Introduction to IT for UCL Astrophysicists

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Where to find this presentation

Find the presentation at https://tinyurl.com/y8lyyg5r.
Note that the third character is a lower-case ‘el’.
On this page click on ‘Download’ to get a copy of the presentation.

Overall goals of presentation

- What software you might find useful
- Pointers to where to get more information (UCL courses, web, etc.)
- UCL-specific information (e.g. login details)
- Hands-on work

Specific contents

- Accessing Astrophysics group machines
- Using the Linux console
- Basics of Python
- Commonly used programs (LaTeX, DS9, IRAF,...)
- Using High-Performance Computing (HPC) machines
- HPC best practices

Information on the Web

Astrophysics Wiki

https://wiki.ucl.ac.uk/display/PhysAstAstPhysGrp/Main+Page

This Wiki is freely viewable and editable by all members of the department. Please use it to record information that you think will be useful to others (including your future self). Be bold!

UCL Research Computing Platforms

https://wiki.rc.ucl.ac.uk/wiki/Main_Page

Stack Overflow

http://stackoverflow.com/

Computing Environment for Astrophysics

- Large datasets requiring substantial processing followed by sophisticated statistical analysis
- Calculations often done on specialised ‘high-performance computing’ (HPC) machines having large filesystems and large RAM; calculations are often broken into pieces that can be run simultaneously (‘in parallel’) across many processors.
- Much useful software is made freely available within the community. Software quality is usually high; documentation quality is more variable.
- Many users write their own software.

Local Computing Environment

You will have your own local machine, which might be:

- PC (Windows)
- Mac
- Linux

Also there are shared Linux machines:

- General purpose Astrophysics server available from outside UCL: `zuserver1`
- UCL Cosmology HPC cluster: `splinter`
- Other UCL HPC clusters: `Grace` and `Legion`
- National HPC cluster: `DiRAC`

Work patterns

Several work patterns are possible:

- Write and test a program on your local machine; use the local machine to remotely connect to `splinter`; upload the program to `splinter` and run it there;
- Or do all your work locally (requires small data sets);
- Or use the local machine to remotely connect to `splinter` and do all your work there.

Remote connections

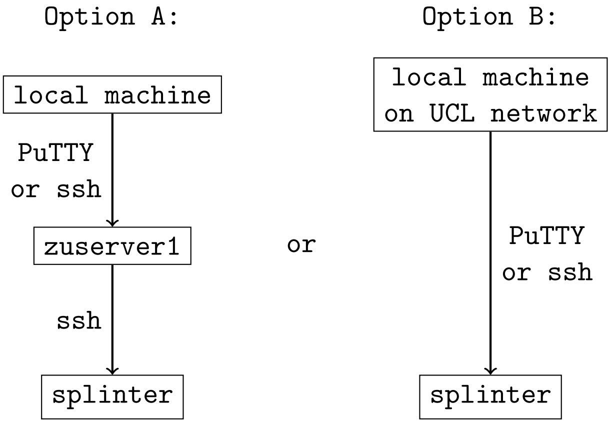
How to connect to a shared machine

- Windows PC: use PuTTY;
- Mac: go to the Terminal window and use `ssh`;
- Linux machine: go to the Terminal window and use `ssh`.

Visibility

If you are not on the UCL network then you cannot connect to `splinter` directly; instead you must go via `zuserver1`.

Two methods for accessing splinter



Accessing remote machines

Credentials

- You will need a *username* and *password* for `splinter` (and, if you are using Option A, for `zuserver1` as well).
- If you do not have these already then we can give guest credentials to be used during this course.

The full names of the servers are:

- `zuserver1.star.ucl.ac.uk`
- `splinter-login.star.ucl.ac.uk`

Using PuTTY for remote connections from Windows

- If you don't have PuTTY you can download it from `http://www.putty.org/`.
- On the 'Connection/SSH/X11' tab, click on 'enable X11 forwarding' and set 'X display location' to 'localhost:0' - this is necessary for handling graphical output.
- On the Session tab, set the Host Name as appropriate: `zuserver1.star.ucl.ac.uk` (Option A) or `splinter-login.star.ucl.ac.uk` (Option B).

Using ssh for remote connections from Mac and Linux

- Syntax: `ssh -YC username@servername`
- The ‘Y’ option is necessary for handling graphical output.

