Load Sharing Facility (LSF)

Minerva Scientific Computing Environment

https://labs.icahn.mssm.edu/minervalab

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Icahn School of Medicine at **Mount Sinai**

Outline

- LSF introduction and basic/helpful LSF commands
- Job submission and monitoring
- Interactive job
- Dependent job
- Parallel jobs: parallel processing and GPUs
- Job arrays and Self-scheduler
- Tips for efficient usage of the queuing system

Minerva cluster @ Mount Sinai

Chimera Compute Partition:

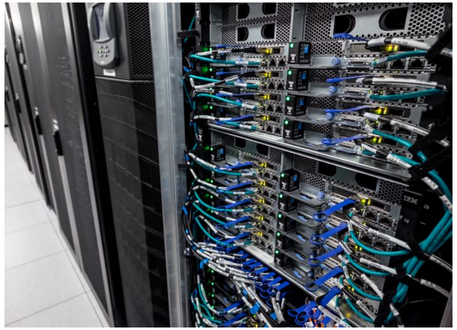
- 4x **login nodes** - Intel Emerald Rapids 8568Y+, 2.3GHz – 96 cores with 512 GB memory per node.
- Compute nodes -
  - 146 **high memory nodes** - Intel Emerald Rapids 8568Y+, 2.3GHz - 96 cores with **1.5 TB** memory per node.)
  - 37 **high memory nodes** - Intel 8168/8268, 2.7/2.9GHz - **1.5 TB** mem/node
  - **GPU nodes:**
    - 12 -Intel 6142, 2.6GHz - 384 GB memory - 4x V100-**16 GB** GPU
    - 8 - Intel 8268, 2.9 GHz - 384 GB memory - 4x A100-**40 GB** GPU
    - 2 - Intel 8358,2.6GHz - 2 TB memory - 4x A100-**80 GB** GPU
    - 2 - Intel 8358 2.6 GHz- 500 GB memory - 4x H100-**80 GB** GPU
    - 47 - Intel ER 8568Y+, 2.3GHz - 1.5 TB memory - 4x H100-**80 GB** GPU
    - 4 - AMD Genoa 9334 2.7GHz - 1.5 TB memory - 8x L40S-**48 GB** GPU

NIH FUNDED NODES

- $2M **CATS** awarded by NIH

  55 compute nodes - Intel 8358, 2.6 GHz- 64 cores per node -**1.5 TB** / node
- $2M **AIMS** awarded by NIH

  6X Intel Xeon Platinum 8570 2.1GHz - 2 TB memory - 8x B200-**192 GB** GPU



Storage: **32** PB of high-speed online storage as an IBM General Parallel File System (**GPFS**)

- **Path /sc/arion** : Use the system path environment variable in scripts **$GPFS**

https://labs.icahn.mssm.edu/minervalab/resources/hardware-technical-specs/

Running Jobs on Minerva Compute Nodes

ssh userID@minerva.hpc.mssm → 4 Login nodes

Never run jobs on login nodes

***bsub** < Your_Job_Submission_Script.lsf*

Compute Partition:

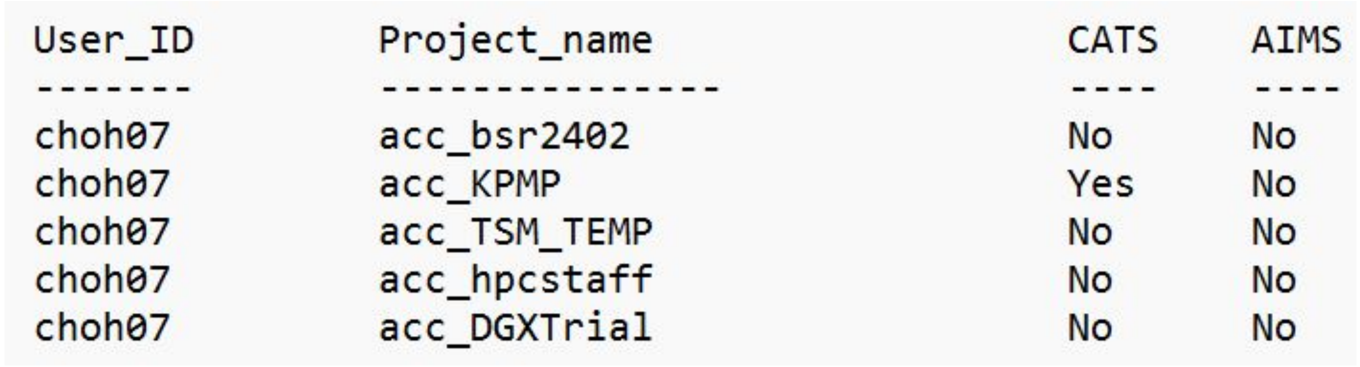
146 Regular nodes
37 High memory nodes
81 GPU nodes (including NIH Funded AIMS B200 nodes)
55 CATS nodes (NIH Funded nodes)

