

# HPRC Cluster: Quick Start User Guide

THIS PAGE CONTAINS OLD INFORMATION - HPC staff will work on updating it soon.

This page is intended as a quick introduction for new users submitting their first job to the HPRC Cluster.

In the typical work flow the user:

1. Logs into [zodiac.hpc.jcu.edu.au](http://zodiac.hpc.jcu.edu.au)
2. Prepares a submission script for their jobs
3. Submits their jobs to the Job Scheduler
4. Monitors their jobs
5. Collects the output of their jobs.

A few things that new users should be aware of:

- Typically, jobs are not run in an interactive manner, except when:
  - users are running small one off jobs
  - evaluating the resources required for bigger jobs
  - using graphical applications like MATLAB
  - Examples of interactive jobs:  
**Content by label**  
  
There is no content with the specified labels
- HPRC Cluster software is not run in a window on their desktop, neither is it launched by clicking on it in a network drive.
- Users need to [log into the cluster](#) and inform the job scheduler about their job and it will run it when it can.

## Quick Start

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## Logging In

The first step in using the HPRC Cluster is to log in to a login node - [ssh1.hpc.jcu.edu.au](http://ssh1.hpc.jcu.edu.au) or [ssh2.hpc.jcu.edu.au](http://ssh2.hpc.jcu.edu.au) ([zodiac.hpc.jcu.edu.au](http://zodiac.hpc.jcu.edu.au) for people still wanting to access the old cluster).

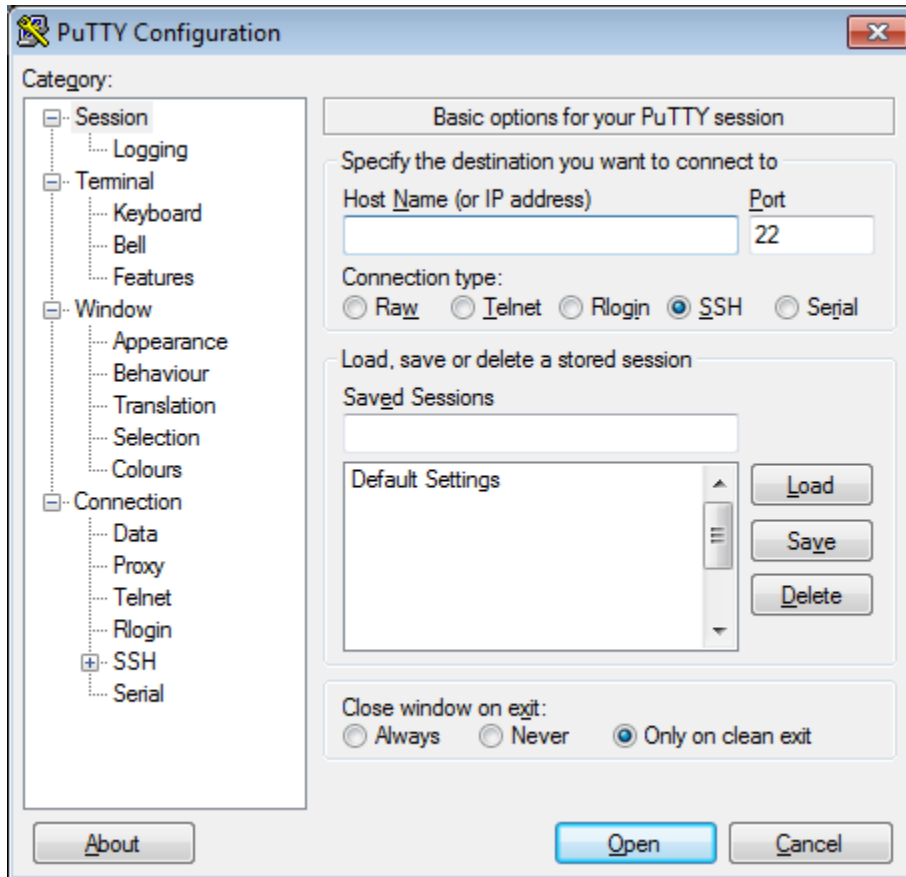
### HPRC Desktop Software - Logging into [zodiac.hpc.jcu.edu.au](http://zodiac.hpc.jcu.edu.au)

The HPC interactive nodes are accessible via the server named [zodiac.hpc.jcu.edu.au](http://zodiac.hpc.jcu.edu.au). See the relevant tabs below of instructions on how to log in to zodiac. Zodiac is a linux based system. To learn more about the linux shell, see the [Software Carpentry Unix Shell tutorials](#).

