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CRUK cluster introduction (II of III)

Using the scheduler for job submission

UNIVERSITY OF CAMBRIDGE

Overview

Our job scheduling system is Platform LSF

In their own words:

> *'LSF provides the capabilities to manage and accelerate workload processing across heterogeneous distributed compute environments. It is comprised of a comprehensive set of intelligent scheduling policies to ensure that the right resources are automatically allocated to the right jobs, for maximum application performance and efficiency.'*
>
> *Version 7.0.4*

LSF will allow you to:

- Submit jobs to the cluster.
- Specify which queue to submit your jobs to.
- Request memory resources for your jobs.
- Set memory limits for your jobs.
- Check the status of the jobs you have submitted.
- Check the status of the hosts within the cluster.
- Kill jobs that you have submitted to the cluster.

The most useful LSF commands

These are:

- **bsub**
- **bjobs**
- **bhosts**
- **bqueues**
- **bkill**

Type command followed by -h for usage details.

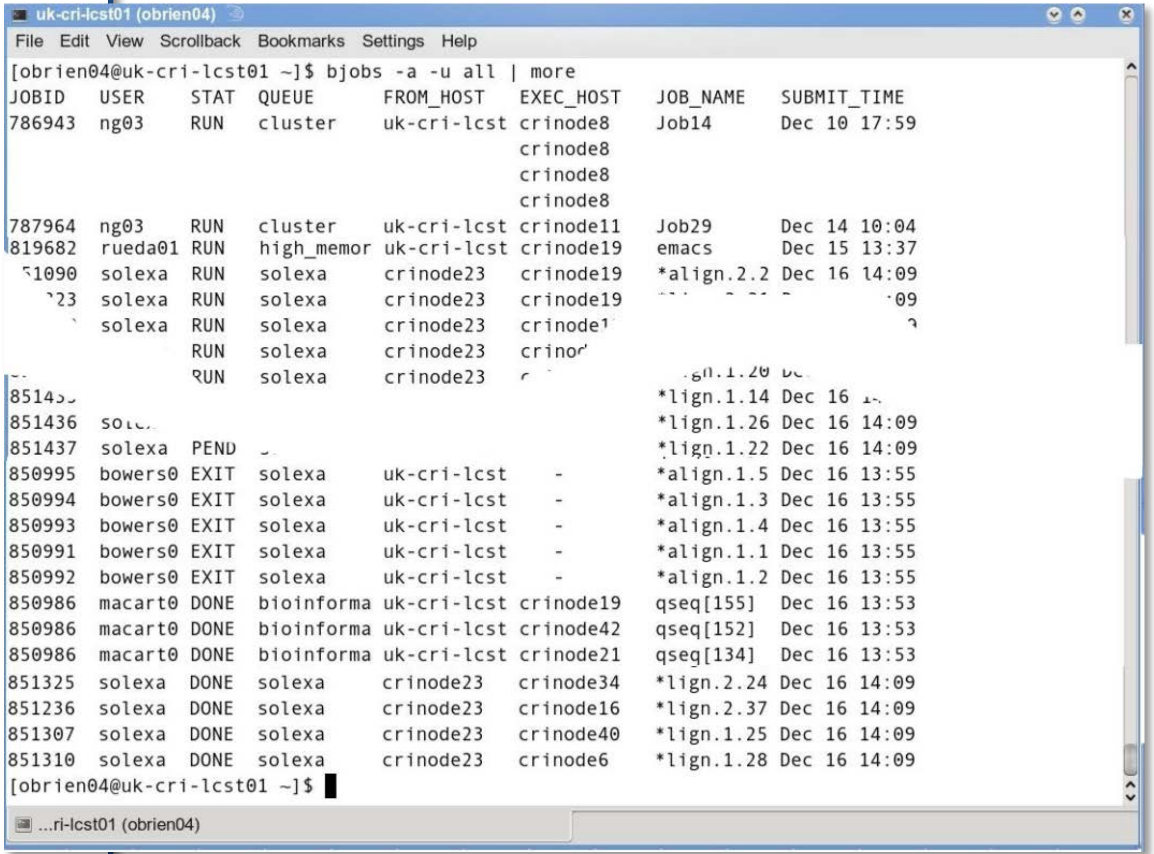
Many LSF commands have shared syntax, i.e. the **-l** (long output), **-u** (User) and **-m** (host) flags.

A Job

A command or series of commands submitted to the cluster with associated resource requirements and limits.