Access to compute resources and job scheduling are managed by IBM Spectrum **LSF** (Load Sharing Facility) batch system.

Prerequisite

- Must have a project allocation account.
- If you don't have one, ask your PI (or project authorizer) send a request at hpchelp@hpc.mssm.edu
- To see a list of accessible project accounts:

  $ **mybalance**



```
User_ID         Project_name                    CATS    AIMS
--------        ----------------                ----    ----
choh07          acc_bsr2402                     No      No
choh07          acc_KPMP                        Yes     No
choh07          acc_TSM_TEMP                    No      No
choh07          acc_hpcstaff                    No      No
choh07          acc_DGXTrial                    No      No
```

Basic LSF commands

• **bsub**	Batch job submission
• **bjobs**	Show your job status. Pending reasons
• **bkill**	Kill a batch job
• **bmod**	Modify the resource requirement of a **pending** job
• **bpeek**	Display the stdout and stderr output of an unfinished job
• **bhist**	Display historical information about a job
• **bqueues**	Display information about queues
• **bhosts**	Display load status information of each compute node

IBM LSF Documentation: https://www.ibm.com/docs/en/spectrum-lsf/10.1.0

Batch job submission example

```
$ cat myfirst.lsf

#!/bin/bash
#BSUB -J myfirstjob                  # Job name
#BSUB -P acc_hpcstaff                # REQUIRED; To get allocation account, type "mybalance"
#BSUB -q premium                     # queue; default queue is premium
#BSUB -n 1                           # number of compute cores (job slots) needed, 1 by default
#BSUB -W 6:00                        # REQUIRED; walltime in HH:MM
#BSUB -R rusage[mem=4000]            # 4000 MB of memory request per "-n"; 3000 MB by default
#BSUB -oo %J.stdout                  # output log (%J : JobID)
#BSUB -eo %J.stderr                  # error log
#BSUB -L /bin/bash                   # Initialize the execution environment

ml gcc                               # Commands that you need to run
cd /sc/arion/work/MyID/my/job/dir/
../mybin/serial_executable < testdata.inp > results.log
```

```
$ bsub < myfirst.lsf
Job <87426883> is submitted to queue <premium>.
```

Batch job submission example (continue)

```
$ cat mysecond.lsf

#!/bin/bash
#BSUB -q premium                    # queue
#BSUB -R rusage[mem=4000]           # 4000 MB of memory request per “-n”; 3000 MB by default
#BSUB -oo %J.stdout                 # output log (%J : JobID)
#BSUB -eo %J.stderr                 # error log
#BSUB -L /bin/bash                  # Initialize the execution environment
ml gcc                              # Commands that you need to run
cd /sc/arion/work/MyID/my/job/dir/
../mybin/serial_executable < testdata.inp > results.log
```

```
$ bsub -q express -J mysecondjob -P acc_hpcstaff -n 1 -W 30 < mysecond.lsf
Job <87426921> is submitted to queue <premium>.
```

If an option is given on both the bsub command line and in the job script, the command line option overrides the option in the script.

bsub major options

-P accountName	of the form: **acc**_projectName
-q queuename	submission queue
-n ncpu	number of cpu's requested (default: 1)
-W wallClockTime	in form of HH:MM
-R rusage[mem=...]	amount of memory requested **per "-n"** in *MB* *Standard abbreviations (MB, GB, …) can also be used.* max memory per node: ~1.4TB (Chimera, CATS, GPU H100, L40S), ~325GB (GPU V100, A100) , ~1.9TB (himem-GPU A100-80GB, B200), ~435GB(GPU H100-80GB)