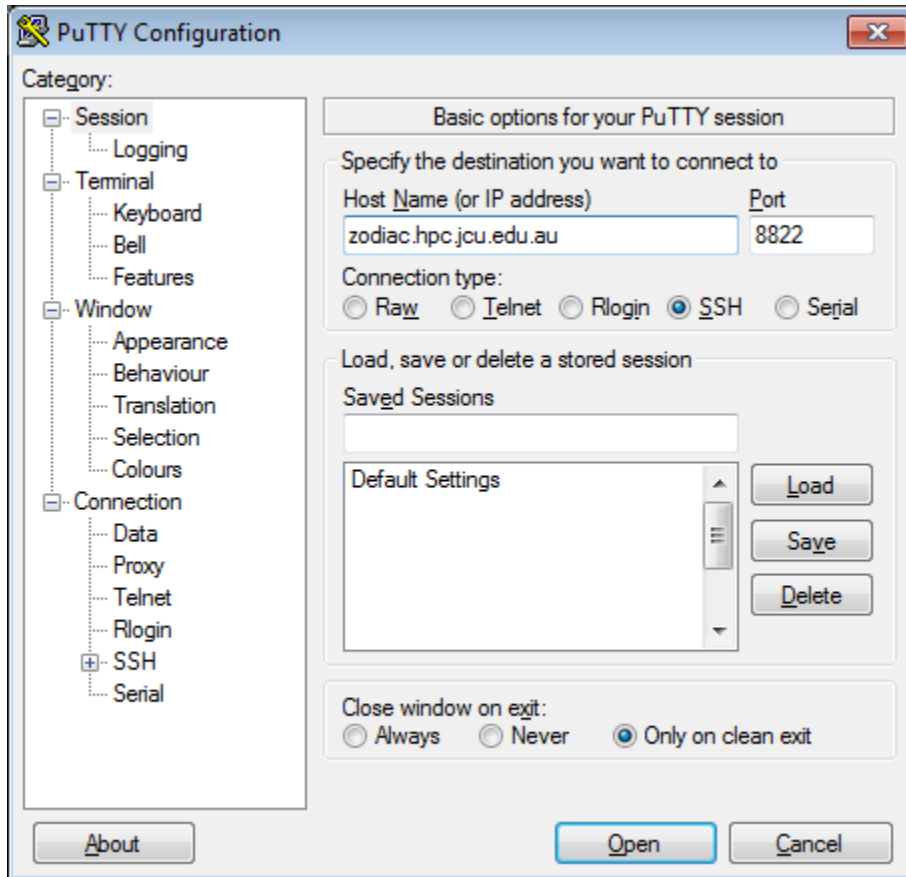
#### Windows

1. Unable to render {include} The included page could not be found.

2. Starting PuTTY will show this window:

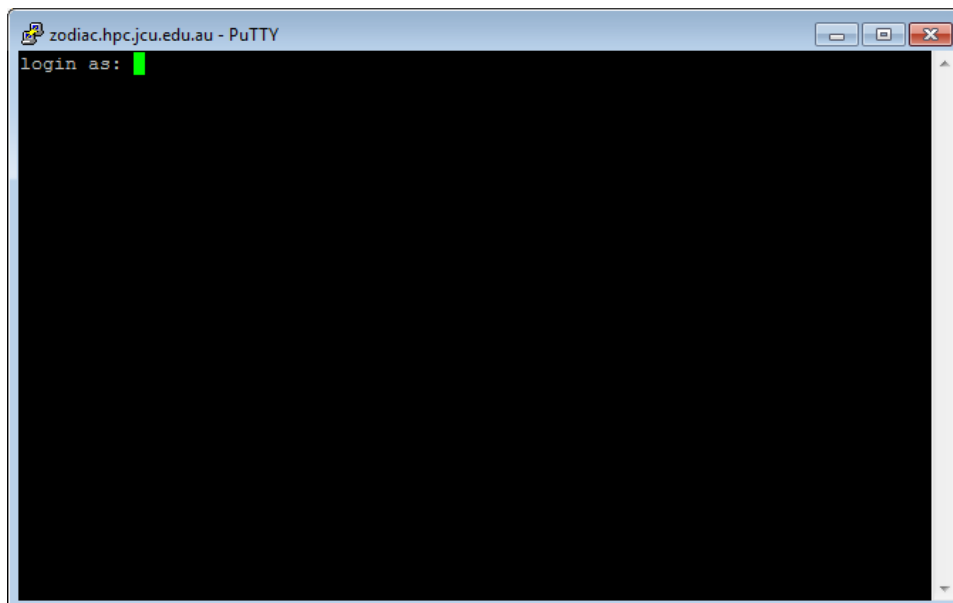


3. Enter the hostname (zodiac.hpc.jcu.edu.au) and the port 8822

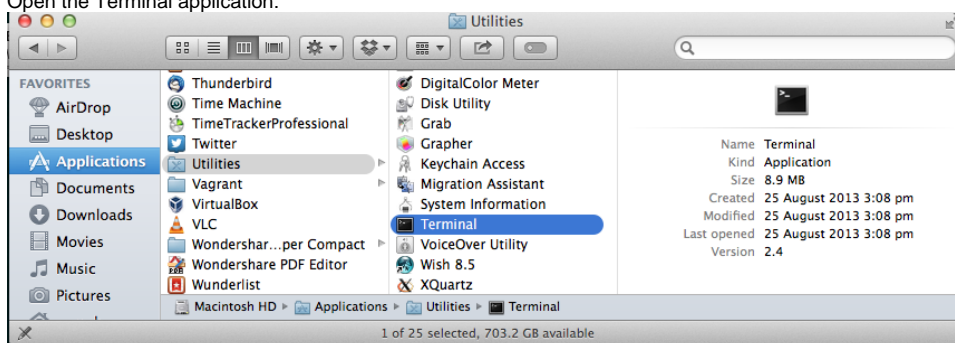


The default port for ssh is port 22, which you can use if you are accessing the cluster from on campus, however if you are accessing it from off campus you need to use port 8822.

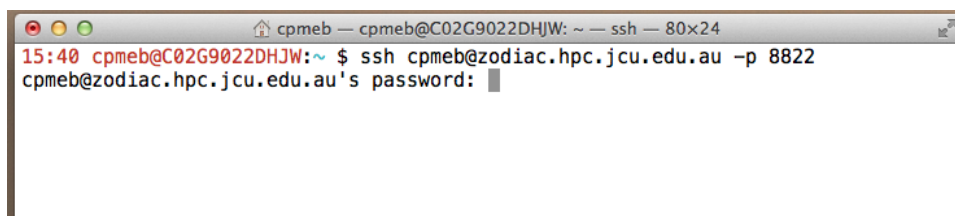
4. Then you will be prompted for your username and password, use your standard JCU credentials (username and password)



1. Open the Terminal application:



2. In the Terminal window run the ssh command: `ssh <username>@zodiac.jcu.edu.au` (add `-p 8822` if you are connecting from outside the JCU network) and you will be asked for your password



3. You are now logged in to the HPC interactive node.

## Software Packages

The HPRC Cluster uses environment modules to manage the available software packages. This allows multiple versions of the same software to be installed without interfering with each other. To enable the `environment` module system the following command needs to be executed on the command line:

```
-bash-4.1$ source /etc/profile.d/modules.sh
```

The software that is available on the HPRC cluster is listed here: [HPRC User Software](#). Alternately you can query the software available on the cluster with the following commands:

| Command                                   | Result  |
|---|---|
| <code>module avail</code>                 | A list of available software is displayed                     |
| <code>module help &lt;software&gt;</code> | Version number and brief synopsis is displayed for <software> |

```

-bash-4.1$ module avail
----- /usr/share/Modules
/modulefiles -----
MPInside/3.5.1      compiler/gcc-4.4.5 module-cvs      modules      mpich2-x86_64
null              perfcatcher
chkfeature        dot                module-info   mpi/intel-4.0 mpt/2.05
perfboost        use.own
----- /etc/modulefiles
-----
compat-openmpi-x86_64 openmpi-x86_64
----- /sw/modules
-----
4ti2              blast/2.2.23      crimap_Monsanto      hdf5          migrate