X-Windows client

- If the remote program that you are running produces graphical output, then you must have a program (an 'X-Windows client') running on your local machine to display this graphical output.
- On Windows you can use XMing (`https://sourceforge.net/projects/xming/`) or Exceed (available on the UCL Desktop).
- On Mac you can use XQuartz.
- On Linux you don't need to do anything special - the graphical interface is already an X-server.

Linux: Command shell

- In Linux you will use a ‘command shell’.
- This is a text-based environment in which you type commands and receive text output.
- Not GUI! Reflects the hardware limitations current when Unix was created. Low-tech and reliable e.g. for remote access.
- Various command shell programs are used: `bash`, `csh`, `tcsh`, `zsh`, etc. To see which one you are using, call `echo $0`.

Linux: Directory structure

- Everything is organised around files (which may be data files or program files i.e. instructions to be executed).
- Files live in directories. There is a hierarchical tree structure of directories.
- Sample file name:
  `/share/splinter/ucapwhi/des/foo.txt`
- Note use of slash '/', not backslash '\' as in Windows.
- Case sensitivity: 'Foo' and 'foo' are different strings.

Linux: Special symbols for directories

Symbol	Meaning
/	Top of the directory tree (the root directory)
.	Current directory
..	Parent of the current directory
~	User's 'home' directory
(TAB)	(Perform autocomplete on directory and file names)

Linux: Environment variables

- The operating system maintains a global namespace of 'environment variables' to store configuration information.
- Use `printenv` (in tcsh) or `set` (in bash) to see all environment variables; use `echo $<variable_name>` to see the value of one environment variable (e.g. `echo $PATH`).
- Use `setenv FOO my_string` (in tcsh) or `export $FOO='my_string'` (in bash) to set `FOO`.
- Variables `PATH` and `PYTHONPATH` are used frequently (to maintain lists of directories in which to search for executable programs and Python modules, respectively).
- Linux has no equivalent of the Windows Registry; configuration is done via the directory structure and the environment variables.

Linux: Structure of commands

Structure

```
[command] -[option(s)] [argument]
```

Examples

```
ls -la
mkdir hello_world
cp hello.cpp new_hello.cpp
```

Linux: command reference

There is a very useful summary of Linux commands at:
`http://www.computerhope.com/unix.htm`

Linux: Basic commands 1

navigation and help

```
pwd
ls -la
cd dir_name
man command_name
info command_name
exit
```

copy or move

```
cp src dest
mv src dest
scp usr@host:file dest
```

create or delete

```
touch file.txt
mkdir dir_name
rm -i file.txt
```

find and system info

```
whereis file
which
echo $VAR_NAME
```

file contents

```
cat file
more file
head file
```

Linux: Basic commands 2

special characters

`&` (background)

`;` (combine)

`\` (next line)

`*` (wildcard)

`|` (pipe)

`>` (output)

`<` (input)

text editors

emacs

vi

gedit

process management

kill, top, nohup

compressed files

gunzip, tar

images

gthumb

ds9

evince

eog

publishing

latex, bibtex

Linux: Exercises I

1. Go to your home directory and create a directory called `level_0`.
2. Change directory to `level_0`.
3. Find the name of the present working directory.
4. Make a directory `level_1`, and move to it.
5. Create a file called `foo.txt` with contents "This file contains the word bar".
6. Add another line in `foo.txt` with contents "This is the second line".
7. Print the contents of `foo.txt` to the screen.
8. Search for the word *bar* in `foo.txt`.
9. Go up one level, then remove the directory `level_1` (and its contents).
10. Find the location of your python installation.

Linux: Exercises II

11. Find the values of the environment variables `PATH` and `LD_LIBRARY_PATH`.
12. Set the environment variable `MY_VAR` to equal the absolute path to `level_0`, and test that it has worked OK.
13. Add (i.e append) to the `PATH` the absolute path to `level_0`, and test that it has worked OK.
14. Use the `man` command to find the option of `ls` that shows file sizes in human readable format.
15. Find the hostname, processor type and operating system version and write this info into a text file called `info.txt`.
16. List the people who are currently logged into the system.
17. Find which process is using the most CPU at the moment.
18. Find the IDs of the processes that you are running.