-R span[#-n's per physical node]

span[ptile=4] - 4 cores per node/host

span[**hosts=1**] - all cores on **same** node/host

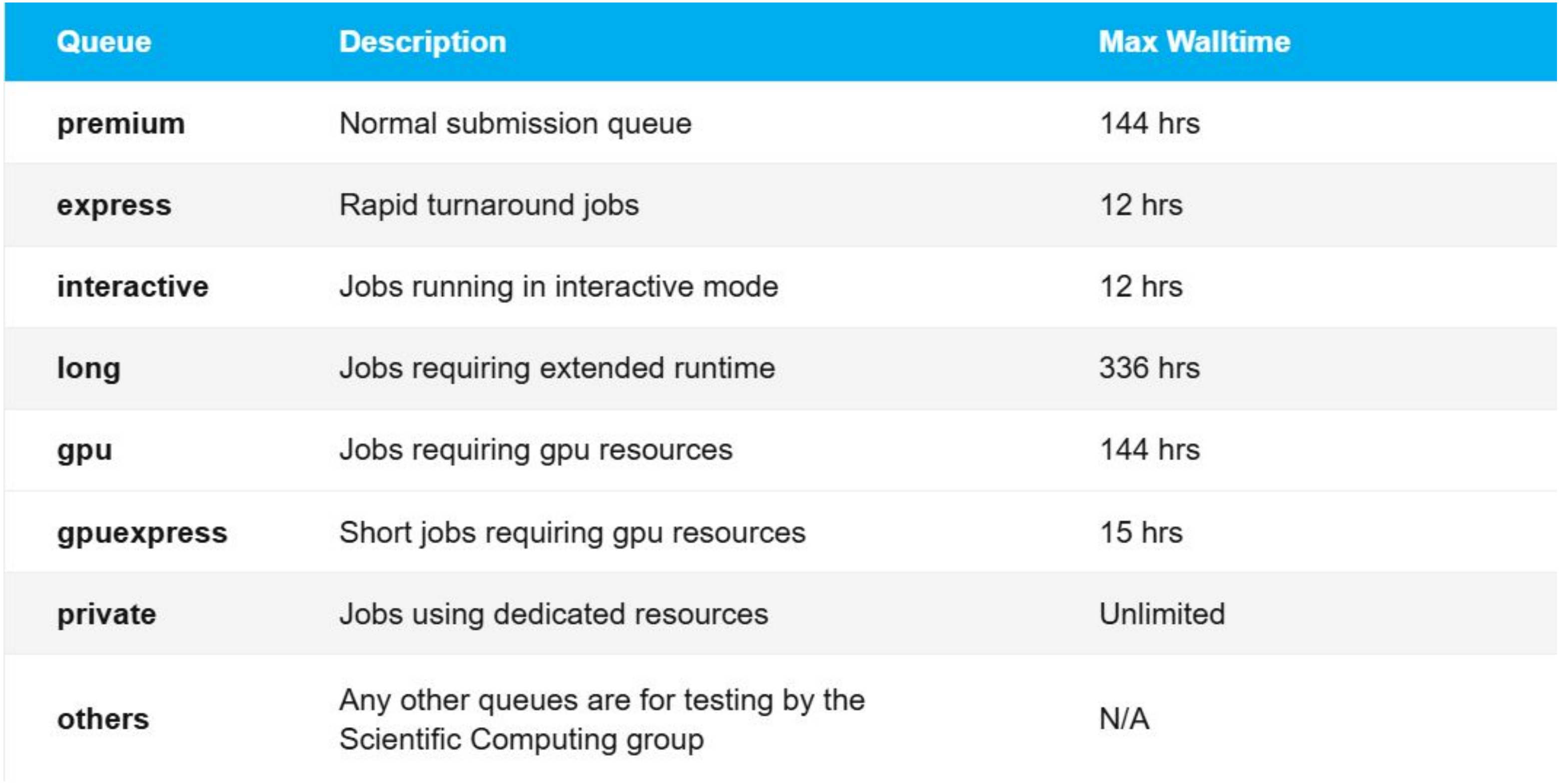
bsub major options

- -o Name of output file (concatenated)
- -oo Name of output file (overwrite)
- -e   Name of error file (concatenated)
- -eo Name of error file (overwrite)

NOTE: Default output is mailed to the user BUT since we have disabled mail response, it goes into the bit bucket.

If -o(o) is specified but not -e, error is appended to output file.