/3.6(default)    picard-tools      tmap/1.1
BEDTools         blast/2.2.29(default) dx                    hmmer
mira             proj              tmhmm
EMBOSS           bowtie            elph                 ima2
modeltest        pvm               topali
GMT              bwa/0.7.4(default) enmtools            jags
molphy           r8s              towhee
Macaulay2        caftools          fasta                java
mpich2           rainbowcrack      towhee-openmpi
Python/2.7       cap3              fastme               jcusmart
mrbayes          rpfits           trans-abyss
R/2.15.1(default) carthagene/1.2.2(default) ffmpeg              jmodeltest
mrmodeltest      ruby/1.9.3        tree-puzzle
R/3.0.0          carthagene/1.3.beta fftw2                lagan
msbayes          ruby/2.0.0        trinityrnaseq
abyss            casacore          fftw3                lamarc
ncar             samtools          udunits
ariadne          cernlib           garli                lapack
netcdf           scalapack         udunits2
arlequin         cfitsio           gdal                 libyaml/0.1.4
netphos          scipy             velvet
asap             chlorop           glimmer              matlab/2008b
numpy            seadas/6.2        wcslib
atlas            clipper           glpk                 matlab/2012a
oases            seg               wise2
bayesass         clustalw          gmp                  matlab/2012b
octave           signalp           wwatch3
beagle           cluster           gnu/4.1.2            matlab/2013a(default)
openbugs         sprng             yasm
beast            cns               gnu/4.4.0            maxent
openjdk          ssaha2            zonation
beast-1.5.4      coils            gnuplot              maxima
openmpi          stacks
bfast            colony2           grass                merlin
pari             structure
blacs            consel           gromacs              migrate/3.2.15
paup            targetp
blas             crimap           hdf                  migrate/3.5.1
phym1           tclreadline/2.1.0

```

## Running Jobs

To run a job on the cluster create a shell script containing the PBS Directives containing the information required by the scheduler to schedule the job, and the job commands.

