories using recursive copy (cp −r)
- Examples
  - cp old.txt new.txt
  - cp old.txt ../Saved/
  - cp old.txt ../Saved/new.txt
  - cp ../Saved/old.txt .
  - cp -R ../Saved ./NewDir
  - cp -R ../Saved ./ExistingDir/ (only if ExistingDir exists)

# Linking rather than copying

- Copy duplicates the data in a file
  - Can be a problem with big data files
  - Can be a problem if you want edits to propagate
- Links are a way to do 'virtual' copies. You can make the same file appear in more than one place.
- Two types of link
  - Hard link completely indistinguishable from a copied file
    - Only works on the same disk (can't span file systems)
    - Only works for files (not directories)
  - Symbolic (or soft) link
    - Is visible as a link, but can still be used as if it is a file
    - Can work across file systems
    - Can be used for directories as well as files
    - Normally the safe option to use

## Creating symbolic links

- Use the  $\mbox{ln}$  command with the  $-\mbox{s}$  modifier
- Usage ln -s [from] [to]
- Exactly the same structure as mv
- When you list a link you can see where it points, but you can use it like a file

\$ cat test.txt
This is a test file

#### \$ ln -s test.txt test2.txt

\$ ls -l test2.txt

lrwxrwxrwx 1 babraham babraham 8 Sep 11 16:27 test2.txt -> test.txt

\$ cat test2.txt
This is a test file

# Deleting files

- Linux has no undo.
- Deleting files has no recycle bin.
- Linux will not ask you "are you sure"
- Files can be deleted with the  $\mbox{rm}$  command
- Directories (and all of their contents) can be deleted with  ${\tt rm}$   $-{\tt r}$
- Examples
  - rm test\_file.txt test\_file2.txt
  - rm \*.txt (be VERY careful using wildcards. Always run is first to see what will go)
  - rm -r Old\_directory/

# Finding files

- From the command line there are two main mechanisms
  - Using locate
    - Uses a pre-built index, so is \*VERY\* quick
    - Needs to be installed and configured (isn't on all distributions)
    - Only works on local drives not network shares
  - Using find
    - Searches fresh each time
    - Can be slow if you're searching large numbers of files
    - Requires no pre-processing

# Using find

- find [options/filters] [place to start] [action]
- Options / Filters
  - -name thisfile.txt
  - -name \*txt
  - -type f -empty
- Action
  - -print
  - -exec (any command include { } for filename need to finish with  $\$ ;)

#### Find examples

- find ~ -name \*fastq.gz -print
- find /etc/ -name \*conf -exec wc -l '{}' \;
- find ~ -type l -print

# Exercise 2

# Finding programs to run



- How does the system know which executable file to run when you just supply a name (like ls in this example) rather than a file path?
- What happens when you have two different programs with the same name?

#### The PATH environment variable

- Two new concepts which will be reused a lot:
  - 1. A search path is a list of directories which the shell will iterate over to try to find something (a program in this case). It is an ordered list and the first hit will be returned.
  - 2. Shells use "environment variables" as a small scale storage and configuration system. They are a set of key/value pairs which provide named pieces of data which influence the behaviour of the shell or programs which it runs. Some environment variables are created by default, but you can modify these, or add your own.

## The PATH environment variable

- You can see the current PATH contents by running:
  - echo \$PATH
  - /usr/local/sbin:/usr/local/bin:/usr/sbin:/usr/bin:/sbin:/bin:/usr/games:/usr/local/games:/snap/bin
- These are the directories which are trusted to contain good programs which you can launch just using their name
- Other programs can be launched using their location (rather than name)
- You can find the location of a named program using which
  - which ls (produces /bin/ls which is where the ls program is)

# Setting the PATH

- PATH is an environment variable, you can set it the same as any other variable, using the export function
- export PATH=/one/folder:/another/folder
- Normally you want to just add to the existing PATH, so you can include the current <code>\$PATH</code> in the definition
- export PATH=/new/folder/:\$PATH
- You can write this into ~/.bashrc to make the change permanent.

# Exercise 3

# More advanced BASH usage

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## What we know already

- How to run existing programs
  - Those which are in the PATH
  - Those which are somewhere else
- How to modify the options for a program using switches
- How to supply data to programs using file paths and wildcards

#### What else can we do

- Record the output of programs
- Check for errors in programs which are running
- Link programs together into small pipelines
- Automate the running of programs over batches of files
- All of these are possible with some simple BASH scripting

# Recording the output of programs

- One of the aspects of POSIX is a standard system for sending data to and from programs.
- Three data streams exist for all Linux programs (though they don't have to use them all)
  - STDIN (Standard Input a way to send data into the program)
  - STDOUT (Standard Output a way to send expected data out of the program)
  - STDERR (Standard Error a way to send errors or warnings out of the program)
- By default STDOUT and STDERR are connected to your shell, so when you see text coming from a program, it's coming from these streams.