Status of jobs running on the cluster can be seen with the command

uk-cri-lcst01 > bjobs -a -u all



```
[obrien04@uk-cri-lcst01 ~]$ bjobs -a -u all | more
JOBID   USER    STAT  QUEUE      FROM_HOST   EXEC_HOST   JOB_NAME   SUBMIT_TIME
786943  ng03    RUN   cluster    uk-cri-lcst crinode8    Job14      Dec 10 17:59
                                             crinode8
                                             crinode8
                                             crinode8
787964  ng03    RUN   cluster    uk-cri-lcst crinode11   Job29      Dec 14 10:04
819682  rueda01 RUN   high_memor uk-cri-lcst crinode19   emacs      Dec 15 13:37
 1090   solexa  RUN   solexa     crinode23   crinode19   *align.2.2 Dec 16 14:09
   23   solexa  RUN   solexa     crinode23   crinode19                     09
        solexa  RUN   solexa     crinode23   crinode1
                RUN   solexa     crinode23   crino
                RUN   solexa     crinode23                gn.1.20  De
85143                                                    *lign.1.14 Dec 16 1
851436  so                                               *lign.1.26 Dec 16 14:09
851437  solexa  PEND                                     *lign.1.22 Dec 16 14:09
850995  bowers0 EXIT  solexa     uk-cri-lcst    -        *align.1.5 Dec 16 13:55
850994  bowers0 EXIT  solexa     uk-cri-lcst    -        *align.1.3 Dec 16 13:55
850993  bowers0 EXIT  solexa     uk-cri-lcst    -        *align.1.4 Dec 16 13:55
850991  bowers0 EXIT  solexa     uk-cri-lcst    -        *align.1.1 Dec 16 13:55
850992  bowers0 EXIT  solexa     uk-cri-lcst    -        *align.1.2 Dec 16 13:55
850986  macart0 DONE  bioinforma uk-cri-lcst crinode19   qseq[155]  Dec 16 13:53
850986  macart0 DONE  bioinforma uk-cri-lcst crinode42   qseq[152]  Dec 16 13:53
850986  macart0 DONE  bioinforma uk-cri-lcst crinode21   qseq[134]  Dec 16 13:53
851325  solexa  DONE  solexa     crinode23   crinode34   *lign.2.24 Dec 16 14:09
851236  solexa  DONE  solexa     crinode23   crinode16   *lign.2.37 Dec 16 14:09
851307  solexa  DONE  solexa     crinode23   crinode40   *lign.1.25 Dec 16 14:09
851310  solexa  DONE  solexa     crinode23   crinode6    *lign.1.28 Dec 16 14:09
[obrien04@uk-cri-lcst01 ~]$
```

The bsub command

A monster, even by unix standards.

```
bsub [ -h ] [ -V ] [ -H ] [ -x ] [ -r ] [ -N ] [ -B ]
[ -I | -Ip | -Is | -K ]
[ -T time_event ]
[ [ -X "exception_cond([params])::action" ] ... ]
[ -w depend_cond ]
[ -q queue_name ... ] [ -a application_name ]
[ -m host_name[+[pref_level]] ... ]
[ -n min_proc[,max_proc] ]
[ -R res_req ]
[ -J job_name_spec ] [ -b begin_time ] [ -t term_time
]
[ -i in_file ] [ -o out_file ] [ -e err_file ]
[ -u mail_user ] [ [ -f "lfile op [ rfile ]" ] ... ]
[ -E "pre_exec_command [ argument ... ]" ]
[ -c cpu_limit[/host_spec ] ] [ -W
run_limit[/host_spec ] ]
[ -F file_limit ] [ -M mem_limit ] [ -D data_limit ]
[ -S stack_limit ] [ -C core_limit ]
[ -k "chkpnt_dir [ chkpnt_period ]" ] [ -w
depend_cond ]
[ -L login_shell ] [ -P project_name ]
[ -G user_group ] [ command [ argument ... ] ]
```

A Queue:

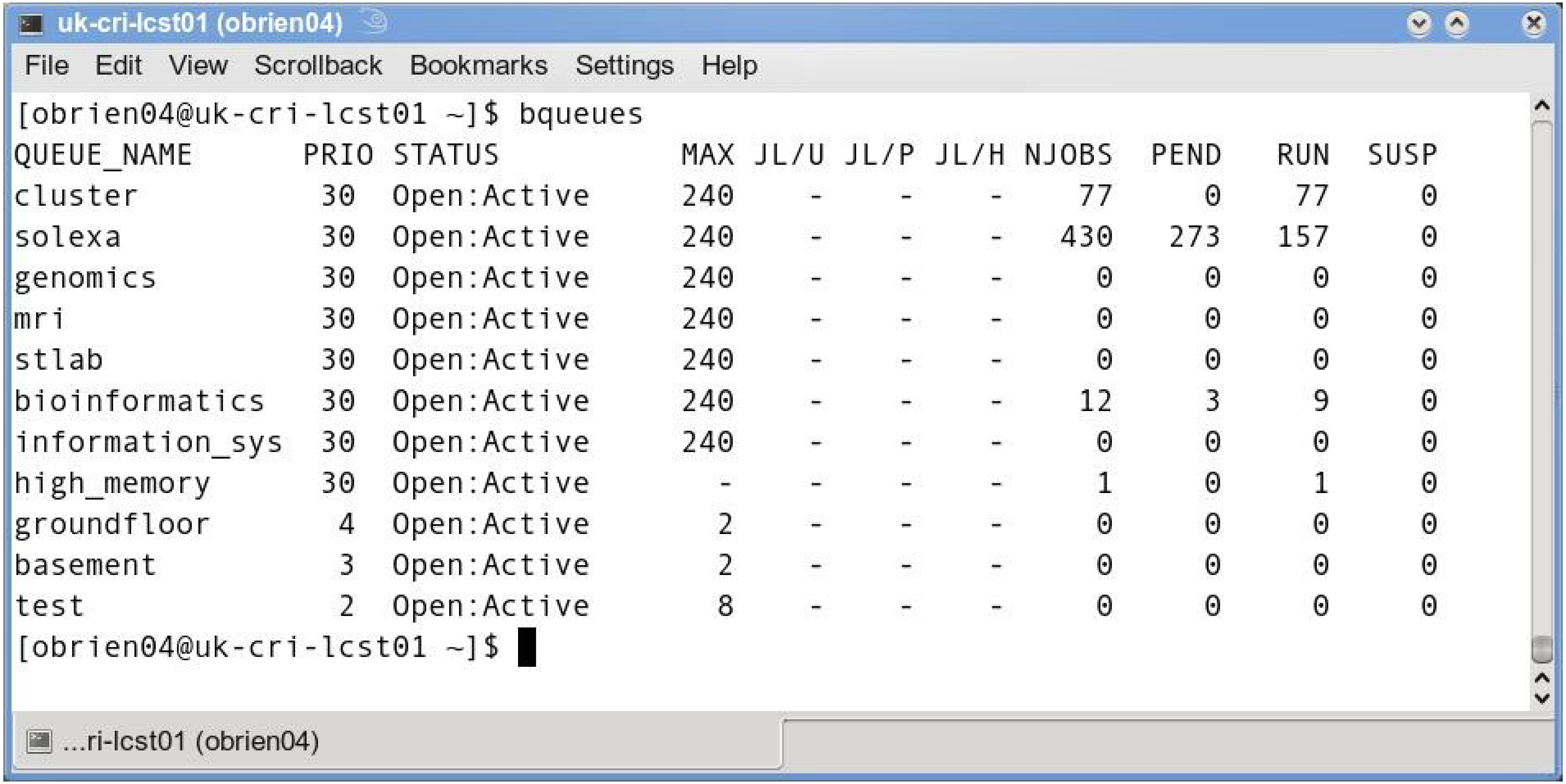
A queue for job submissions associated with specified users and cluster hosts, and providing specified default resources.

You specify the queue to use by adding the
-q <queuename>
option to the bsub command.

Most CRI cluster queues have a default memory resource limit of 2GB per job.
You can override the default by adding the
-M <memory size in KB>
to the bsub
command.

An example submission request to the queue named cluster to run a job which overrides the 2GB memory limit allowing the job to use 4GBs and requesting that the host has/hosts have 4GB memory available, may look like this:

```
uk-cri-lcst01 > bsub -q cluster -M 4194304
-R "rusage[mem=4096]" <command>
```



```
[obrien04@uk-cri-lcst01 ~]$ bqueues
QUEUE_NAME      PRIO STATUS          MAX JL/U JL/P JL/H NJOBS  PEND   RUN  SUSP
cluster          30  Open:Active     240    -    -    -    77     0    77     0
solexa           30  Open:Active     240    -    -    -   430   273   157     0
genomics         30  Open:Active     240    -    -    -     0     0     0     0
mri              30  Open:Active     240    -    -    -     0     0     0     0
stlab            30  Open:Active     240    -    -    -     0     0     0     0
bioinformatics   30  Open:Active     240    -    -    -    12     3     9     0
information_sys  30  Open:Active     240    -    -    -     0     0     0     0
high_memory      30  Open:Active       -    -    -    -     1     0     1     0
groundfloor       4  Open:Active       2    -    -    -     0     0     0     0
basement          3  Open:Active       2    -    -    -     0     0     0     0
test              2  Open:Active       8    -    -    -     0     0     0     0
[obrien04@uk-cri-lcst01 ~]$ 
```

The 'test' queue

We also have a test queue, called test, which comprises one sacrificial host (8 cores).