Example: [paup](#) with the [ML\\_analysis.nex](#) sample file

### Running a job on the HPRC Cluster

In this example we will run [paup](#) with the [ML\\_analysis.nex](#) sample file provided on the [paup sample nexus files](#) page.

After logging into the cluster download the example file with the command:

```
-bash-4.1$ wget http://paup.csit.fsu.edu/data/ML_analysis.nex
--2014-03-11 13:08:16-- http://paup.csit.fsu.edu/data/ML_analysis.nex
Resolving paup.csit.fsu.edu... 144.174.50.3
Connecting to paup.csit.fsu.edu|144.174.50.3|:80... connected.
HTTP request sent, awaiting response... 200 OK
Length: 2990 (2.9K) [text/plain]
Saving to: "ML_analysis.nex"

100%[=====] 2,990 --.-K/s in 0s

2014-03-11 13:08:17 (70.7 MB/s) - "ML_analysis.nex" saved [2990/2990]
```

## Creating the job script

Using a text editor – examples include vim and nano – create your shell script with the filename: `ML_analysis.sh` and the following contents (the colours are only used for illustration purposes below):

```
#!/bin/bash

#
# Checkpointing is to be done on a job at pbs_mom shutdown.
#
#PBS -c s

#
# Merge standard output and standard error streams into the named file.
#
#PBS -j oe

#
# Set the name of the job
#
#PBS -N ML_analysis

#
# Advise the scheduler that the job requires one cpu (ppn) from one node.
#
#PBS -l nodes=1:ppn=1
```

```

#
# Advise the scheduler about the amount of physical memory required.
# kb for kilobytes, mb for megabytes, gb for gigabytes.
#
#PBS -l pmem=5gb

#
# Advise the scheduler that this job will have completed within 10 minutes.
#
#PBS -l walltime=00:10:00

#
# Send mail at batch job abort/exit to the Email address provided.
#
#PBS -m ae
#PBS -M your.name@jcu.edu.au

ncpu=`wc -l $PBS_NODEFILE | awk '{print $1}'`
echo "-----"
echo " This job is allocated "$ncpu" CPU cores on "
cat $PBS_NODEFILE | uniq
echo "-----"
echo "PBS: Submitted to $PBS_QUEUE@$PBS_O_HOST"
echo "PBS: Working directory is $PBS_O_WORKDIR"
echo "PBS: Job identifier is $PBS_JOBID"
echo "PBS: Job name is $PBS_JOBNAME"
echo "-----"

cd $PBS_O_WORKDIR
source /etc/profile.d/modules.sh
module load paup
paup -n ML_analysis.nex

```

Legend:

1. The very first line of the script file is the **Shebang**, the shebang must always be the first line.
2. The second section contains the PBS directives. For more information on PBS directives please see the [HPC PBSPro script files page](#).
3. The third section outputs information about the job, and is only included as an example of what can be done.
4. The fourth section contains the commands that are actually run in the job. In this case we are using a **bash** shell.

## Submitting the Job - qsub

The final step is to submit the job to the job scheduler:

```

-bash-4.1$ qsub ML_analysis.sh
148122.jobmgr.hpc.jcu.edu.au

```

## Monitoring the Job - qstat

Once the job has been submitted you can monitor its progress by using the qstat command.

When you first submit your job it is placed into the job queue, and its status column contains Q, meaning the job is in the queue:

```

-bash-4.1$ qstat 148122.jobmgr.hpc.jcu.edu.au
Job ID          Name          User          Time Use S Queue
-----
148122.jobmgr   ML_analysis   jcxxxxxxx    0 Q normal

```

Once your job starts running its status changes to R:

```

-bash-4.1$ qstat 148122.jobmgr.hpc.jcu.edu.au
Job ID          Name          User          Time Use S Queue
-----
148122.jobmgr   ML_analysis   jcxxxxxxx    0 R normal

```

- You can display all of the jobs you are running:

```
-bash-4.1$ qstat -u jcxxxxx -ln
jobmgr.hpc.jcu.edu.au:

                               Req'd   Req'd
Elap
Job ID          Username   Queue   Jobname          SessID NDS   TSK   Memory   Time   S
Time
-----
148185.jobmgr.hpc.jcu. jcxxxxx   normal  ML_analysis      0      1    1    5gb 500:00:00 R
00:00:17  n026/19
```