Recording the output of programs



 Rather than leaving these streams connected to the screen, you can link them to either files, or other programs to either create logs, or to build small pipelines

## Redirecting standard streams

- You can redirect using arrows at the end of your command
  - > [file] Redirects STDOUT
  - < [file] Redirects STDIN
  - 2> [file] Redirects STDERR
  - 2>&1 Sends STDERR to STDOUT so you only have one output stream

\$ find . -print > file\_list.txt 2> errors.txt

\$ ls

Data Desktop Documents Downloads **errors.txt** examples.desktop **file\_list.txt** Music Pictures Public Templates Videos

\$ head file\_list.txt

- / -
- ./Downloads ./Pictures
- ./Public
- ./Public
- ./Music
- ./.bash\_logout
- ./.local
- ./.local/share
- ./.local/share/icc
- ./.local/share/icc/edid-33d524c378824a7b78c6c679234da6b1.icc

# Throwing stuff away

- Sometimes you want to be able to hide output
  - STDOUT I just want to test whether something worked
  - STDERR I want to hide progress / error messages
- Linux defines a special file /dev/null which you can write to but just discards all data sent to it
  - might\_fail > /dev/null
  - chatty\_app 2> /dev/null

# Linking programs together

- Part of the original UNIX design was to have lots of small programs doing specific jobs, and then to link them together to perform more advanced tasks.
- There are a couple of mechanisms to do this
  - Pipes
  - Backticks

# Linking programs together using pipes

- Pipes are a mechanism to connect the STDOUT of one program to the STDIN of another. You can use them to build small pipelines
- To create a pipe just use a pipe character | between programs
- pr1 | pr2 is the equivalent to pr1 > temp; pr2 < temp

\$ ls | head -2 Data Desktop

# Useful programs for pipes

- Whilst you can theoretically use pipes to link any programs, there are some which are particularly useful, these are things like:
  - $\mathsf{wc}\,$  to do word and line counting
  - grep to do pattern searching
  - sort to sort things
  - uniq to deduplicate things
  - less to read large amounts of output
  - zcat/gunzip/gzip to do decompression or compression

# Small example pipeline

 Take a compressed fastq sequence file, extract from it all of the entries containing the telomere repeat sequence (TTAGGG) and count them

#### • zcat file.fq.gz | grep TTAGGGTTAGGG | wc -1

```
$ zcat file.fq.gz | wc -1
179536960
```

```
$ zcat file.fq.gz | grep TTAGGGTTAGGG | wc -1
3925
```

## Using backticks to capture output

- Pipes are great to link streams of data together, but they need to be supported by both programs
- In some cases you want to use the output of one program as an argument to another one.
- You can do this using backticks these are like quotes, but their contents are executed, and the contents are replaced with the STDOUT of the executed code

## Backticks example

- I want to find out where a program (fastqc) is installed, and I want to find out whether that location is a real file, or a symlink to somewhere else.
- I can do this in 2 separate steps, but this involves copy/paste
  - which fastqc
  - ls -l [whatever came out of step 1]
- Backticks let you do this in a single step.

\$ ls -1 `which fastqc`
-rwxr-xr-x 1 andrewss bioinf 14400 Dec 21 2017 /bi/apps/fastqc/0.11.7/fastqc

#### Iterating over files

- When processing data it is common to need to re-run the same command multiple times for different input/output files.
- Some programs will support being provided with multiple input files, but many will not.
- You can use the automation features of the BASH shell to automate the running of these types of programs
### The BASH for loop

- Simple looping construct
  - Loop over a set of files
  - Loop over a set of values
- Creates a temporary environment variable which you can use when creating commands

### Examples of for loops

```
for value in {5,10,20,50}
    do
    run_simulation --iterations=$value > ${value}_iterations.log 2>&1
    done
```

```
for value in {10..100}
    do
    run_simulation --iterations=$value > ${value}_iterations.log 2>&1
    done
```

```
for file in *txt
   do
   echo $file
   grep .sam $file | wc -l
   done
```

### Job Control

- By default you run one job at at time in a shell
  - Shells support multiple running jobs
- States of job
  - Running foreground (shell has the attention of the job)
  - Running background (output goes to the shell but other jobs can run)
  - Suspended background (job exists but is paused, consumes no CPU)
  - Running disconnected (output is no longer attached to the shell)

### Job Control

- prog\_to\_run (starts in foreground)
- •prog\_to\_run &

(starts in background)

- Control of running jobs
  - jobs (lists the jobs in this shell)
  - Control + Z (suspends the current job)
  - $\operatorname{bg}$  (puts the current suspended job into the background
  - fg [number] (puts the selected job back in the foreground)

### Job Control - nohup

- nohup prog\_to\_run
  - Merges STDOUT and STDERR
  - Disconnects from the terminal
  - Can't be killed when the terminal exits
  - Output appended to nohup.out
  - Can redirect with > logfile.txt

### Job Control - listing and killing processes

ps
ps -fu [username]
ps -ef
(list my processes associated with this shell)
(list all processes for user [username])
(list all processes on the system)

```
$ ps -fu andrewss
UTD
         PTD PPTD
                   C STIME TTY
                                       TIME CMD
andrewss 14510 1
                   0 Sep26 ?
                                   00:00:02 ls --color=auto
andrewss 15496 15494 0 10:21 ?
                                   00:00:00 sshd: andrewss@pts/36
andrewss 15497 15496
                   0 10:21 pts/36
                                   00:00:00 -bash
andrewss 17195 1 0 Sep26 ?
                                   00:00:11 /usr/libexec/openssh/sftp-
server
andrewss 17955 1 0 Sep26 ?
                                  00:00:11 ls --color=auto
andrewss 20618 15497 0 11:03 pts/36
                                  00:00:00 ps -fu andrewss
```

### Job Control - listing and killing processes

- You can only kill your own processes
- kill [PID] (Nicely ask this process to stop)
  kill -9 [PID] (Force this process to abruptly stop)

# Exercise 4

# Installing and Managing Software

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## Different types of software

- Software comes in different types
  - Interpreted scripts
  - Pre-compiled binary software
  - Source code requiring compilation
- Software comes from different sources
  - Distributed with your operating system
  - Distributed by some other software management system
  - Downloaded from a specific site on the internet

### Users, roles and permissions

- Software can be installed just for an individual user
- Most software is installed in a way which allows all users to run it
- You need to understand users, roles and permissions to install software