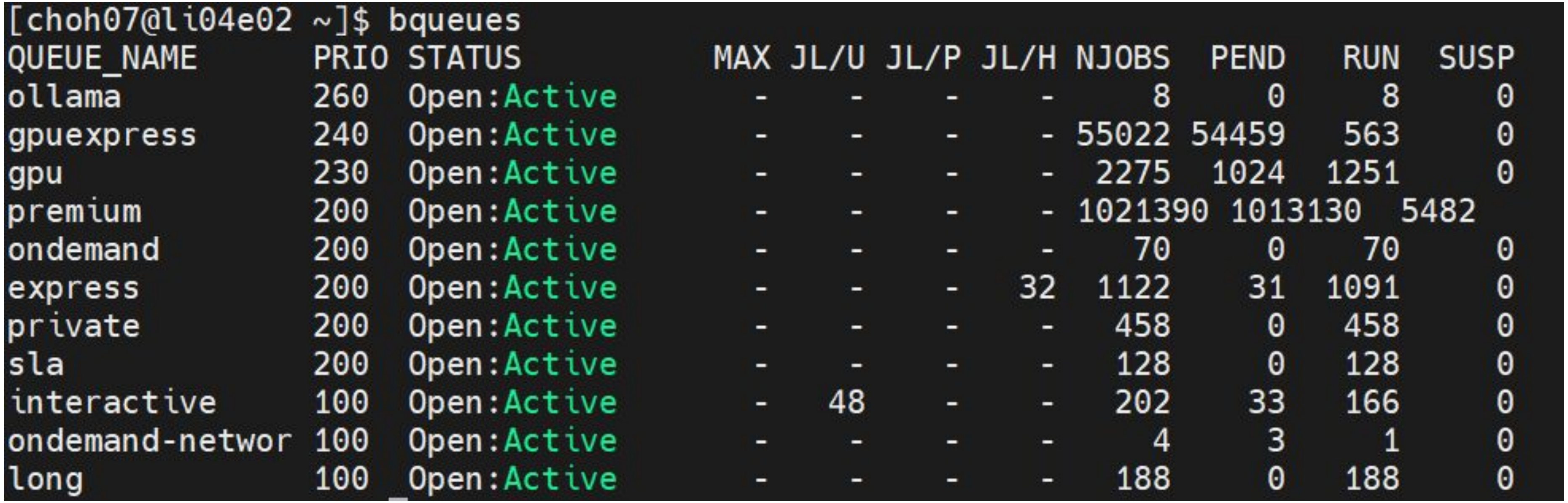
Minerva LSF queue structure



Queue	Description	Max Walltime
premium	Normal submission queue	144 hrs
express	Rapid turnaround jobs	12 hrs
interactive	Jobs running in interactive mode	12 hrs
long	Jobs requiring extended runtime	336 hrs
gpu	Jobs requiring gpu resources	144 hrs
gpuexpress	Short jobs requiring gpu resources	15 hrs
private	Jobs using dedicated resources	Unlimited
others	Any other queues are for testing by the Scientific Computing group	N/A