Programming: Languages

High-level languages - fast to code

- Python
- IDL
- Matlib, Mathematica, R

Low-level languages - fast to run

- C, C++
- Fortran
- Assembler

Python

Python has become popular:

- Good trade-off between ease-of-use and performance
- Many add-in libraries, so sophisticated programs can often be built easily [`https://xkcd.com/353/`].

Python Features and Aspects

- Two slightly-incompatible versions: 2 and 3 (currently 2.7 and 3.6). Still lots of users of 2; better to use 3 if you can.
- Can be used interactively or compiled.
- Duck typing (type of variable is inferred at run-time)...
- ... and hence generic programming (in which a function can take many different types of variables as inputs).
- Object-orientation.
- Exceptions (try, raise, except) for handling error conditions.
- Automatic garbage collection (so no need to worry about memory management).

Python for Astrophysicists

Use Python plus the following add-in libraries:

- Numpy: array processing for numbers and strings
- Scipy: scientific library
- Astropy: astronomical library
- Matplotlib: plotting

All of these libraries (plus many others) are available in one package called Anaconda:

`https://www.continuum.io/downloads`.

Using Python on `splinter`

- To initialize your `splinter` session so that it will use Python 3 and so that it can find all the necessary libraries, run: `module load dev_tools/oct2016/python-Anaconda-3-4.2.0`
- This will set the necessary environment variables.
- We will explain in more detail later about the `module` command.

Python: Interactive

- Begin an interactive Python session by calling `ipython`
- You can then type Python commands on successive lines, such as

```
print 2+2
a = 7
print a**2
exit
```

Python: Compiled

- Create a Python program by writing code in a text file (say called my_program.py).
- Then execute the program by calling `python my_program.py`
- Even better:
  - Put `#!/usr/bin/env python` as the first line in my_program.py
  - Run `chmod +x my_program.py`

  Then execute the program by calling `./my_program.py`

Python: sample program

```python
#!/usr/bin/env python
# Use the `#' to indicate a comment

# Import library and give it a
# short name for convenience
import numpy as np


a = np.arange(10) # The array [0, 1, ..., 9]
b = f(a) # f is a subroutine defined below
print b

def f(x):
    # The whitespace at the beginning
    # of the next line is crucial.
    return x**2
```

Python

Dictionaries

Useful to do key-value mapping and can be created using `dict()`
Can access keys using `dictionary.keys()` and values using `dictionary.values()` or `dictionary[key]`

Functions

```
def function_name(arg1, arg_opt=1, *args, **kwargs):
```

`arg_opt` is an optional argument, and if you don't want to specify the number of arguments use `*args` for a list of arguments and `**kwargs` for a dictionary. Example:

```
function_name(100.0, *[1, 2, 3], **{`foo':`bar'})
```

Classes

Can create objects with functions, but must initialise the arguments:

```
class class_name:
    def __init__(self, arg):
        self.argument = arg
```

NumPy

NumPy Arrays

Can create NumPy arrays in many ways; `np.array([])`, `np.empty(())`, `np.zeros([])`, `np.ones([])`, `np.arange()`, `np.linspace()`, ...

Basic Statistics

`np.mean()`, `np.median()`, `np.min()`, `np.max()`, `np.std()`, `np.argmin()`, `np.argmax()`

Shape Manipulation

Can change arrays to be different shapes and size; `np.reshape()`, `np.flatten()`, `np.shape()`, array slicing (next slide...)

Sorting

Can use `np.sort()` to sort arrays along different axes, and `np.argsort()` to return the arguments of the sorted arrays

I/O

Can use `np.loadtxt()` and `np.genfromtxt()` to get values from a data files. Can choose data type, delimiter, to skip header/footer/rows, to unpack the data into multiple variables, etc.