### Users and Roles

- For security and privacy most users run with restricted privileges most of the time
  - They can only read some parts of the file system (eg: not other users data for)
  - They can only write to some parts of the file system (eg: can't overwrite important programs)
- The 'root' user is an account which has full privileges on the system and is used for administrative purposes

### Using the root account

- Log in as root requires knowledge of the root account password. Quite dangerous as everything runs with full privileges.
- Use su to move from a user account to the root account. Can be done within a session, but still requires the root account password.
- Use sudo to selectively run some commands as root. Can restrict which commands can be run and log them. Can use the users own password to authenticate
- Running programs with the suid or sgid permissions set on them

## File / Directory Permissions

- Every file and directory has a number of permissions. There are 3 types
  - 1. Read permission
  - 2. Write permission
  - 3. Execute permission (list permission on directory)
- The permissions apply to 3 classes of user
  - 1. The owner of the file/directory
  - 2. The members of the file/directories group
  - 3. Everyone else

### File / Directory Permissions





## Changing permissions / ownership

### • chmod

- u (user) / g (group) / a (all)
- + / (add or remove permission)
- r (read) / w (write) / x (execute/list)
- File/directory list

chmod g+wx my.file chmod ga-x my.file chmod -R u-w my.dir

• Can add -R to change permissions for a directory and all of its contents

### Special permission bits

- User level special bit (SUID)
  - Applies to executable files
  - Will execute as root, even for a normal user
- Group level special bit (SGID)
  - Can apply to executables or directories
  - On executables executes as the group of the file
  - On directories it forces any newly created files to inherit the group of the parent
- chmod u+s [file]
- chmod g+s [file]

### Where to install software

- In theory you can install software anywhere on the system, but there are places where software is expected to be installed.
- If you don't have admin access, or you are installing just for yourself you can install into your home directory.
- For site-wide packages you should follow the rules set out by the File Hierarchy Standard (FHS), which defines the expected locations of software on a POSIX system

### FHS Locations

- There are two types of application
  - Those which follow a standard structure for dividing the files they use between a set of related directories. These will be all system software and some add in packages
    - bin executable files things you'd actually run
    - lib library files code which is shared between programs and doesn't run directly
    - share other data files used by applications
  - Those which bundle all of their code and data under a single directory and don't split it up
    - These will be the majority of scientific applications and other non-core software

### FHS Installation Locations

- If software follows the FHS division of sub-folders then it can go in a few places
  - /bin and /sbin are only for vital software packaged by the operating system, software in /sbin is to be used only by admins
  - /usr/bin and /usr/sbin are similar, but are for non-vital software
  - /usr/local (with executables in /usr/local/bin) is for software installed outside the operating systems package manager, but for software which follows the FHS standard
- Non-FHS packages are generally recommended to be installed under  $/\operatorname{opt}$

## Installing operating system packages

- Nearly all Linux distributions come with a set of optional software packages for a wide range of applications
- They use a package manager program to allow you to add and remove packages
- Package managers handle installation of the required software as well as any dependencies. They also handle updates.
- There are two main package managers
  - Apt (advanced packaging tool) Ubuntu, Debian, Mint
  - Yum (Yum updater modified) RedHat, CentOS, Fedora

# Using a package manager (command line)

All operations (except searches) need to run under sudo

### APT

- apt install [package name]
- apt search [search term]
- apt upgrade
- apt purge [package name]

### YUM

- yum install [package name]
- yum search [search term]
- yum update
- yum remove [package name]

## The good and bad of OS packages

Good

• Very easy to install

Bad

• Limited software availability

- Will resolve dependencies and install them
- Only one version of any package
- Sometimes not up to date
- Guaranteed compatible with the rest of your system
- More difficult to get support from authors

### OS Package Example - JRE (Java)

### # apt install default-jre

Reading package lists... Done The following additional packages will be installed: ca-certificates-java default-jre-headless fonts-dejavu-extra java-common libatk-wrapper-java libatk-wrapper-java-jni libgif7 openjdk-11-jre openjdk-11-jre-headless Suggested packages: default-java-plugin fonts-ipafont-gothic fonts-ipafont-mincho fonts-wgy-microhei | fonts-wgy-zenhei The following NEW packages will be installed ca-certificates-java default-jre default-jre-headless fonts-dejavu-extra java-common libatk-wrapper-java libatkwrapper-java-jni libgif7 openjdk-11-jre openjdk-11-jre-headless 0 to upgrade, 10 to newly install, 0 to remove and 0 not to upgrade. Need to get 41.6 MB of archives. After this operation, 191 MB of additional disk space will be used. Do you want to continue? [Y/n] **Y** Get:1 http://gb.archive.ubuntu.com/ubuntu bionic/main amd64 java-common all 0.63ubuntu1~02 [7,032 B] Unpacking java-common (0.63ubuntu1~02) ... Setting up default-jre (2:1.10-63ubuntu1~02) ... Processing triggers for libc-bin (2.27-3ubuntul) ... Processing triggers for ca-certificates (20180409) ...

0 added, 0 removed; done.

Running hooks in /etc/ca-certificates/update.d...

# Exercise 5

### Installing pre-compiled binaries

- These are the easiest type of installation to perform
- You need to make sure that you have the correct download for your operating system and architecture (32bit vs 64bit)
- Installation is normally just extracting the files from the archive
- You can add the new directory to the PATH, or link the executables to a location already in <code>\$PATH</code> to make them easier to work with
- You *might* need to check for library compatibility

### Some useful related functions

- Downloading files from the internet via command line
- Compression systems and archive files

### Downloading via command line

- The first stage in most installations is to download the packaged software from the project web site.
- To do this from the command line you can use the wget program which simply takes the URL you want to download as an argument

\$ wget https://www.bioinformatics.babraham.ac.uk/projects/fastqc/fastqc\_v0.11.7.zip

## Extracting from archive files

- Most software is distributed as a single archive file to make it simpler, and to allow it to be compressed
- The two major formats used are:
  - Zip a container which is compressed by default
  - Tar a container which can optionally be compressed
    - tar.gz = gzip compression
    - tar.bz2 = bzip compression
- The first step in most software installations is to extract from the archive

## Extracting from zip files

• Use the unzip program. Very simple. Don't normally supply options.