* shared

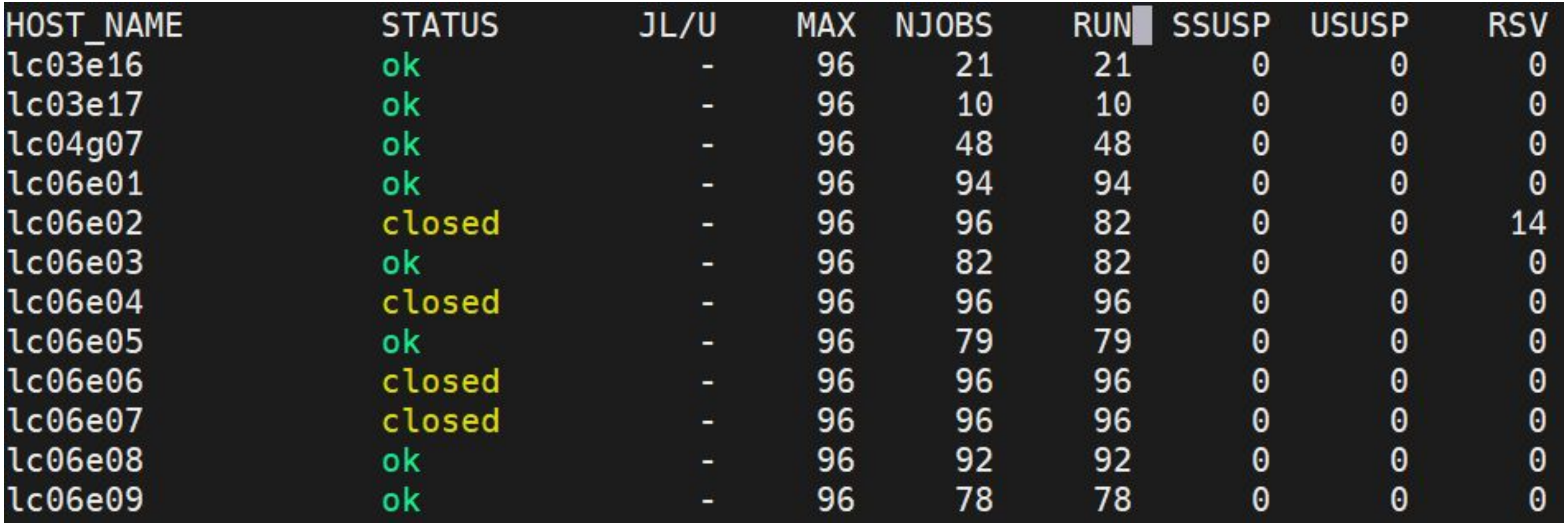
bqueues : information about all the available queues



```
[choh07@li04e02 ~]$ bqueues
QUEUE_NAME      PRIO STATUS          MAX JL/U JL/P JL/H NJOBS  PEND   RUN  SUSP
ollama          260  Open:Active       -    -    -    -     8     0     8     0
gpuexpress      240  Open:Active       -    -    -    - 55022 54459   563     0
gpu             230  Open:Active       -    -    -    -  2275  1024  1251     0
premium         200  Open:Active       -    -    -    - 1021390 1013130  5482
ondemand        200  Open:Active       -    -    -    -    70     0    70     0
express         200  Open:Active       -    -    -   32  1122    31  1091     0
private         200  Open:Active       -    -    -    -   458     0   458     0
sla             200  Open:Active       -    -    -    -   128     0   128     0
interactive     100  Open:Active       -   48    -    -   202    33   166     0
ondemand-networ 100  Open:Active       -    -    -    -     4     3     1     0
long            100  Open:Active       -    -    -    -   188     0   188     0
```

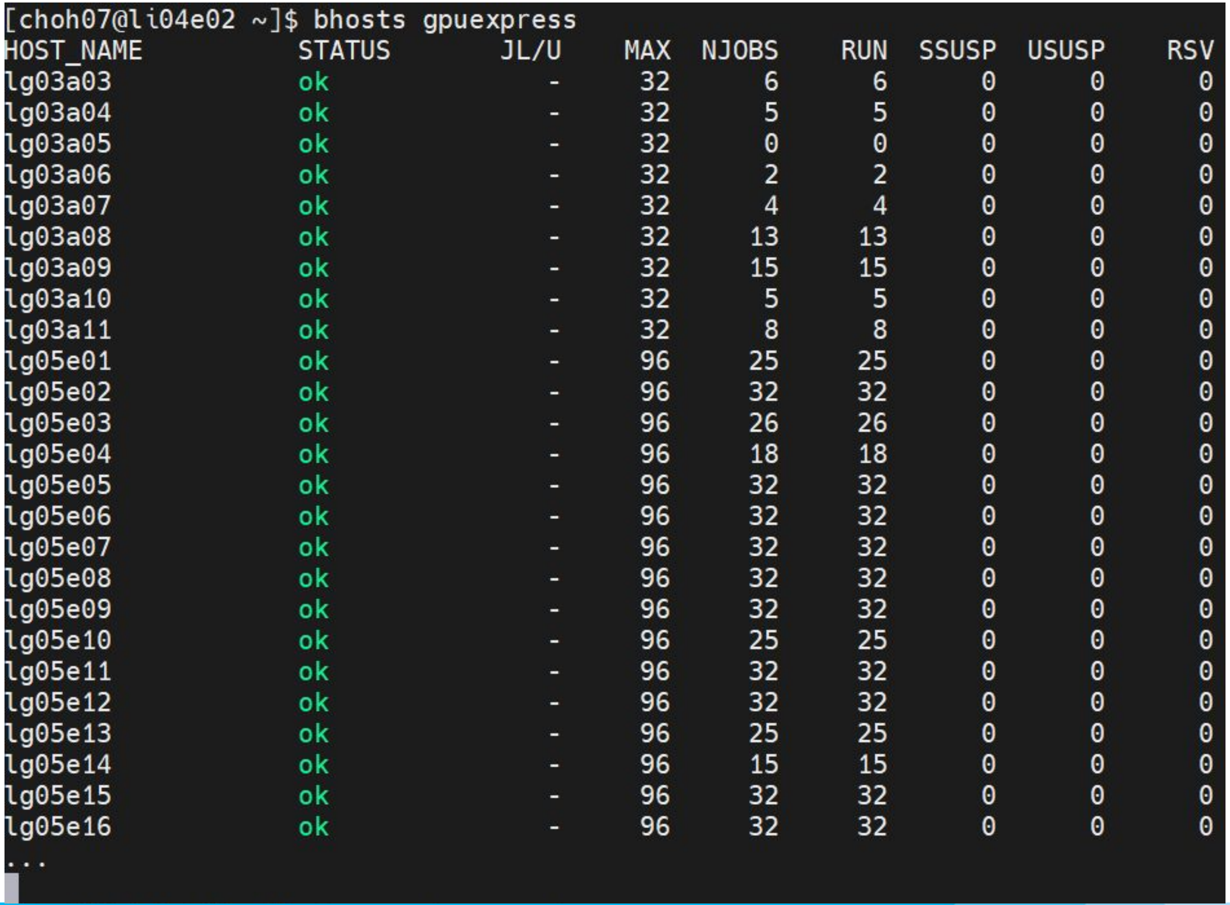
bhosts : Displays nodes and their load status