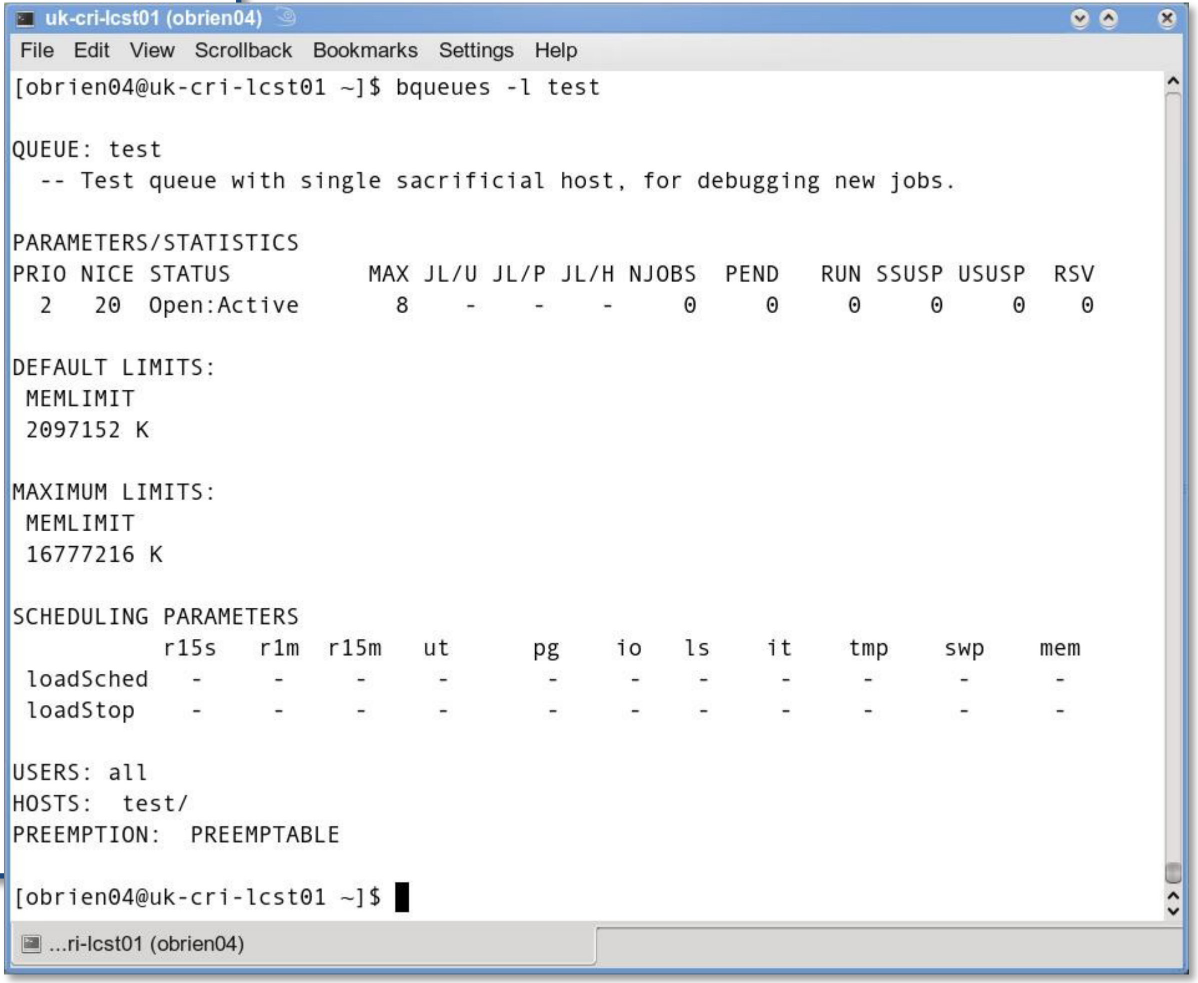
Please submit brand new jobs, and jobs that you feel might have become rogue after tweaking, to this queue before setting them loose on the cluster. If it kills the host, let us know and we'll restart it ready for further testing.

(Of course, if your job does kill the test host, please don't release it to the cluster in general until it has been debugged and shown to behave itself in the test environment.)

Viewing the test queue properties

Use the long version of the bqueues command.