\$ unzip fastqc\_v0.11.7.zip Archive: fastqc\_v0.11.7.zip creating: FastQC/ inflating: FastQC/cisd-jhdf5.jar creating: FastQC/Configuration/ inflating: FastQC/Configuration/adapter\_list.txt inflating: FastQC/Configuration/contaminant\_list.txt inflating: FastQC/Configuration/limits.txt inflating: FastQC/Configuration/limits.txt inflating: FastQC/fastqc inflating: FastQC/fastqc\_icon.ico creating: FastQC/Help/ etc...

### Extracting from tar files

- $\bullet$  Uses the <code>tar</code> program with the following options
  - -x (extract data)
  - -v (be verbose show what you're extracting optional)
  - -z (decompress gzipped archive for tar.gz files)
  - -j (decompress bzipped argive for tar.bz files)
  - -f [file] (the tar file to extract from)

#### \$ tar -xzvf bismark\_v0.20.0.tar.gz Bismark\_v0.20.0/ Bismark\_v0.20.0/bismark Bismark\_v0.20.0/coverage2cytosine Bismark\_v0.20.0/bismark2report Bismark\_v0.20.0/bismark2report Bismark\_v0.20.0/deduplicate\_bismark Bismark\_v0.20.0/bismark2summary Bismark\_v0.20.0/bismark2summary Bismark\_v0.20.0/bismark2bedGraph Bismark\_v0.20.0/Docs/ Bismark\_v0.20.0/Docs/ Bismark\_v0.20.0/plotly/ Bismark\_v0.20.0/plotly/ Bismark\_v0.20.0/plotly/ Bismark\_v0.20.0/bismark\_methylation\_extractor

### Binary install example - bowtie2

• This is a short read aligner, distributed as a binary zip file

Home / Browse / Development / Text Processing / Bowtie / Files Bowtie Brought to you by: ben_langmead, ch4rr0, ctrapnell, mcschatz													
Summary	Files	Reviews	Support	Wiki	Mailing Lists	Tickets 🔹	Discussion	Code					
Download Latest Version bowtie2-2.3.4.2-source.zip (5.7 MB)       Get Updates         Home / bowtie2 / 2.3.4.2       Image: Comparison of the source state of the source st													
Name 🖨				I	Modified ≑	Size 🖨	Downloads / \	Week 🖨					
Parent folder													
bowtie2-2.3.4.2-macos-x86_64.zip				2	2018-08-08	11.5 MB	114 🛌	(i)					
bowtie2-2.3.4.2-linux-x86_64.zip				2	2018-08-08	54.8 MB	359 🔟	(i)					
bowtie2-2.3.	4.2-sourc	e.zip		2	2018-08-08	5.7 MB	319 🔛	(i)					
Totals: 3 Item	ıs					72.0 MB	792						



Be careful which download link you select

The main (green) link here is for the source code, not the Linux binaries

### Binary install example - bowtie2

We need to be root as we're installing outside our home

\$ sudo su

cd /opt/

It's a self-contained app, so goes in /opt

# wget https://kent.dl.sourceforge.net/project/bowtie-bio/bowtie2/2.3.4.2/bowtie2-2.3.4.2-linux-x86\_64.zip

2018-09-12 14:22:14 (3.00 MB/s) - 'bowtie2-2.3.4.2-linux-x86\_64.zip' saved [54761153/54761153]

#### # unzip bowtie2-2.3.4.2-linux-x86\_64.zip

Archive: bowtie2-2.3.4.2-linux-x86\_64.zip creating: bowtie2-2.3.4.2-linux-x86\_64/ inflating: bowtie2-2.3.4.2-linux-x86\_64/bowtie2-align-l inflating: bowtie2-2.3.4.2-linux-x86\_64/bowtie2-align-l-debug

#### # cd bowtie2-2.3.4.2-linux-x86\_64

### # **ls**

AUTHORS	bowtie2-align-s	bowtie2-build-l-debug	bowtie2-inspect-l	doc	MANUAL.markdown	VERSION
bowtie2	bowtie2-align-s-debug	bowtie2-build-s	bowtie2-inspect-l-debug	example	NEWS	
bowtie2-align-l	bowtie2-build	bowtie2-build-s-debug	bowtie2-inspect-s	LICENSE	scripts	
bowtie2-align-l-debug	bowtie2-build-l	bowtie2-inspect	bowtie2-inspect-s-debug	MANUAL	TUTORIAL	

./bowtie2 --help It's not in PATH, so we need to use ./bowtie2 to launch it

Bowtie 2 version 2.3.4.2 by Ben Langmead (langmea@cs.jhu.edu, www.cs.jhu.edu/~langmea) Usage:

bowtie2 [options]\* -x <bt2-idx> {-1 <m1> -2 <m2> | -U <r> | --interleaved <i>} [-S <sam>]

# ln -s /opt/bowtie2-2.3.4.2-linux-x86\_64/bowtie2 /usr/local/bin/

We can link the executable into a directory in PATH

### Libraries

- Most binary applications make use of dynamic linking
- Some functionality is not in the application but is taken from 'library' files
  - Come with the operating system
  - Distributed with the application
- Libraries allow for
  - Updating without rebuilding the application
  - Removal of duplicate code
## Checking library compatibility

