

# 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).

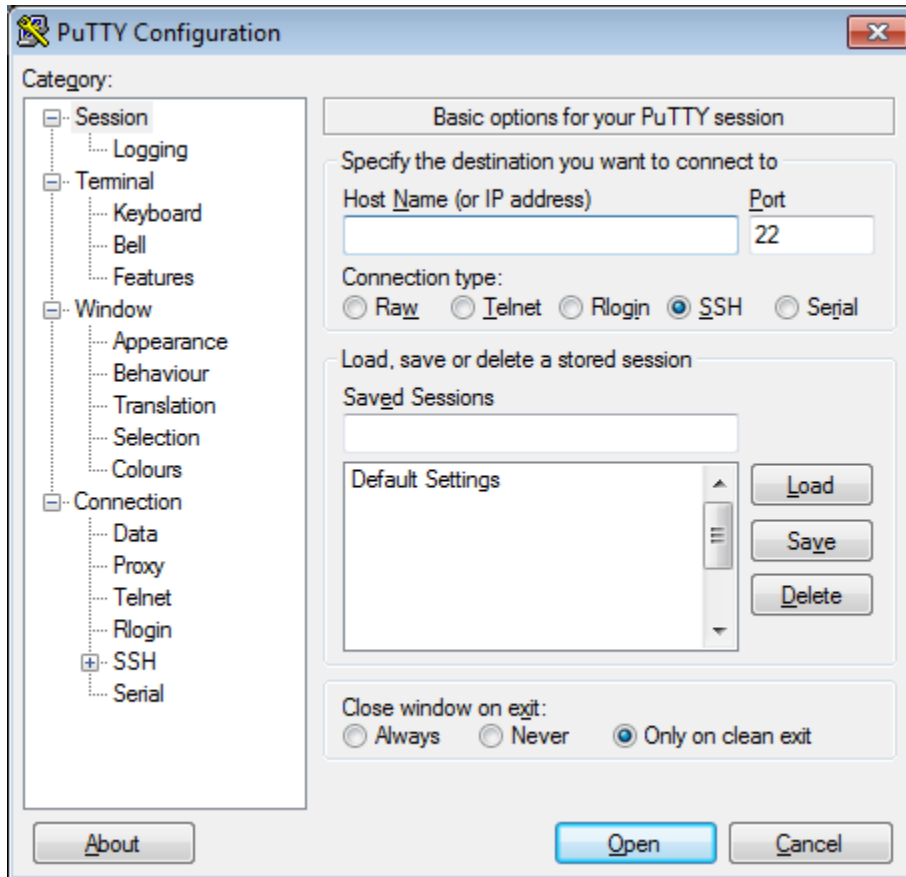
### HPRC Desktop Software - Logging into [zodiac.hpc.jcu.edu.au](http://zodiac.hpc.jcu.edu.au)

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](#).