- All of the jobs running on the cluster:

```
-bash-4.1$ qstat
Job ID          Name          User          Time Use S Queue
-----
132501.jobmgr  DDWoodpcaL   jcxxxxx      581:37:3 R normal
132502.jobmgr  DDWoodpca0.1L jcxxxxx      581:11:0 R normal
132503.jobmgr  DDWoodpca0.01L jcxxxxx      581:02:3 R normal
132504.jobmgr  DDWoodpca0.001L jcxxxxx      581:05:1 R normal
132560.jobmgr  IBWoodpcaL   jcxxxxx      575:36:2 R normal
132561.jobmgr  IBWoodpca0.1L jcxxxxx      550:28:1 R normal
132562.jobmgr  IBWoodpca0.01L jcxxxxx      573:21:3 R normal
132563.jobmgr  IBWoodpca0.001L jcxxxxx      575:25:3 R normal
142918.jobmgr  DDpca0.001pcb1LL jcxxxxx      275:22:4 R normal
144744.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      3597:28: R bigmem
144745.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      2279:22: R bigmem
144746.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      1098:06: R normal
144747.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      928:26:1 R normal
144748.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      942:19:5 R normal
144753.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      1434:04: R normal
144754.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      927:20:1 R normal
144756.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      938:07:5 R normal
145377.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      1145:52: R normal
145379.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      1286:49: R normal
145381.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      1034:06: R normal
145382.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      740:05:5 R normal
145384.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      1285:28: R normal
145386.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      1028:30: R normal
145387.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      1070:39: R normal
145390.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      1238:34: R normal
145391.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      2018:17: R normal
145392.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      1585:10: R normal
145708.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      1159:11: R normal
145756.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      835:32:4 R normal
145790.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      1083:20: R normal
146395.jobmgr  ...001pcb2500LL jcxxxxx      145:38:3 R normal
146396.jobmgr  ...001pcb7500LL jcxxxxx      145:00:3 R normal
146397.jobmgr  ...001pcb12500LL jcxxxxx      152:09:2 R normal
146398.jobmgr  ...001pcb5000LL jcxxxxx      151:49:3 R normal
146399.jobmgr  ...001pcb15000LL jcxxxxx      143:16:2 R normal
146527.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      547:57:0 R normal
147055.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      362:59:2 R normal
147059.jobmgr  ..._567_bfw0_PBS jcxxxxx      46:57:34 R normal
147060.jobmgr  ..._547_bfw0_PBS jcxxxxx      46:56:16 R normal
147063.jobmgr  ..._543_bfw0_PBS jcxxxxx      46:59:03 R normal
147065.jobmgr  ...fw0_PBS_CG1.3 jcxxxxx      297:58:1 R normal
147070.jobmgr  ..._573_bfw0_PBS jcxxxxx      51:54:44 R normal
147071.jobmgr  ..._549_bfw0_PBS jcxxxxx      51:45:14 R normal
147072.jobmgr  ..._550_bfw0_PBS jcxxxxx      46:32:31 R normal
147073.jobmgr  ..._532_bfw0_PBS jcxxxxx      51:36:30 R normal
147074.jobmgr  ..._575_bfw0_PBS jcxxxxx      50:08:14 R normal
147096.jobmgr  ..._582_bfw0_PBS jcxxxxx      51:10:26 R normal
147097.jobmgr  ..._578_bfw0_PBS jcxxxxx      51:08:43 R normal
147101.jobmgr  ..._568_bfw0_PBS jcxxxxx      46:43:19 R normal
147106.jobmgr  ..._539_bfw0_PBS jcxxxxx      46:40:11 R normal
147115.jobmgr  ...es.1km_1km.sh jcxxxxx      50:46:46 R normal
```