- Most binaries are dynamically linked
  - Additional functionality pulled from system libraries at runtime
- If the libraries are missing / wrong versions then the application won't work
- Installing the missing libraries will usually fix things.
- You can see the requirements with ldd

## Example of Idd usage

#### \$ ldd `which ssh`

linux-vdso.so.1 (0x00007ffef7598000) libselinux.so.1 => /lib/x86 64-linux-gnu/libselinux.so.1 (0x00007f68e7899000) libcrypto.so.1.0.0 => /usr/lib/x86\_64-linux-gnu/libcrypto.so.1.0.0 (0x00007f68e7456000) libdl.so.2 => /lib/x86\_64-linux-gnu/libdl.so.2 (0x00007f68e7252000) libz.so.1 => /lib/x86 64-linux-gnu/libz.so.1 (0x00007f68e7035000) libresolv.so.2 => /lib/x86\_64-linux-gnu/libresolv.so.2 (0x00007f68e6e1a000) libgssapi krb5.so.2 => /usr/lib/x86 64-linux-gnu/libgssapi krb5.so.2 (0x00007f68e6bcf000) libc.so.6 => /lib/x86 64-linux-gnu/libc.so.6 (0x00007f68e67de000) libpcre.so.3 => /lib/x86 64-linux-gnu/libpcre.so.3 (0x00007f68e656c000) /lib64/ld-linux-x86-64.so.2 (0x00007f68e7d77000) libkrb5.so.3 => /usr/lib/x86 64-linux-gnu/libkrb5.so.3 (0x00007f68e6296000) libk5crypto.so.3 => /usr/lib/x86 64-linux-gnu/libk5crypto.so.3 (0x00007f68e6064000) libcom err.so.2 => /lib/x86 64-linux-gnu/libcom err.so.2 (0x00007f68e5e60000) libkrb5support.so.0 => /usr/lib/x86\_64-linux-gnu/libkrb5support.so.0 (0x00007f68e5c55000) libpthread.so.0 => /lib/x86 64-linux-gnu/libpthread.so.0 (0x00007f68e5a36000) libkeyutils.so.1 => /lib/x86 64-linux-gnu/libkeyutils.so.1 (0x00007f68e5832000)

## Library search path

- Libraries are identified by using a search path
  - Some hard-coded components
  - Some components added by the application
  - Some components can be configured by the user
- System library directories (/lib /usr/lib)
- Application library directories (usually relative to the application itself)
- User components (via the LD\_LIBRARY\_PATH environment variable)

## Library search path

#### \$ ldd jellyfish Linux-vdso.so.1 => (0x00007ffd4a352000) libpthread.so.0 => /lib64/libpthread.so.0 (0x00000376b400000) libjellyfish-2.0.so.2 => not found libstdc++.so.6 => /usr/lib64/libstdc++.so.6 (0x000003770400000) libm.so.6 => /lib64/libm.so.6 (0x00000376ac00000) libgcc\_s.so.1 => /lib64/libgcc\_s.so.1 (0x00000376f000000) libc.so.6 => /lib64/libc.so.6 (0x00000376a800000) /lib64/ld-Linux-x86-64.so.2 (0x00000376a400000)

## Installing script files

- Some software is written as cross-platform scripts.
- These are distributed as source code, but do not need to be compiled to run. They are written in interpreted languages such as perl, python, ruby etc.
- Installation is similar to that for binary executables

## Script install example - bismark

\$ sudo su

# cd /opt

# wget http://www.bioinformatics.babraham.ac.uk/projects/bismark/bismark\_v0.20.0.tar.gz

2018-09-12 14:49:19 (60.6 MB/s) - 'bismark v0.20.0.tar.gz' saved [1411124/1411124]

# tar -xzvf bismark\_v0.20.0.tar.gz Bismark\_v0.20.0/ Bismark\_v0.20.0/bismark Bismark\_v0.20.0/coverage2cytosine Bismark\_v0.20.0/bismark2report

# cd Bismark\_v0.20.0/
# ./bismark --help

DESCRIPTION

The following is a brief description of command line options and arguments to control the Bismark bisulfite mapper and methylation caller. Bismark takes in FastA or FastQ files and aligns the reads to a specified bisulfite genome. Sequence reads are transformed into a bisulfite converted

# export PATH=/opt/Bismark\_v0.20.0/:\$PATH

## Running script based programs

### • Two methods:

- Call the interpreter and pass the script
- Execute the script directly interpreter taken from the first line

```
# perl bismark --version
Bismark - Bisulfite Mapper and Methylation Caller.
Bismark Version: v0.20.0
# bismark --version
Bismark - Bisulfite Mapper and Methylation Caller.
```

Bismark Version: v0.20.0

## Script 'shebang' lines

- The first line of a script file starts with #! [interpreter]
- If your interpreter is in a different location you can edit the first line
- You can also use the env program to take the first instance from your PATH

#!/usr/bin/perl

#!/opt/perl\_5.28.0/bin/perl

#!/usr/bin/env perl

# Exercise 6

## Installing from source code

- Most software distributed as source code is written in C or C++
- Should come with a BUILD.txt or INSTALL.txt file
- Most programs will use a build system to manage compilation
  - make
  - cmake
- Many will use the autotools system to manage differences in configuration
- Compilation will require various accessory packages to work

## Anatomy of C/C++ compilation



## Libraries and headers

- We mentioned libraries earlier, as a way to include common code in several applications without duplicating it
- At runtime a "dynamically linked" application needs the binary libraries to be available
- During compilation, code which uses libraries will also need the library "header" file - a text file describing the capabilities of the library. These will not normally be installed, but will be available from the OS
- For each library package there will be a corresponding 'dev' package containing the headers. These will be needed for compilation.