- List *all* the compute nodes on Minerva



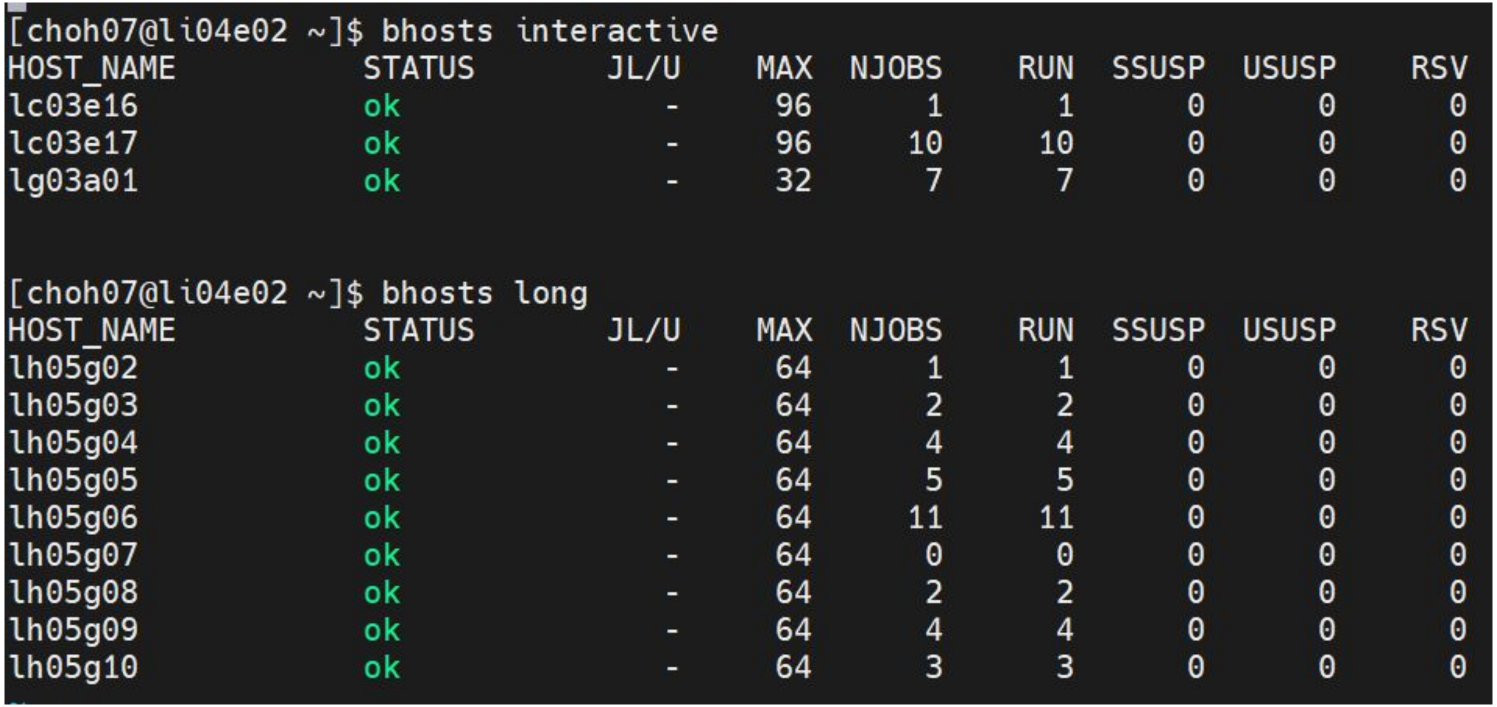
```
HOST_NAME          STATUS       JL/U    MAX  NJOBS    RUN  SSUSP  USUSP    RSV
lc03e16            ok              -     96     21     21      0      0      0
lc03e17            ok              -     96     10     10      0      0      0
lc04g07            ok              -     96     48     48      0      0      0
lc06e01            ok              -     96     94     94      0      0      0
lc06e02            closed          -     96     96     82      0      0     14
lc06e03            ok              -     96     82     82      0      0      0
lc06e04            closed          -     96     96     96      0      0      0
lc06e05            ok              -     96     79     79      0      0      0
lc06e06            closed          -     96     96     96      0      0      0
lc06e07            closed          -     96     96     96      0      0      0
lc06e08            ok              -     96     92     92      0      0      0
lc06e09            ok              -     96     78     78      0      0      0
```