|               |                  |          |          |   |        |
|---------------|------------------|----------|----------|---|--------|
| 147203.jobmgr | NarrowBoxParent  | jcxxxxxx | 140:35:0 | R | normal |
| 147206.jobmgr | NarrowBoxParent  | jcxxxxxx | 150:53:4 | R | normal |
| 147207.jobmgr | NarrowBoxParent  | jcxxxxxx | 125:10:5 | R | normal |
| 147212.jobmgr | NarrowBoxParent  | jcxxxxxx | 151:57:4 | R | normal |
| 147213.jobmgr | NarrowBoxParent  | jcxxxxxx | 164:20:4 | R | normal |
| 147215.jobmgr | NarrowBoxParent  | jcxxxxxx | 160:11:4 | R | normal |
| 147216.jobmgr | NarrowBoxParent  | jcxxxxxx | 157:02:1 | R | normal |
| 147217.jobmgr | NarrowBoxParent  | jcxxxxxx | 163:39:0 | R | normal |
| 147218.jobmgr | NarrowBoxParent  | jcxxxxxx | 156:11:5 | R | normal |
| 147219.jobmgr | NarrowBoxParent  | jcxxxxxx | 140:37:4 | R | normal |
| 147220.jobmgr | NarrowBoxParent  | jcxxxxxx | 149:46:1 | R | normal |
| 147221.jobmgr | NarrowBoxParent  | jcxxxxxx | 141:12:4 | R | normal |
| 147222.jobmgr | NarrowBoxParent  | jcxxxxxx | 136:42:2 | R | normal |
| 147224.jobmgr | NarrowBoxParent  | jcxxxxxx | 132:20:5 | R | normal |
| 147225.jobmgr | NarrowBoxParent  | jcxxxxxx | 153:33:0 | R | normal |
| 147274.jobmgr | NarrowBox        | jcxxxxxx | 138:18:2 | R | normal |
| 147275.jobmgr | NarrowBox        | jcxxxxxx | 142:08:0 | R | normal |
| 147318.jobmgr | ..._bFw0_PBS_1.2 | jcxxxxxx | 39:59:20 | R | normal |
| 147325.jobmgr | NarrowBox        | jcxxxxxx | 148:00:2 | R | normal |
| 147331.jobmgr | ...fw0_PBS_CG1.3 | jcxxxxxx | 248:00:3 | R | normal |
| 147332.jobmgr | ...fw0_PBS_CG1.3 | jcxxxxxx | 229:03:3 | R | normal |
| 147391.jobmgr | NarrowBox        | jcxxxxxx | 126:32:5 | R | normal |
| 147398.jobmgr | NarrowBox        | jcxxxxxx | 125:48:5 | R | normal |
| 147470.jobmgr | ...fw0_PBS_CG1.3 | jcxxxxxx | 232:50:4 | R | normal |
| 147471.jobmgr | ...fw0_PBS_CG1.3 | jcxxxxxx | 196:34:1 | R | normal |
| 147472.jobmgr | ...fw0_PBS_CG1.3 | jcxxxxxx | 415:56:4 | R | normal |
| 147494.jobmgr | ...or.lkm_lkm.sh | jcxxxxxx | 25:36:45 | R | normal |
| 147495.jobmgr | ...us.lkm_lkm.sh | jcxxxxxx | 26:03:45 | R | normal |
| 147496.jobmgr | ...us.lkm_lkm.sh | jcxxxxxx | 26:04:44 | R | normal |
| 147498.jobmgr | ...us.lkm_lkm.sh | jcxxxxxx | 25:59:16 | R | normal |
| 147499.jobmgr | ...ii.lkm_lkm.sh | jcxxxxxx | 11:43:42 | R | normal |
| 147502.jobmgr | ...fw0_PBS_CG1.3 | jcxxxxxx | 131:28:4 | R | normal |
| 147576.jobmgr | NarrowBox        | jcxxxxxx | 60:24:11 | R | normal |
| 147577.jobmgr | NarrowBox        | jcxxxxxx | 60:36:39 | R | normal |
| 147584.jobmgr | NarrowBox        | jcxxxxxx | 52:12:36 | R | normal |
| 147590.jobmgr | NarrowBox        | jcxxxxxx | 49:06:43 | R | normal |
| 147616.jobmgr | NarrowBox        | jcxxxxxx | 33:08:43 | R | normal |
| 147619.jobmgr | NarrowBox        | jcxxxxxx | 30:28:18 | R | normal |
| 147621.jobmgr | NarrowBox        | jcxxxxxx | 30:33:22 | R | normal |
| 147629.jobmgr | ...es.lkm_lkm.sh | jcxxxxxx | 07:04:15 | R | normal |
| 147630.jobmgr | ...ae.lkm_lkm.sh | jcxxxxxx | 07:15:13 | R | normal |
| 147631.jobmgr | ...ra.lkm_lkm.sh | jcxxxxxx | 0        | Q | normal |
| 147632.jobmgr | ...ii.lkm_lkm.sh | jcxxxxxx | 0        | Q | normal |
| 147634.jobmgr | ...ta.lkm_lkm.sh | jcxxxxxx | 0        | Q | normal |
| 147635.jobmgr | ...mi.lkm_lkm.sh | jcxxxxxx | 0        | Q | normal |
| 147636.jobmgr | ...ii.lkm_lkm.sh | jcxxxxxx | 0        | Q | normal |
| 147637.jobmgr | ...ei.lkm_lkm.sh | jcxxxxxx | 07:02:52 | R | normal |
| 147647.jobmgr | NarrowBox        | jcxxxxxx | 13:28:24 | R | normal |
| 147651.jobmgr | run_RSEM.sh      | jcxxxxxx | 21:46:18 | R | normal |
| 147652.jobmgr | NarrowBox        | jcxxxxxx | 19:52:35 | R | normal |
| 147657.jobmgr | NarrowBox        | jcxxxxxx | 18:04:53 | R | normal |
| 147665.jobmgr | NarrowBox        | jcxxxxxx | 16:17:01 | R | normal |
| 147702.jobmgr | NarrowBox        | jcxxxxxx | 13:03:45 | R | normal |
| 147820.jobmgr | NarrowBox        | jcxxxxxx | 10:16:38 | R | normal |
| 148021.jobmgr | NarrowBox        | jcxxxxxx | 08:41:26 | R | normal |
| 148022.jobmgr | NarrowBox        | jcxxxxxx | 08:42:34 | R | normal |
| 148087.jobmgr | NarrowBox        | jcxxxxxx | 07:45:33 | R | normal |
| 148095.jobmgr | NarrowBox        | jcxxxxxx | 07:03:12 | R | normal |
| 148096.jobmgr | NarrowBox        | jcxxxxxx | 07:10:18 | R | normal |
| 148099.jobmgr | NarrowBox        | jcxxxxxx | 06:54:12 | R | normal |
| 148100.jobmgr | NarrowBox        | jcxxxxxx | 06:38:54 | R | normal |
| 148101.jobmgr | NarrowBox        | jcxxxxxx | 06:46:31 | R | normal |
| 148108.jobmgr | NarrowBox        | jcxxxxxx | 05:57:17 | R | normal |
| 148124.jobmgr | NarrowBox        | jcxxxxxx | 05:11:52 | R | normal |
| 148126.jobmgr | NarrowBox        | jcxxxxxx | 04:49:25 | R | normal |
| 148138.jobmgr | NarrowBox        | jcxxxxxx | 04:30:48 | R | normal |
| 148150.jobmgr | NarrowBox        | jcxxxxxx | 03:46:22 | R | normal |
| 148154.jobmgr | NarrowBox        | jcxxxxxx | 03:19:45 | R | normal |
| 148179.jobmgr | NarrowBox        | jcxxxxxx | 00:10:33 | R | normal |
| 148180.jobmgr | NarrowBox        | jcxxxxxx | 00:10:57 | R | normal |
| 148182.jobmgr | NarrowBox        | jcxxxxxx | 00:30:19 | R | normal |