## Setting up a build environment

- Get all of the basic tools in one go
  - Ubuntu/Debian etc
    - sudo apt install build-essential
  - CentOS/Redhat etc.
    - sudo yum groupinstall "Development tools"

## Standard autotools / make compilation

## • Four steps

- configure Checks library dependencies and the capabilities of your system. Writes out a custom 'makefile' which should work for you. Allows for some customisation
- make
   make test
   Make test
   Does the actual compilation
   Runs a test suite to make sure the binaries work (not always present)
- make install Moves the compiled binaries to their final location
- All of the steps involving make (but particularly the compilation) can be parallelised over multiple CPUs

## Options for autotools

- Configure
  - Some programs will offer custom options. Try ./configure --help
  - Main option here is to set the location for the installed files. By default these will go into the directories under /usr/local/. If you want to put them somewhere else you specify the --prefix option. Other options might be described in BUILD.txt
  - ./configure --prefix=/opt/custom/
- Make
  - You can set the number of CPU cores to split the compilation over using the -j parameter

make -j 10

\$ wget -q ftp://emboss.open-bio.org/pub/EMBOSS/EMBOSS-6.6.0.tar.gz
\$ tar -xzf EMBOSS-6.6.0.tar.gz
\$ cd EMBOSS-6.6.0/

\$ ./configure --prefix=/opt/EMBOSS/ > configure.log 2>&1

```
checking for X11/Xlib.h... no
```

X11 graphics have been selected but no X11 header files have been found.

\$ sudo apt install libx11-dev

\$ ./configure --prefix=/opt/EMBOSS/ > configure.log 2>&1

checking for X11/Xlib.h... yes

\$ make -j 4 > make.log 2>&1 &

\$ tail -f make.log

\$ make test
make: Nothing to be done for 'test'.

\$ sudo make install

#### \$ ls /opt/EMBOSS/

bin include lib share

#### \$ /opt/EMBOSS/bin/embossversion

Report the current EMBOSS version number 6.6.0.0

# Installing EMBOSS

1. Configure

2. Make

3. Make test

4. Make install

## Standard cmake installation

- Slightly simpler than autotools
  - Create a build directory inside the source directory
  - Move into the build directory
  - Run cmake with the target being the directory above (cmake ...)
    - Add -DCMAKE\_INSTALL\_PREFIX=/my/custom/dir if wanted
  - Run make, the same as for autotools

\$ wget https://github.com/pezmaster31/bamtools/archive/v2.5.1.tar.gz
\$ tar -xzf v2.5.1.tar.gz
\$ cd bamtools-2.5.1/

\$ mkdir build
\$ cd build

\$ sudo apt install cmake

\$ cmake -DCMAKE INSTALL PREFIX=/opt/bamtools/ .. > cmake.log 2>&1

Could NOT find ZLIB (missing: ZLIB\_LIBRARY ZLIB\_INCLUDE\_DIR)

\$ sudo apt install zlib1g-dev

\$ cmake -DCMAKE INSTALL PREFIX=/opt/bamtools/ .. > cmake.log 2>&1

Found ZLIB: /usr/lib/x86 64-linux-gnu/libz.so (found version "1.2.11")

\$ make -j 4 > make.log 2>&1 &

\$ make test
make: \*\*\* No rule to make target 'test'. Stop.

\$ sudo make install

\$ /opt/bamtools/bin/bamtools --version

bamtools 2.5.1
Part of BamTools API and toolkit
Primary authors: Derek Barnett, Erik Garrison, Michael Stromberg
(c) 2009-2012 Marth Lab, Biology Dept., Boston College

## Installing BamTools

# Exercise 7

# Extending Languages

v2018-11





## Extending Languages

- Most commonly used languages will have extensions which can be installed to provide new functionality
- The extensions may not be written in the same language
  - C or C++ extensions to scripted languages are very common
- We will look at how to extend different languages
  - R
  - Perl
  - Python

# R packages

## Installing R packages

- Standard locations are either in site-wide R package folder, eg /usr/lib/R or in ~/R/
- Installation through a package repository
  - CRAN
  - BioConductor
- Manual installation from any source
  - Project site
  - Github etc.

## R Library Paths

- .libPaths() (R function to show the current search path)
- Controlled by environment variables
  - R\_LIBS
  - R\_LIBS\_USER
  - Set the root of a R library tree
- Default personal directory is
  - ~/R/R.[version]\$[platform]-library/

## Installing R packages through CRAN

- Installer and dependency resolution built into the language
- Can install both binary and source packages
  - Source packages my have OS dependencies which will need to be fixed
- From within R
  - install.packages("packagename")
  - Use sudo to launch R if you want to install for all users

## Installing R packages from BioConductor

- Independent, bioinformatics oriented package repository
- Has its own installer which you need to load
- Different processes for different R versions
  - Older R (<3.5.0)
    - source("https://bioconductor.org/biocLite.R")
    - biocLite()
  - Newer R (>=3.5.0)
    - install.packages("BiocManager")
    - BiocManager::install()

## Installing R packages from BioConductor

- Additional packages can be installed with
  - Old system
    - biocLite("packagename")
  - New system
    - BiocManager::install("packagename")
  - Will handle dependency resolution both within Bioconductor and to CRAN repositories.