uk-cri-lcst01 > **bqueues -l test**

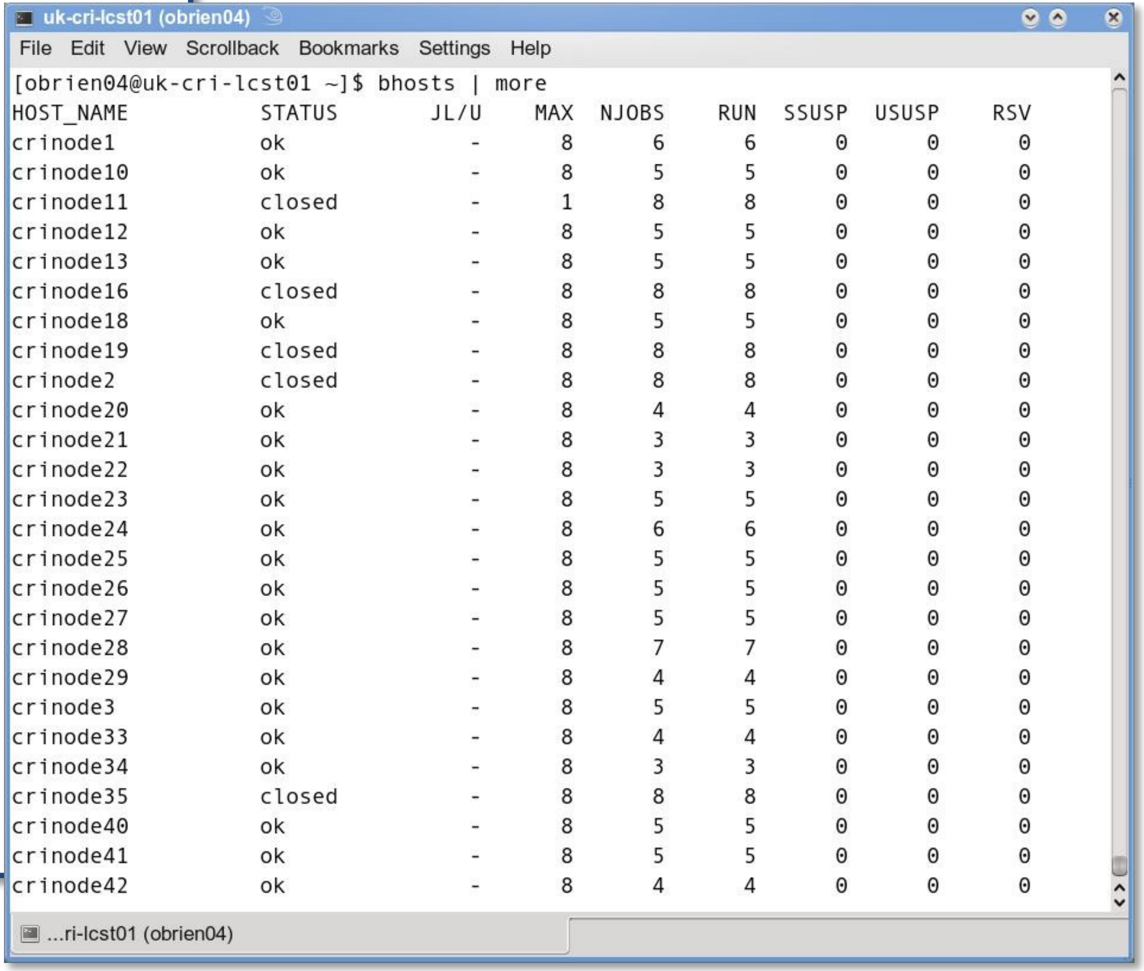


```
[obrien04@uk-cri-lcst01 ~]$ bqueues -l test

QUEUE: test
  -- Test queue with single sacrificial host, for debugging new jobs.

PARAMETERS/STATISTICS
PRIO NICE STATUS          MAX JL/U JL/P JL/H NJOBS  PEND   RUN SSUSP USUSP  RSV
  2   20  Open:Active       8    -    -    -     0     0     0     0     0    0

DEFAULT LIMITS:
 MEMLIMIT
 2097152 K

MAXIMUM LIMITS:
 MEMLIMIT
 16777216 K

SCHEDULING PARAMETERS
           r15s   r1m  r15m   ut      pg    io   ls    it    tmp    swp    mem
 loadSched   -     -     -     -       -     -    -     -     -      -      -
 loadStop    -     -     -     -       -     -    -     -     -      -      -

USERS: all
HOSTS:  test/
PREEMPTION:  PREEMPTABLE

[obrien04@uk-cri-lcst01 ~]$
```