## Deleting a job - qdel

If you need to your job you can use the qdel command

```
-bash-4.1$ qdel 148122.jobmgr.hpc.jcu.edu.au
```

## Your job's Output

Different programs have different ways of outputting their data. If they output data directly to a file then your results will be in whatever file you specified. If, however, the results are printed out to the standard out (as is the case for this example) then PBS captures them into a file for you.

```
-----  
This job is allocated 1 CPU cores on  
n025nfs  
-----
```

```
PBS: Submitted to normal@n029.default.domain  
PBS: Working directory is /home/jcxxxxx/paup  
PBS: Job identifier is 148122.jobmgr.hpc.jcu.edu.au  
PBS: Job name is ML_analysis  
-----
```

```
P A U P *  
Portable version 4.0b10 for Unix  
Tue Mar 11 13:36:52 2014
```

```
-----NOTICE-----  
This is a beta-test version. Please report any crashes,  
apparent calculation errors, or other anomalous results.  
There are no restrictions on publication of results obtained  
with this version, but you should check the WWW site  
frequently for bug announcements and/or updated versions.  
See the README file on the distribution media for details.  
-----
```

Processing of file "~/ML\_analysis.nex" begins...

Data read in DNA format

Data matrix has 8 taxa, 200 characters  
Valid character-state symbols: ACGT  
Missing data identified by '?'  
"Equate" macros in effect:

```
R,r ==> {AG}  
Y,y ==> {CT}  
M,m ==> {AC}  
K,k ==> {GT}  
S,s ==> {CG}  
W,w ==> {AT}  
H,h ==> {ACT}  
B,b ==> {CGT}  
V,v ==> {ACG}  
D,d ==> {AGT}  
N,n ==> {ACGT}
```

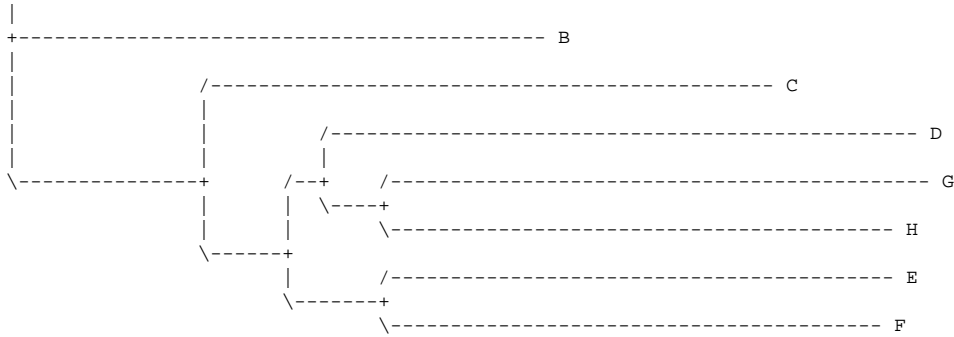
Neighbor-joining search settings:

```
Ties (if encountered) will be broken systematically  
Distance measure = uncorrected ("p")  
(Tree is unrooted)
```

```
Tree found by neighbor-joining method stored in tree buffer  
Time used = <1 sec (CPU time = 0.00 sec)
```