## Installing R packages from other sources

- Download the tar.gz file for the package
- Run:
  - R CMD INSTALL package.tar.gz
- Direct installation from github
  - Install the devtools package
  - library(devtools)
  - install\_github("user/repository")

# Exercise 8

# Perl Modules

## Installing Perl modules

- Install from your OS repository
  - Structured naming format, Example::Module would be perl-example-module
  - Won't be pulled from here any other way
  - May end up with duplicates
- Automated install using CPAN.pm
  - Use a module to install modules.
  - Ships alongside Perl
- Manual installation
  - Follows a standard recipe

## Perl module search path

### • Searches through directories in @INC

- Can see these with perl -V
- Can add locations using PERL5LIB environment variable

@INC:

```
/bi/apps/perl_modules/lib/perl5/x86_64-linux-thread-multi
/bi/apps/perl_modules/lib/perl5/
/bi/apps/perl_modules/lib/perl5/x86_64-linux-thread-multi
/bi/apps/perl_modules/lib64/perl5
/usr/local/lib64/perl5
/usr/local/share/perl5
/usr/lib64/perl5/vendor_perl
/usr/lib64/perl5/vendor_perl
/usr/lib64/perl5
```

## Installing Perl modules - Using cpan

- Run cpan install Example::Module
  - Automated download, configuration and installation
  - Does the same steps as a manual install
  - Can resolve dependencies

### • Configuration on first use

To install modules, you need to configure a local Perl library directory or escalate your privileges. CPAN can help you by bootstrapping the local::lib module or by configuring itself to use 'sudo' (if available). You may also resolve this problem manually if you need to customize your setup.

What approach do you want? (Choose 'local::lib', 'sudo' or 'manual') [local::lib]

Manual Perl Module installation (after download and un-tarring)

#### MakeMaker

- perl Makefile.PL
- make
- make test
- make install (with
   sudo?)

#### Build

- perl Build.PL
- ./Build
- ./Build test
- ./Build install (with sudo?)

## Installing in non-standard locations

- perl -V (look at @INC)
- @INC:
- /usr/local/share/perl/5.26.1
- /usr/share/perl/5.26
- /usr/local/lib/site\_perl
- Add folders to PERL5LIB environment variable

perl Makefile.PL INSTALL\_BASE=/my/dir

perl Build.PL --install\_base=/my/dir
# Exercise 9

# Python packages

## Installing python packages

#### • Several options

- 1. OS system packages
- 2. Automated install with pip
- 3. Manual install
- 4. Install from source code repository

#### Python package locations

- Searches in directories in sys.path
- Can add directories by modifying PYTHONPATH

```
$ python
Python 2.7.3 (default, Feb 15 2013, 11:09:45)
[GCC 4.4.6 20110731 (Red Hat 4.4.6-3)] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> import sys
>>> print ("\n".join(sys.path))
```

```
/bi/apps/python/2.7.3/lib/python27.zip
/bi/apps/python/2.7.3/lib/python2.7
/bi/apps/python/2.7.3/lib/python2.7/plat-linux2
/bi/apps/python/2.7.3/lib/python2.7/lib-tk
/bi/apps/python/2.7.3/lib/python2.7/lib-old
/bi/apps/python/2.7.3/lib/python2.7/site-packages
/bi/apps/python/2.7.3/lib/python2.7/site-packages/ipython-0.13.1-py2.7.egg
/bi/apps/python/2.7.3/lib/python2.7/site-packages/ply-3.4-py2.7.egg
/bi/apps/cellprofiler/CellProfiler-2.2.0
/bi/apps/python/2.7.3/lib/python2.7/site-packages/gtk-2.0
/bi/apps/python/2.7.3/lib/python2.7/site-packages
```

#### Installing python packages with pip

- apt/yum install python-pip
- pip install numpy
- pip install --user numpy
- pip install --upgrade numpy
- Check pip vs pip3

Manual python package installation (after download and un-tarring)

- python setup.py install
- python3 setup.py install --prefix=/my/folder
  - Will fail initially as final destination isn't in PYTHONPATH
  - Will tell you what folder to add
  - Rerun install after fixing PYTHONPATH
  - If the custom location is outside your home directory then you'll need to modify the global PYTHONPATH by editing /etc/bashrc (or one of the other global shell config files)

# Exercise 10

# Automated installers and Containers

v2018-11





#### Automated Installers

- Like a package manager, but independent of Operating System
- Some will operate from source, distributing recipes
- Some will distribute pre-compiled binaries
- Most common examples
  - Conda (https://conda.io)
  - Easy Build (https://easybuild.readthedocs.io)

#### Conda

- Package management system
- Originally for python packages, but now covers all types of software
- Several Implementations
  - Anaconda (original distribution, with a full python environment)
  - Miniconda (small distribution, just for running conda)
- Add-in repositories for more packages
  - BioConda (<u>https://bioconda.github.io/</u>)

### Using conda

- Install a conda providing environment (probably miniconda)
- Set up some channels (bioconda)
- Install some packages
  - Use the packages

#### Installing miniconda

- Go to <a href="https://conda.io/miniconda.html">https://conda.io/miniconda.html</a>
- Download the shell script for your platform
- Run it
- Will install into your home directory each user gets a separate install
- Will offer to modify your PATH to include the miniconda bin directory  $^{\ast}$

\*Be careful about this!!

#### Adding bioconda channels

- conda config --add channels bioconda
- conda config --add channels conda-forge
- Bioconda will now be searched for new installs

#### Installing packages with conda

- Simple installs [but don't do this]
  - conda install bwa
  - conda install bwa=0.7.4
- Custom environments
  - conda create -n aligners
  - source activate aligners
  - conda install bwa bowtie2 hisat2
  - source deactivate

### Problems with conda?

- Only software available in the repositories
  - Pretty comprehensive these days
- Closed environment
  - Can't mix and match with things from the base OS (well you can, but stuff will break!)
- Duplication
  - Every user (and every environment) gets their own copy of everything
- Duplication (again)
  - Will install its own R / perl / python etc and will put it first in the path
  - Can break non-conda applications in odd ways
  - Always use a named environment

# Exercise 11

# Containers

#### Containers

- A method for bundling software and data together into a single item which can be ported easily between users/computers
- Can provide an isolated environment similar to a VM or a conda environment, or make a suite of programs/data look like an application
- Main systems
  - Docker\*