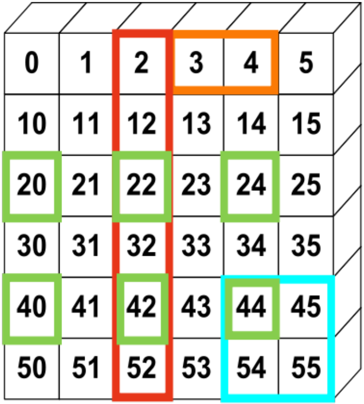
Array Slicing

```
a = np.arange(60).reshape(6,10)[:,0:6]
>>> a[0,3:5]
array([3,4])

>>> a[4:,4:]
array([[44, 45],
       [54, 55]])

>>> a[:,2]
array([2,22,52])

>>> a[2::2,::2]
array([[20,22,24]
       [40,42,44]])
```



Scipy/Astropy/PyFITS/SymPy

Constants and Conversions

For example: `scipy.constants.c`, `scipy.constants.hbar`, `scipy.constants.lambda2nu(550*scipy.constants.nano)`

More Stats

Various stats tool using `scipy.stats`, such as calculating mean, variance, skew, and probability and cumulative density functions

Optimising and Fitting

Can use `scipy.optimize` to find minima (`.fmin_bfgs`), find roots of a function (`.fsolve`), and fitting (`.curve_fit`)

PyFits

Using `pyfits`, can import (`.open()`), read (`.info()`/`.header()`), and write (`.PrimaryHDU()` and `.writeto()`) FITS files

World Coordinate Systems

Can find the RA and Dec of pixels using `astropy.wcs.WCS` and and convert RA and Dec to pixels using `astropy.wcs.WCS.wcs_sky2pix()`

Symbolic Calculus

Differentiation, Integration, Linear Algebra, Series Expansion, and Equation Simplifying using `sympy`

Information on the Web

Documentation

http://scipy.org/
http://matplotlib.org/
http://www.astropy.org/

SciPy Tutorials (Also NumPy and Matplotlib)

https://conference.scipy.org/scipy2013/tutorials.php

SciPy Lectures (Also NumPy and Matplotlib)

http://www.scipy-lectures.org/

Stanford's Introduction to Scientific Python

http://web.stanford.edu/~arbenson/cme193.html

Matplotlib

- Powerful plotting library. See `http://matplotlib.org/gallery.html` for range of examples.
- Two interfaces: one similar to MATLAB (for interactive use; relies on global state), and one object-oriented. Typically the latter is to be preferred.
- Read the introduction at `http://matplotlib.org/faq/usage_faq.html` as this clarifies many points of terminology and usage.
- Alas the documentation could be better. StackOverflow clarifies many of the more subtle points.

Matplotlib Example

```python
import numpy as np
import matplotlib.pyplot as plt

x = np.arange(0, 2*np.pi, 0.1)
y = np.sin(x)

plt.figure()
plt.scatter(x, y) # Or plt.plot...
plt.show()
```

Matplotlib Features

Different Plotting Styles

Can edit marker style, colour, edge colour, size and opaqueness, errorbar style and colour.
Can annotate plots with text and arrows.
Can include colour maps and bars (see next slide).
Can plot in polar and World Coordinate System coordinates (with the help of `astropy`).

Image Plotting

Can read and plot an image using `plt.imshow`. Beware of orientation!

Multiple Subplots

Using `plt.subplot()` you can create multiple subplots, for example the following creates two side-by-side subplots that share x and y axes:

```
plt.subplots_adjust(hspace=0.5)
ax1 = plt.subplot(121)
ax2 = plt.subplot(122, sharex=ax1, sharey=ax1)
```

Matplotlib Colormaps

- Plotting mutiple-dimensional data is hard. You can use colour to indicate one of the data dimensions e.g. a contour map with colour shading for elevation above and below sea level.
- This requires a mapping (a 'colormap') that associates a colour with each data value. The Matplotlib default way of doing this is 'rainbow': map data values to wavelength (between 'red' and 'blue'). This is simple, elegant, physically well-motivated...
- ... but suboptimal in practice (because human perception of colour is complicated and involves non-linearities).
- Don't use the default colormap; instead, explicitly specify an alternative (`https://matplotlib.org/examples/color/colormaps_reference.html`). See also `http://www.research.ibm.com/people/l/lloydt/color/color.HTM`.

Matplotlib: Exercises I

- Use the SDSS data file (compressed FITS format) `/share/splinter/ucapwhi/Linux_training/demo.fits.gz`.
- Use the pyfits library (`import astropy.io.fits as pyfits`) to manipulate file columns as numpy arrays.
- Use the open command to get a handle to the file (`h = pyfits.open(...)`). Then get e.g. the `Dist` column via `x = h[1].data.field('Dist')`.