Checking the status of hosts within the cluster

Check hosts status using the bhosts command

uk-cri-lcst01 > bhosts

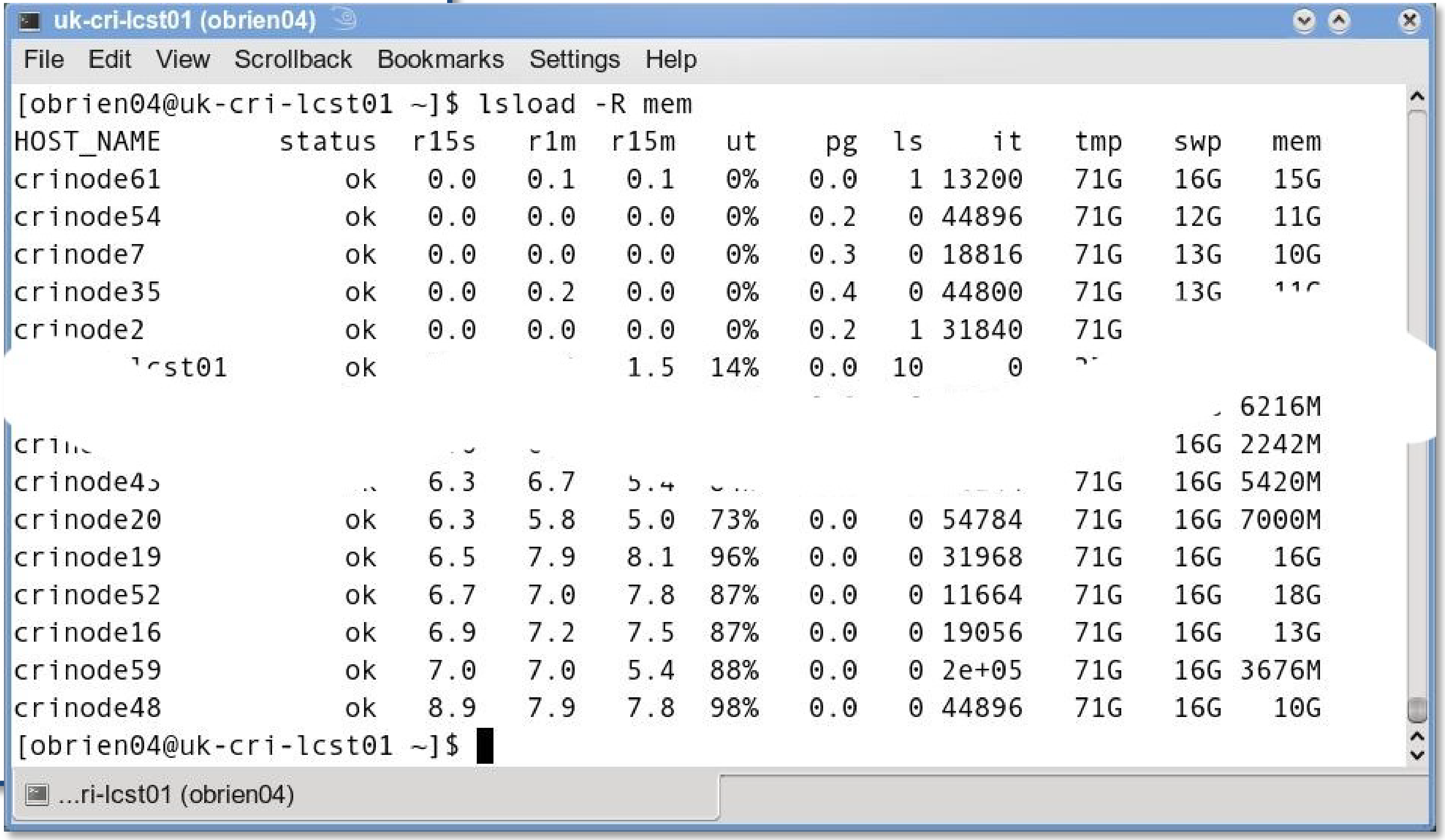


```
[obrien04@uk-cri-lcst01 ~]$ bhosts | more
HOST_NAME          STATUS       JL/U    MAX  NJOBS    RUN  SSUSP  USUSP    RSV
crinode1           ok              -      8      6      6      0      0      0
crinode10          ok              -      8      5      5      0      0      0
crinode11          closed          -      1      8      8      0      0      0
crinode12          ok              -      8      5      5      0      0      0
crinode13          ok              -      8      5      5      0      0      0
crinode16          closed          -      8      8      8      0      0      0
crinode18          ok              -      8      5      5      0      0      0
crinode19          closed          -      8      8      8      0      0      0
crinode2           closed          -      8      8      8      0      0      0
crinode20          ok              -      8      4      4      0      0      0
crinode21          ok              -      8      3      3      0      0      0
crinode22          ok              -      8      3      3      0      0      0
crinode23          ok              -      8      5      5      0      0      0
crinode24          ok              -      8      6      6      0      0      0
crinode25          ok              -      8      5      5      0      0      0
crinode26          ok              -      8      5      5      0      0      0
crinode27          ok              -      8      5      5      0      0      0
crinode28          ok              -      8      7      7      0      0      0
crinode29          ok              -      8      4      4      0      0      0
crinode3           ok              -      8      5      5      0      0      0
crinode33          ok              -      8      4      4      0      0      0
crinode34          ok              -      8      3      3      0      0      0
crinode35          closed          -      8      8      8      0      0      0
crinode40          ok              -      8      5      5      0      0      0
crinode41          ok              -      8      5      5      0      0      0
crinode42          ok              -      8      4      4      0      0      0
```