(https://www.docker.com/)

Singularity<sup>\*</sup>

(https://www.sylabs.io/singularity/)

\*They play nicely together

#### Finding a container

- DockerHub (<u>https://hub.docker.com</u>)
- SingularityHub (<u>https://singularity-hub.org</u>)
- Search for the application / user / container you want
  - Find the address (user/name) eg vsoch/hello-world

#### Installing singularity

- Available from apt in Debian/Ubuntu
  - sudo apt install singularity-container
  - Note that just "singularity" is a game!
- Compile from source (<u>https://github.com/sylabs/singularity/releases</u>)
  - v2.6.0 is autotools based similar install to previous apps
  - v3.0.0 is re-written in GOLang so has a custom install procedure

#### Installing a container

- Download from a repository and install onto your machine
- singularity pull shub://dleehr/qiime2-singularity
- singularity pull docker://qiime2/core
- File names can get a bit long, so:
- singularity pull --name qiime.simg docker://qiime2/core
- Produces a .simg file on your machine

#### Using a container

- Different options. You can start a shell in the environment of the container
  - singularity shell qiime.simg
- You can run a script which the image provides
  - singularity run qiime.simg
  - ./qiime.simg

# Exercise 12

# Different types of Linux installation

v2018-11





## Types of Linux installation

- Bare metal
  - Physical hardware
  - CD / DVD / USB / Network installation
- Virtual Machine
  - Runs within another operating system
  - Portable / disposable
  - Install from ISO / Network
- Cloud
  - Virtual machine on someone else's hardware
  - Amazon / Google are the main providers
  - Range of available hardware and OS images available

#### Installing bare metal or in a VM

- Essentially the same process
- Uses an installer provided by the Linux distribution
- Two main types
  - Live image
    - Boot into a working OS from a CD/DVD/USB
    - Copy the image to a hard drive and boot from there
    - Little to no configuration options need to modify post install
  - Real installer
    - Guided installation process in a custom installer
    - Many options (software, networking, disk partitioning etc.)
    - More flexibility, but more hassle

#### Installing into a VirtualBox VM

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# Exercise 14

#### Creating an Amazon EC2 server

- Create an AWS account (will require a credit card, but test servers can be run for free)
  - <u>https://aws.amazon.com</u>
- Create a key pair
- Create an EC2 instance
- Connect to the image using the key
- Do what you want
- Shut it down (so you stop being charged!)

#### Create a key pair

- Key Pairs > Create Key Pair
  - Give it a name
  - Download the .pem file which it creates

Opening CourseTest.pem								
You have chosen to open:								
CourseTest.pem								
which is: Text Document								
from: https://eu-west-2.console.aws.amazon.com								
What should Firefox do with this file?								
Save File								
Do this <u>a</u> utomatically for files like this from now on.								
OK Cancel								

#### Create an EC2 instance

- Instances > Launch Instance
  - Select hardware and base OS



#### Launch instance and set keys



#### Find instance details

#### Under instances



#### • Find username

- For Amazon Linux 2 or the Amazon Linux AMI, the user name is ec2-user.
- For a Centos AMI, the user name is centos.
- For a Debian AMI, the user name is admin or root.
- For a Fedora AMI, the user name is ec2-user or fedora.
- For a RHEL AMI, the user name is ec2-user or root.
- For a SUSE AMI, the user name is ec2-user or root.
- For an Ubuntu AMI, the user name is ubuntu.

#### Connect to the instance via SSH using your key

• ssh -i [key\_file.pem] username@address.from.ec2

```
X
                                                                    ubuntu@ip-172-31-3-143: ~
andrewss@BI1803 MINGW64 /c/Users/andrewss/Documents/Amazon Keys
$ ssh -i CourseTest.pem ubuntu@ec2-3-8-122-6.eu-west-2.compute.amazonaws.com
The authenticity of host 'ec2-3-8-122-6.eu-west-2.compute.amazonaws.com (3.8.122
.6)' can't be established.
ECDSA key fingerprint is SHA256:9AG34mEW4StJL7w6KapigsSWjX9yQ7Ds3WtsbXhs+tM.
Are you sure you want to continue connecting (yes/no)? yes
Warning: Permanently added 'ec2-3-8-122-6.eu-west-2.compute.amazonaws.com,3.8.12
2.6' (ECDSA) to the list of known hosts.
Welcome to Ubuntu 18.04.1 LTS (GNU/Linux 4.15.0-1021-aws x86_64)
 * Documentation: https://help.ubuntu.com
                  https://landscape.canonical.com
 * Management:
                  https://ubuntu.com/advantage
 * Support:
  System information as of Fri Nov 2 10:11:18 UTC 2018
  System load: 0.0
                                                      84
                                 Processes:
  Usage of /: 13.3% of 7.69GB Users logged in:
                                                      0
                                 IP address for eth0: 172.31.3.143
  Memory usage: 13%
  Swap usage:
               0%
 * Security certifications for Ubuntu!
   We now have FIPS, STIG, CC and a CIS Benchmark.
```
## Terminate your instance

- Instances > Right click > Terminate
- Will be warned about deleting the underlying storage



## Storage

- Simple instances come with limited, temporary storage
- For serious work you want additional storage
  - Configure storage bins
  - Add them to one (or more) images
  - Add data to them
- Storage bins exist independently of the compute instances
  - Simple stores for applications or databases
    Elastic Block Store (EBS)
    \$\$\$
  - File system storage for concurrent access Elastic File System (EFS)
  - Large data storage and processing/archiving
  - Long term archiving

Simple Storage Service (S3)\$\$Glacier\$

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## Exercise 15