1. Create a scatter plot of distance (`'Dist'`) as a function of r-band absolute magnitude (`'rMAG'`). Do you think that this data set is a subset of a larger data set?
2. Make a map by scatter-plotting declination (`'DEdeg'`) as a function of right ascension (`'RAdeg'`). Use small dots. Why is the density lower at the top? Why should the plot really be flipped left/right?

Matplotlib: Exercises II

3. Use astropy to redo the last plot so that it uses an equal area all-sky projection such as ‘mollweide’.

Jupyter

Jupyter is a framework for creating interactive web pages in which source code (written in Python or other high-level language) appears together with the corresponding output (text or graphics). This is an excellent environment for demonstrating how your code works.
See `http://jupyter.org/`.

UCL Software Carpentry Workshop

UCL training course in programming skills

`https://www.ucl.ac.uk/isd/services/research-it/training`

Upcoming courses

- 31st October - 1st November 2017
- 14th - 15th December 2017

Source control system

- A source control system is a repository for successive versions of documents (e.g. source code for computer programs).
- Versions can be compared and old versions restored if needed (e.g. to undo recent bad changes).
- Multiple developers are able to make changes to the same file, with automatic merging of edits from different developers (but if there is an *edit conflict* i.e. two developers change the same line then manual intervention will be needed).
- Any serious development that you do (even if just for yourself) should be under the control of a source control system.

Git

- We often use the source control system ‘Git’.
- Git is non-trivial to learn (see `https://xkcd.com/1597/`) but is very powerful. It is useful to have a clear idea of Git’s internal workings before attempting to do even simple things.
- Git uses a ‘distributed’ model (as opposed to a ‘client/server’ model used e.g. by SVN). All copies of a repository are ‘peers’ (i.e. no one copy is special as far is Git is concerned).

Git workstyles

- Git can be used in support of various work styles.
- For most projects that you will encounter, it is sufficent to put a repository somewhere on the Internet and think of this as the 'official' copy. You can then 'clone' this repository locally, make your changes, and then 'push' this pack to the official repository. Your colleagues will be doing the same, and Git will handle the necessary merging.
- On larger projects you begin by copying the official repository to a new 'forked' copy (also on the Internet). You can then develop (as above) in this fork. Later you can ask for your forked copy be merged back into the official copy ('pull request'). This gives the official owners more control over changes.

GitHub and BitBucket

- GitHub (`https://github.com`) and BitBucket (`https://bitbucket.org`) make available Internet-accessible storage space for git repositories.
- Both give Web Browser access to repositories.
- With both you can install Git locally (command-line interface) and both provide a user-friendly GUI interface to the local Git software.

Common and Useful Programs

- LaTeX
- DS9
- IRAF
- SExtractor/SWarp
- CosmoSIS

LaTeX

Features

- LaTeXis text processing software.
- Not WYSIWYG. Source files are text files (which LaTeXthen compiles into pdf); as a result e.g. it is easy to merge two sets of changes.
- Optimised for good display of mathematics.
- Required for submissions to arXiv.
- Use ‘beamer’ to produce presentations (e.g. this one).
- Use ‘tikz’ to produce diagrams (as in this presentation).

Websites

`http://www.tug.org/texworks/`

DS9

Features

- Viewer for FITS and othjer files
- Aligning with WCS (World Coordinate System)
- Scaling image contrast
- Funky colour sets (and inverse or negative)
- Regions and annotating the image
- Multiple frames; blinking and matching
- Contour plots

Website

`http://ds9.si.edu/site/Home.html`

Image Reduction and Analysis Facility (IRAF)

Features

- *'IRAF is a collection of software geared towards the reduction of astronomical images in pixel array form ... from imaging array detectors such as CCDs.'*
- *'IRAF commands (known as tasks) are organized into package structures. Additional packages may be added to IRAF. There are many packages ... focusing on a particular branch of research or facility.'*
- Example package: STSDAS (for analysing Hubble Space Telescope data).