check host resources

Use the lsload command

uk-cri-lcst01 > lsload -R mem



```
[obrien04@uk-cri-lcst01 ~]$ lsload -R mem
HOST_NAME         status  r15s   r1m  r15m   ut    pg  ls    it   tmp   swp   mem
crinode61             ok   0.0   0.1   0.1   0%   0.0   1 13200   71G   16G   15G
crinode54             ok   0.0   0.0   0.0   0%   0.2   0 44896   71G   12G   11G
crinode7              ok   0.0   0.0   0.0   0%   0.3   0 18816   71G   13G   10G
crinode35             ok   0.0   0.2   0.0   0%   0.4   0 44800   71G   13G   11G
crinode2              ok   0.0   0.0   0.0   0%   0.2   1 31840   71G
        lcst01        ok               1.5  14%   0.0  10     0
                                                                          6216M
crin                                                                16G 2242M
crinode45                6.3   6.7   5.4                          71G   16G 5420M
crinode20             ok   6.3   5.8   5.0  73%   0.0   0 54784   71G   16G 7000M
crinode19             ok   6.5   7.9   8.1  96%   0.0   0 31968   71G   16G   16G
crinode52             ok   6.7   7.0   7.8  87%   0.0   0 11664   71G   16G   18G
crinode16             ok   6.9   7.2   7.5  87%   0.0   0 19056   71G   16G   13G
crinode59             ok   7.0   7.0   5.4  88%   0.0   0 2e+05   71G   16G 3676M
crinode48             ok   8.9   7.9   7.8  98%   0.0   0 44896   71G   16G   10G
[obrien04@uk-cri-lcst01 ~]$
```

Killing jobs with bkill

You can kill your own jobs if they appear not to be running as intended.

LSF also allows for jobs to be stopped and restarted (provided they were submitted with the **bsub -r** flag).

```
bstop [ -h ] [ -V ] [ -q queue_name ] [ -m host_name ]
[ -u user_name | all ] [ -J job_name ] [ jobId |
"jobId[index_list]" ... ]

bresume [ -h ] [ -V ] [ -q queue_name ] [ -m host_name ]
[ -u user_name | all ] [ -J job_name ] [ jobId |
"jobId[index_list]" ... ]

bkill [ -h ] [ -V ] [ -l ] [ -s (signal_value | signal_name ) ]
[ -q queue_name ] [ -m host_name ] [ -u (user_name | all) ]
[ -J job_name ] [ jobId | "jobId[index_list]" ... ]
```

Running scripts with LSF

Script must be executable, the linux chmod command can be used
to set the executable attribute

```
uk-cri-lcst01> chmod u+x /lustre/xxlab/xxuser/xxscript.sh
```

The script can then also be run by redirecting it to the bsub command using one of the linux redirection operators "<“

```
uk-cri-lcst01> bsub -q cluster -M 4194304 -R "rusage[mem=4096]" < xxscript.sh
```

You can also include BSUB options within the script i.e.

```
#!/bin/sh
#BSUB -o myoutput.log
#BSUB -e myerror.log
#BSUB -a R
cd /lustre/xxlab/xxuser
<command>
```