Neighbor-joining tree:

```
/----- A
```



Likelihood scores of tree(s) in memory:

Likelihood settings:

Number of substitution types = 2 (HKY85 variant)  
 Transition/transversion ratio estimated via ML  
 Assumed nucleotide frequencies (empirical frequencies):  
 A=0.35000 C=0.28813 G=0.20563 T=0.15625  
 Among-site rate variation:  
 Assumed proportion of invariable sites = none  
 Distribution of rates at variable sites = gamma (discrete approximation)  
 Shape parameter (alpha) = estimated  
 Number of rate categories = 4  
 Representation of average rate for each category = mean  
 These settings correspond to the HKY85+G model  
 Number of distinct data patterns under this model = 152  
 Molecular clock not enforced  
 Starting branch lengths obtained using Rogers-Swofford approximation method  
 Branch-length optimization = one-dimensional Newton-Raphson with pass  
 limit=20, delta=1e-06  
 -ln L (unconstrained) = 936.27218

| Tree       | 1          |
|------------|------------|
| -ln L      | 1646.41982 |
| Ti/tv:     |            |
| exp. ratio | 4.167819   |
| kappa      | 8.796257   |
| Shape      | 0.429541   |

Time used to compute likelihoods = 1 sec (CPU time = 0.79 sec)

Optimality criterion set to likelihood.

Heuristic search settings:

Optimality criterion = likelihood

Likelihood settings:

Number of substitution types = 2 (HKY85 variant)  
 Transition/transversion ratio = 4.16782 (kappa = 8.7962568)  
 Assumed nucleotide frequencies (empirical frequencies):  
 A=0.35000 C=0.28813 G=0.20563 T=0.15625  
 Among-site rate variation:  
 Assumed proportion of invariable sites = none  
 Distribution of rates at variable sites = gamma (discrete approximation)  
 Shape parameter (alpha) = 0.429541  
 Number of rate categories = 4  
 Representation of average rate for each category = mean  
 These settings correspond to the HKY85+G model  
 Number of distinct data patterns under this model = 152  
 Molecular clock not enforced  
 Starting branch lengths obtained using Rogers-Swofford approximation method  
 Trees with approximate likelihoods 5% or further from the target score are rejected without additional iteration  
 Branch-length optimization = one-dimensional Newton-Raphson with pass  
 limit=20, delta=1e-06  
 -ln L (unconstrained) = 936.27218

Starting tree(s) obtained via stepwise addition

Addition sequence: random

Number of replicates = 5

Starting seed = 1412047148

Number of trees held at each step during stepwise addition = 1

Branch-swapping algorithm: tree-bisection-reconnection (TBR)

```
Steepest descent option not in effect
Initial 'MaxTrees' setting = 100
Branches collapsed (creating polytomies) if branch length is less than or
equal to 1e-08
'MulTrees' option in effect
Topological constraints not enforced
Trees are unrooted
```

```
Heuristic search completed
Total number of rearrangements tried = 128
Score of best tree(s) found = 1645.76314
Number of trees retained = 1
Time used = 4 sec (CPU time = 3.49 sec)
```

Tree-island profile:

| Island | Size | First tree | Last tree | Score      | First replicate | Times hit |
|--------|------|------------|-----------|------------|-----------------|-----------|
| 1      | 1    | 1          | 1         | 1645.76314 | 1               | 5         |

Processing of file "~/ML\_analysis.nex" completed.

## Other Examples

- [Running a job on the HPRC Cluster](#)
- [Running R Jobs on the HPRC Cluster](#)

## Job Resources

It is important to match resources requested with the PBS Directives in your script and the resource usage of your job. There can be consequences for incorrectly specifying these resource requirements

- **Walltime:** your job can be killed if it exceeds the specified wall time.
- **Memory:** overusing memory can cause the compute node's memory to be pushed into swap space, slowing down all jobs on that node. This has also killed compute nodes in the past, destroying
- **CPUs:** using more cpus than requested can slow down all jobs running on that node.

## Furthur Reading

1. [HPRC Cluster Explained](#)
2. [HPRC Cluster Job Management Explained](#)
3. [HPC PBSPro script files](#)