Websites

http://iraf.noao.edu/
http://iraf.net/irafdocs/

SExtractor/SWarp

Features

- *'SExtractor is a program that builds a catalogue of objects from an astronomical image. Although it is particularly oriented towards reduction of large scale galaxy-survey data, it can perform reasonably well on moderately crowded star fields.'*
- *'SWarp is a program that resamples and co-adds together FITS images using any arbitrary astrometric projection defined in the WCS standard.'*

Websites

http://www.astromatic.net/software/sextractor
http://www.astromatic.net/software/swarp

CosmoSIS

Features

- *'CosmoSIS is a cosmological parameter estimation code. It is a framework for structuring cosmological parameter estimation in a way that eases re-usability, debugging, verifiability, and code sharing in the form of calculation modules. It consolidates and connects together existing code for predicting cosmic observables, and makes mapping out experimental likelihoods with a range of different techniques much more accessible.'*

Websites

`https://bitbucket.org/joezuntz/cosmosis/wiki/Home`
`https://wiki.ucl.ac.uk/display/PhysAstAstPhysGrp/Installing+and+Running+CosmoSIS`

ASCL.net

There's more: the Astrophysics Source Code Library (`http://ascl.net/`) lists over 1000 astronomical programs that you can download.

HPC: Information on the Web

Introduction to Parallel Computing (Presentation)

`https://wiki.ucl.ac.uk/display/PhysAstAstPhysGrp/Computing+and+Programming`

UCL Astrophysics Wiki information on `splinter`

`https://wiki.ucl.ac.uk/display/PhysAstAstPhysGrp/Splinter+User+Guide`

UCL Research Computing Platforms

`https://wiki.rc.ucl.ac.uk/wiki/Main_Page`

DiRAC

`http://www.dirac.ac.uk/`

HPC: splinter mailing list

`https://www.mailinglists.ucl.ac.uk/mailman/listinfo/splinter-users`

- Please subscribe
- Post any issues regarding `splinter`

HPC: Cluster structure

A HPC cluster (such as `splinter`) consists of many nodes (= 'boxes' = machines).

- One node is the 'login' node; it hosts the command session that you get when you log in.
- Another node is the 'head'; it runs the software that controls how the cluster operates.
- All the other nodes are 'compute' nodes; they do the actual work.
- The nodes can talk to each other via an Ethernet network.

HPC: Node structure

Each node has:

- Several cores (= processors). Each core can run computer code independently of each other.
- Memory (RAM) that can be allocated to the cores. If necessary some memory can be used by several cores at once.
- Its own file space.

HPC: `splinter` nodes and cores

Currently `splinter` has 29 nodes and 456 cores:

- 8 nodes each with 12 cores and 48GB RAM
- 20 nodes each with 16 cores and 128GB RAM
- 1 node with 40 cores and 1TB RAM

HPC: Program structure

- A simple program runs code sequentially using just one core.
- More complex programs run more quickly by running several ‘threads’ of code in parallel on several cores within one node - one thread per core.
- So the simple programs are ‘single-threaded’ and the more complex are ‘multi-threaded’.
- A multi-threaded program can run on just one core if necessary - the threads will execute one after another and the program will run more slowly.

HPC: How to parallelize

Method 1:

- Write a single-threaded program.
- Run many copies of it at once; each uses one core.
- Run time depends on total number of cores.
- Single-threaded programs are easy to write and debug.
- No fast way for the various running copies to talk to each other during processing. Therefore this method is useful only when the problem can be divided into independent chunks. Such problems are called 'embarrassingly parallel'.
- Easy to submit many jobs at once using a 'Job Array' - see `splinter` user guide.

HPC: How to parallelize

Method 2:

- Write a multi-threaded program.
- Run it on one node, using all the cores on that node.
- Run time depends on maximum number of cores on one node.
- Multi-threaded programs are hard to write and debug. Tools called 'OpenMP' and 'MPI' help.
- The threads can share memory hence can talk to each other during processing; for certain problems this is crucial. Need to be careful that the threads don't conflict when updating shared memory.

HPC: Workspaces I

`/home/user_name`

- This is your home directory
- Login scripts can be put here
- 1GB quota
- Private

`/share/splinter/user_name`

- Create the directory if it is not already there
- Can be used as a workspace
- No quota
- Public unless made private

HPC: Workspaces II

`/share/data1`

- For storing large data
- You can create a directory for your, .e.g, `/share/data1/SKA`

`/share/apps`

- For installing software
- Module files

HPC: Login script

- There is a file called `.login` in your `$HOME` directory
- Every time you login this file will be executed
- You can load modules, envvars, etc.