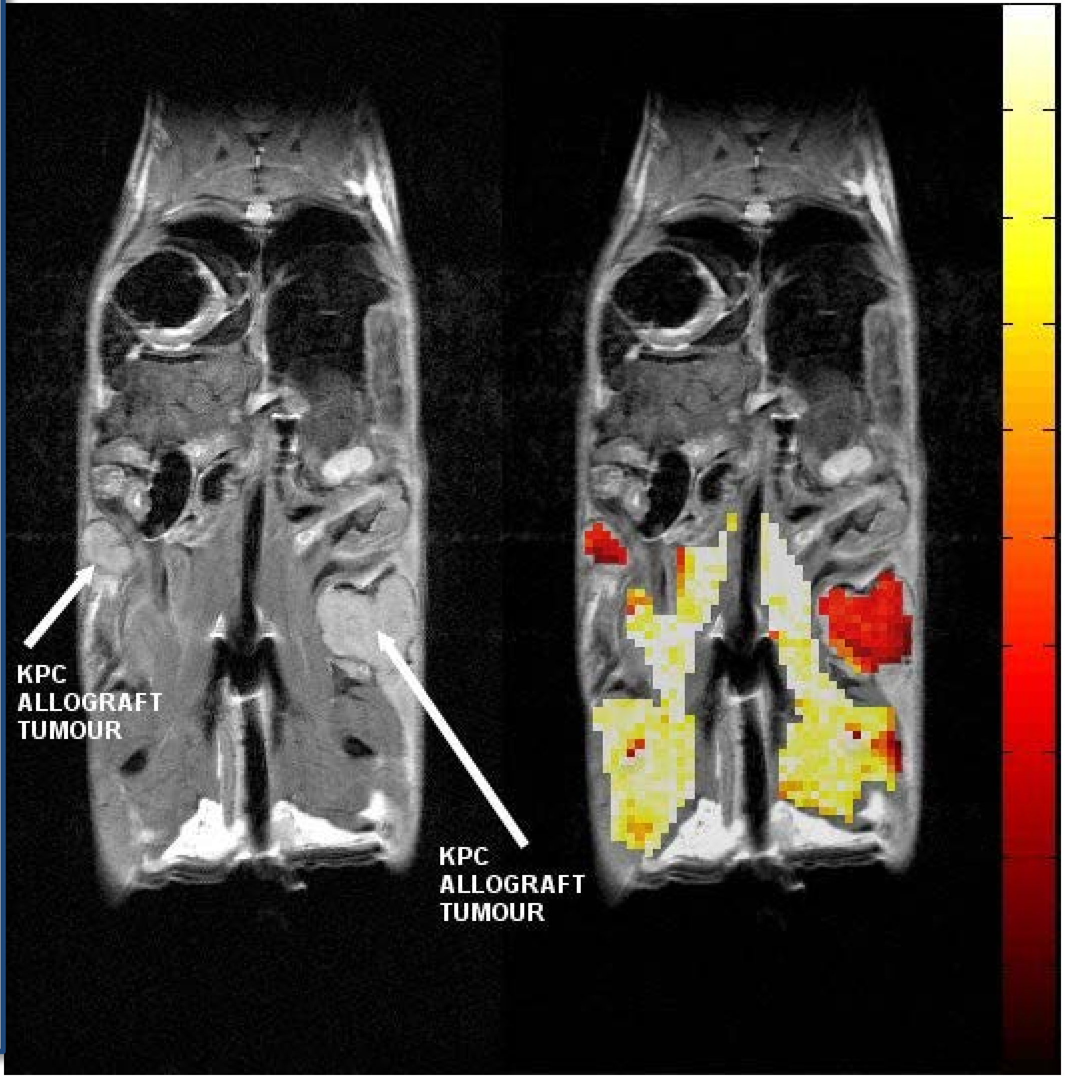
Simple Parallel Computing

Most HPC at CRI consists of breaking up your dataset into chunks and firing off a separate job for each chunk.

' Magnetisation Transfer Map Example

Here small groups of pixels from T2 weighted image slices are processed to calculate the elements of the MT map.'

(Example courtesy of Dominick McIntyre, Griffiths Group)



Message Passing parallel jobs

Uses the generic PJL (Parallel Job Launcher) framework. You can easily recognise it because of the use of the -a openmpi flag and mpirun.lsf

```
uk-cri-lcst01 > bsub -o %J.out -e %J.err -n 4 -R "span[ptile=1]"
-a openmpi mpirun.lsf ./test
```

In recent versions of LSF, another framework is also available, and it permits a tight (native) integration with the MPIs (this is why there is the OpenMPI integration)

```
uk-cri-lcst01 > bsub -o %J.out -e %J.err -n 4 -R "span[ptile=1]"
mpirun ./test
```

A job submission example

from Ben Davis, bioinformatics

> *‘This is a shell command line loop I ran recently... quite a good example as the actual thing running is just creating checksum files so doesn’t distract.’*

```
for f in `seq 1 16`; do bsub -n 1 -M 1048576 -R 'span[hosts=1]
select[mem>=1024 && tmp>=2000] rusage[mem=1024, tmp=2000]' -o md5cs-%J.out
-J md5cs$f -q solexa md5sum -c SJD_$f.md5;done;
```

> *‘Here multiple named jobs are submitted to the solexa queue. Each checks a single file specified by numeric indices incorporated in the file title and creates a named output file where the title contains the job ID.’*

Job array example

from Stewart MacArthur, bioinformatics

> *'Here is a self contained example of the basics of using job arrays. The main benefit in this case is the not speed but the ability to control the number of jobs running at any one time, using the %50 notation in the bsub ... I find job arrays particularly useful for running lots of small jobs, as there is only a single job submission there is little LSF overhead, compared to submitting 1000 separate jobs, which takes some time. Also being able to control the number of running jobs stops you swamping your queue with jobs and leaves space for others to get jobs running.'*

```
### Generate a random big file that we want to sort, 10 Million lines
perl -e 'for (1..1E7){printf("%.0f\n",rand()*1E7)};' > bigFile
### Split the file up into chunks with 10,000 lines in each chunk
split -a 3 -d -l 10000 bigFile split
### rename the files on a 1-1000 scheme not 0-999
for f in split*;do mv ${f} $(echo ${f} |perl -ne 'm/split(0*)(\d+)/g;print
"Split",$2+1,"\n";');done
### submit a job array, allowing 50 jobs to be run at anyone time
bsub -J "sort[1-1000]%50" "sort -n Split\$LSB_JOBINDEX >Split\
$LSB_JOBINDEX.sorted"
### merge the sorted files together once all the jobs are finished
sort -n -m *.sorted >bigFile.sorted
### Delete the temp files
rm -f Split*
```

Job dependency

-w 'dependency_expression‘

LSF does not place your job unless the dependency expression evaluates to TRUE. The dependency expression is a logical expression composed of one or more dependency conditions.

To make dependency expression of multiple conditions, use the following logical operators:
&& (AND) **||** (OR) **!** (NOT)

Use the * with dependency conditions to define one-to-one dependency among job array elements such that each element of one array depends on the corresponding element of another array. The job array size must be identical.

For example:

```
bsub      -w "done(myarrayA[*])"
          -J "myArrayB[1-10]"
          myJob2
```

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Practical session II

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