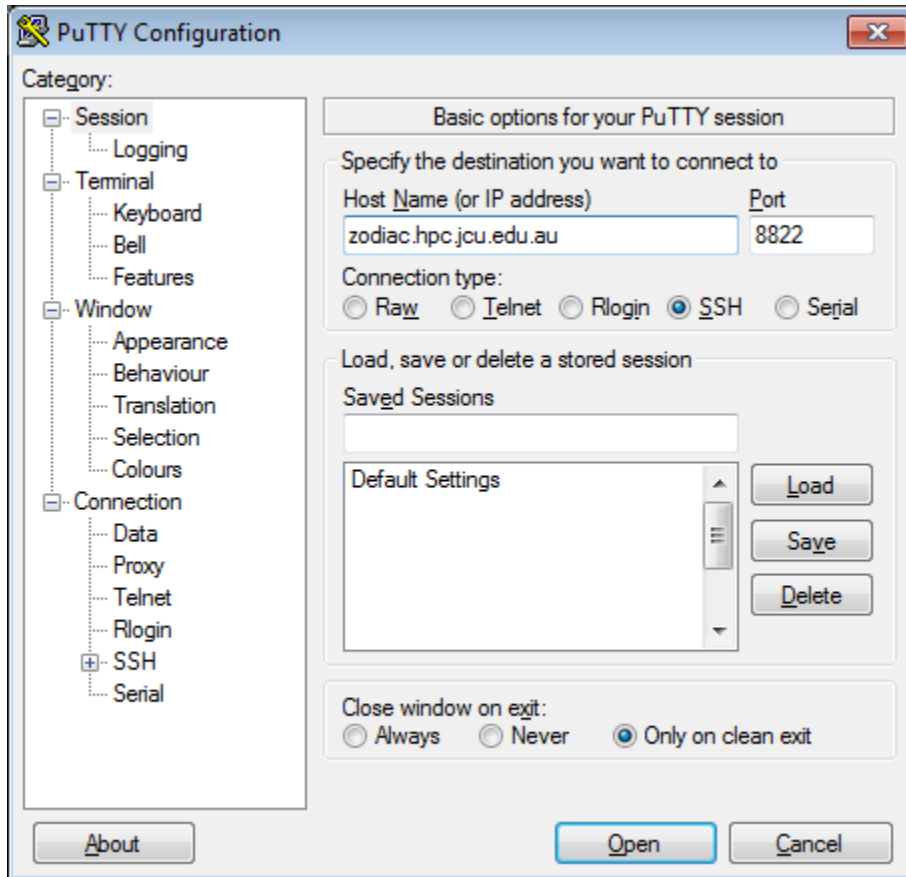
#### Windows

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

2. Starting PuTTY will show this window:

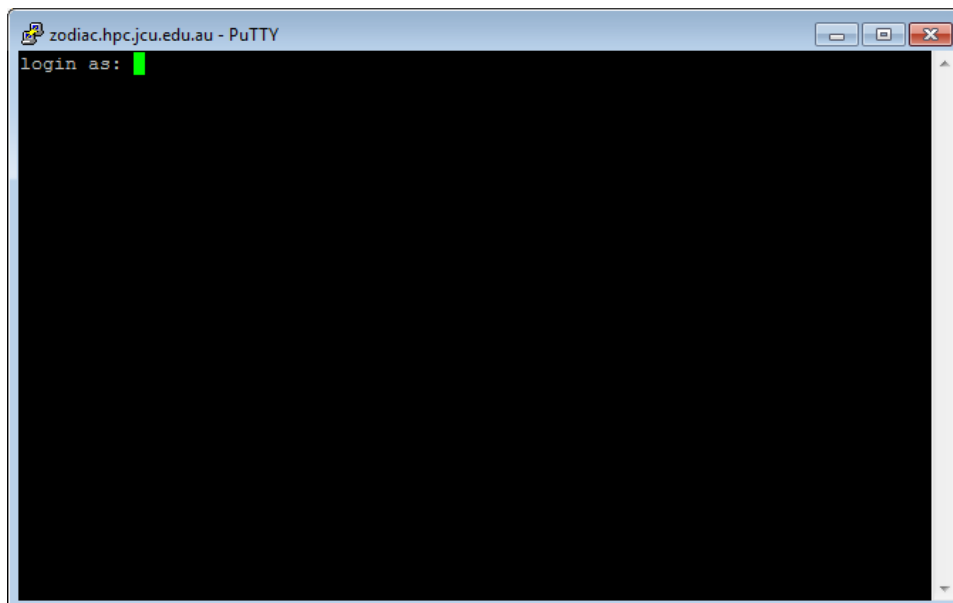


3. Enter the hostname (zodiac.hpc.jcu.edu.au) and the port 8822

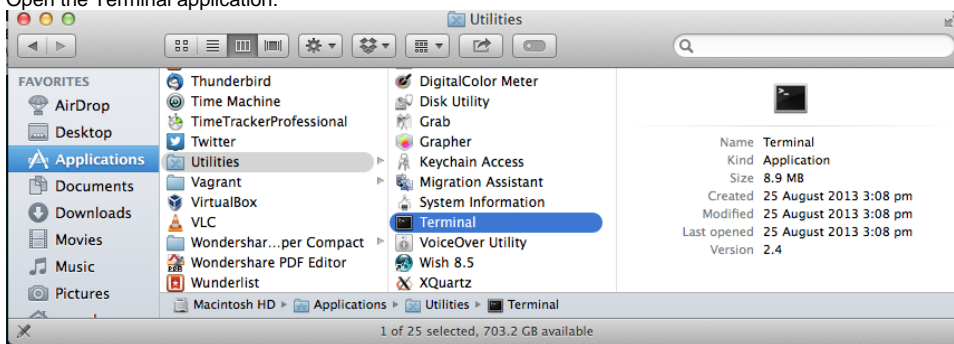


The default port for ssh is port 22, which you can use if you are accessing the cluster from on campus, however if you are accessing it from off campus you need to use port 8822.

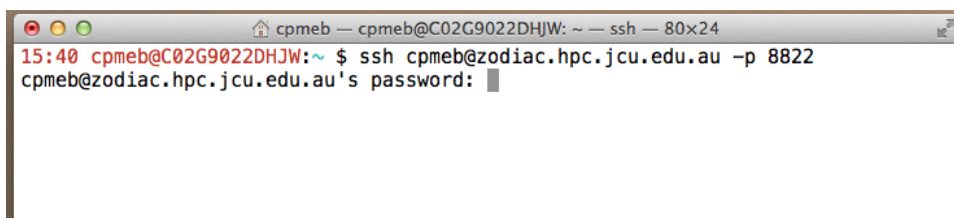
4. Then you will be prompted for your username and password, use your standard JCU credentials (username and password)



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   DDWoodpca1L        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   IBWoodpca1L       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:

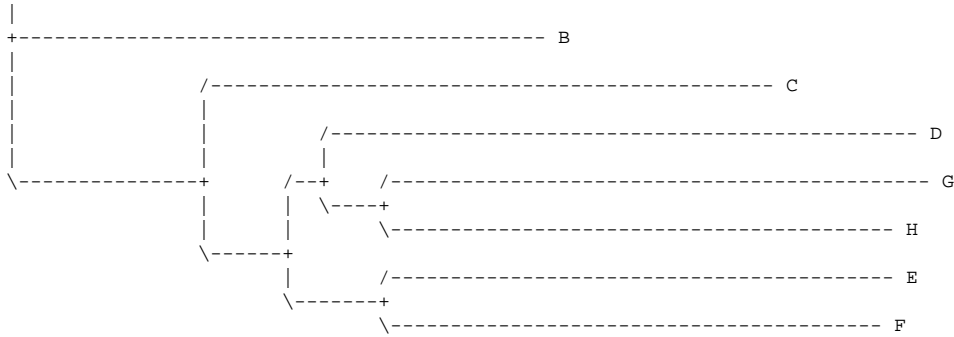
```
R,r ==> {AG}  
Y,y ==> {CT}  
M,m ==> {AC}  
K,k ==> {GT}  
S,s ==> {CG}  
W,w ==> {AT}  
H,h ==> {ACT}  
B,b ==> {CGT}  
V,v ==> {ACG}  
D,d ==> {AGT}  
N,n ==> {ACGT}
```

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](#)