Examples

Load my aliases

```
source ~/aliases.csh
```

Load python

```
module load dev_tools/oct2016/python-Anaconda-3-4.2.0
```

HPC: Modules

- A module file sets environment variables required to run a program. This makes it easy e.g. to switch between different versions of a program.
- Available to everyone in `splinter`

Examples

Print the available modules

```
module avail
```

Load a module

```
module load module_name
```

List the loaded modules

```
module list
```

Unload a module

```
module unload module_name
```

Unload all modules

```
module purge
```

Help

```
module --help
```

HPC: Submitting jobs

- Computing jobs should be submitted to the scheduler.
- To do this you will need to write a 'job script'.
- Alternatively you can start an interactive session on a compute node.
- Don't run heavy programs on the login node!

Examples

Submit a job

```
qsub job_script
```

Start an interactive session

```
qsub -IX
```

Check the status of a job

```
checkjob job_id
```

List the status of all jobs

```
qstat
```

Show the queue

```
showq
```

Delete a job

```
qdel job_id
```

HPC: Queues

When submitting a job you can specify a queue (= subset of nodes) to ensure that your job is processed only on nodes with sufficient resources. Available queues are:

- `compute` (all nodes)
- `cores16` (all 16 core nodes)
- `cores12` (all 12 core nodes)
- `smp` (all 40 core nodes (there's only one))

HPC: Structure of a job script

```
#!/bin/tcsh
#PBS -S /bin/tcsh
#PBS -q cores12
#PBS -N a_name_for_your_job
#PBS -l nodes=1:ppn=6
#PBS -l mem=32gb
#PBS -l walltime=120:00:00
```

Set environment variables if needed

```
setenv OMP_NUM_THREADS 6
```

Load module files if needed

```
module load dev_tools/oct2016/python-Anaconda-3-4.2.0
```

Run the program

```
/home/username/hello_world.exe
```

HPC: Jobscripts: things to remember

- Choose the correct queue
- Choose the correct number of `nodes` and `ppn`
- Specify the memory required
- Always specify the walltime
- If your program is not parallel, please use `nodes=1,ppn=1`
- Use the `compute` queue for single processor jobs
- Use `qsub -IX` for an interactive session
- If using most of the resources, please send an email to the mailing list.

HPC: More PBS commands

Specify output

```
# PBS -o path/to/file.out
```

Specify error output

```
# PBS -e path/to/file.err
```

Mail alert at (b)eginning, (e)nd, and (a)bortion of execution

```
# PBS -m bea
```

Send mail to the following address

```
# PBS -M your_email_id@ucl.ac.uk
```

HPC: Using *Ganglia*

`http://splinter.star.ucl.ac.uk/ganglia/`

- A tool for analysing `splinter`.
- Can only be loaded from `splinter` (using Firefox).
- Will give you load/memory information.
- Can look into nodes.

HPC: Collaborative projects

- For collaborations between two splinter users you can share common data in `/share/data1/my_collaboration`
- Give read/write permission to other users using `chmod`

HPC: Best practices

- Choose the compute nodes that are suited for your problem
- Read the User Guide
- Do not run your programs in the login node
- Install common software locally if and only if absolutely necessary
- Request optimum resources
- Minimise data transfer between nodes
- Backup anything that you would hate to lose

HPC: Exercises

1. Start an interactive session. Find which node you have been assigned.
2. Still in the interactive session, run ‘ipython‘ and run some Python commands. Then exit ipython and the interactive session.
3. Write a job script to run a ‘hello world‘ program in Python and submit it to the queue.
4. Amend the job file so that the output goes to a file.
5. Using the above example, check the job status using ‘qstat‘ and ‘checkjob‘.

Extra Slides - Python Examples

Dictionary example:

```
dc = dict(a=1, b=''Hello World'', c=(1, 2, 3))
print dc.keys(), dc.values(), dc[''b'']
```

Function example:

```
def my_first_func(arg1, arg_vol=1, *args, **kwargs):
    print arg1, arg_vol
    for a in args:
        print a
    for key, value in kwargs.iteritems():
        print key, value
```

Class example:

```
class my_first_class:
    def __init__(self, arg):
        self.argument = arg

    def print_arg(self):
        return self.argument

instance = my_first_class(42)
print instance.method()
```

Extra Slides - NumPy Examples

Shape Manipulation examples:

```
a = numpy.arange(60).reshape(6,10)
print a.shape
print a.flatten()
print a.reshape(2, -1, 3)
```

Sorting examples:

```
a = numpy.array([2, 6, 5, 1, 6, 3, 3])
print numpy.sort(a)
print numpy.argsort(a)

data_type = [(''wavelength'', int), (''flux'', float)]
values = [(31, 210), (45, 3400), (18, 150), (7, 50), (21, 100)]
array = numpy.array(values, dtype=data_type)
print numpy.sort(array, order=''wavelength'')
```

I/O examples:

```
data = numpy.genfromtxt(file_name, dtype=data_type,
    delimiter=delimiter_character, skip_header=number_of_lines_to_skip)
data1, data2 = np.loadtxt(file_name, skiprows=number_of_lines_to_skip,
    unpack=True)
```

Extra Slides - Scipy/Astropy/PyFITS/SymPy Examples 1

Constants and conversions example:

```
x = scipy.constants.find('Newton')
print scipy.constants.value(x[0]), scipy.constants.unit(x[0])
```

More stats examples:

```
bell = scipy.stats.norm(loc=centre, scale=standard_deviation)
print bell.stats(moments='mvs')
print bell.pdf([value, value_2, value_3])
print bell.cdf([value, value_2, value_3])
```

Optimising and Fitting examples:

```
minima1 = scipy.optimize.fmin_bfgs(function, initial_guess)
minima2 = scipy.optimize.brute(function, (search_grid,))

r1 = scipy.optimize.fsolve(function, initial_guess)
r2 = scipy.optimize.newton_krylov(function, initial_guess, verbose=True)

opt_values, covariance_matrix = scipy.optimise.curve_fit(function, x_data, y_data)
plt.plot(x_data, y_data, 'bo', label='data')
plt.plot(x_data, function(x_data, opt_values[0], opt_values[1]), 'r-', label='fit')
```

Extra Slides - Scipy/Astropy/PyFITS/SymPy Examples 2

PyFITS examples:

```
fh = pyfits.open(file_name)
print fh.info(), fh[1].header()

hdu = pyfits.PrimaryHDU(data)
hdu.writeto(new_image_name, clobber=True)
```

World Coordinate System examples:

```
wcs = astropy.wcs.WCS(header=pyfits.open(file_name)[1].header)
pixcrd = numpy.array([[coord1_x, coord1_y], [coord2_x, coord2_y]], numpy.float_)
sky = wcs.wcs_pix2sky(pixcrd, 1)
print sky

pixcrd2 = wcs.wcs_sky2pix(sky, 1)
print pixcrd2
```

Symbolic Calculus examples:

```
a = sympy.Symbol(''a'')
b = sympy.Symbol(''b'')
e = (a + 2*b)**5
e.diff(b)
sympy.integrate(a**2 * sympy.cos(a), a)
sympy.simplify((a + a*b)/a)
sympy.series(sympy.cos(a), a)
```

Extra Slides - Matplotlib Examples

Annotate examples:

http://matplotlib.org/examples/pylab_examples/annotation_demo2.html

Polar and color/size/opaqueness example:

```
plt.figure(figsize=(10,10))
ax = plt.subplot(111, polar=True)
c = scatter(angles, radii, c=colors, s=sizes, alpha=opaqueness)
plt.show()
```

Image plot example:

```
datafile = matplotlib.cbook.get_sample_data(file_name, asfileobj=True)
A = fromstring(datafile.read(), uint16).astype(float)
A *= 1.0/max(A)
A.shape = 512, 512
im = plt.imshow(A, cmap=cm.hot, origin='upper', extent=plot_size)
plt.show()
```

Subplot and colour bar example:

```
fig, axes = plt.subplots(nrows=2, ncols=2)
for dat, ax in zip(data, axes.flat):
    im = ax.imshow(dat, vmin=colour_min, vmax=colour_max)
cax = fig.add_axes([left, bottom, width, height])
fig.colorbar(im, cax=cax)
plt.show()
```