bhosts (continue)



```
[choh07@li04e02 ~]$ bhosts gpuexpress
HOST_NAME          STATUS       JL/U    MAX  NJOBS    RUN  SSUSP  USUSP    RSV
lg03a03            ok              -     32      6      6      0      0      0
lg03a04            ok              -     32      5      5      0      0      0
lg03a05            ok              -     32      0      0      0      0      0
lg03a06            ok              -     32      2      2      0      0      0
lg03a07            ok              -     32      4      4      0      0      0
lg03a08            ok              -     32     13     13      0      0      0
lg03a09            ok              -     32     15     15      0      0      0
lg03a10            ok              -     32      5      5      0      0      0
lg03a11            ok              -     32      8      8      0      0      0
lg05e01            ok              -     96     25     25      0      0      0
lg05e02            ok              -     96     32     32      0      0      0
lg05e03            ok              -     96     26     26      0      0      0
lg05e04            ok              -     96     18     18      0      0      0
lg05e05            ok              -     96     32     32      0      0      0
lg05e06            ok              -     96     32     32      0      0      0
lg05e07            ok              -     96     32     32      0      0      0
lg05e08            ok              -     96     32     32      0      0      0
lg05e09            ok              -     96     32     32      0      0      0
lg05e10            ok              -     96     25     25      0      0      0
lg05e11            ok              -     96     32     32      0      0      0
lg05e12            ok              -     96     32     32      0      0      0
lg05e13            ok              -     96     25     25      0      0      0
lg05e14            ok              -     96     15     15      0      0      0
lg05e15            ok              -     96     32     32      0      0      0
lg05e16            ok              -     96     32     32      0      0      0
...
```

bhosts (continue)



```
[choh07@li04e02 ~]$ bhosts interactive
HOST_NAME          STATUS       JL/U    MAX  NJOBS    RUN  SSUSP  USUSP    RSV
lc03e16            ok              -     96      1      1      0      0      0
lc03e17            ok              -     96     10     10      0      0      0
lg03a01            ok              -     32      7      7      0      0      0


[choh07@li04e02 ~]$ bhosts long
HOST_NAME          STATUS       JL/U    MAX  NJOBS    RUN  SSUSP  USUSP    RSV
lh05g02            ok              -     64      1      1      0      0      0
lh05g03            ok              -     64      2      2      0      0      0
lh05g04            ok              -     64      4      4      0      0      0
lh05g05            ok              -     64      5      5      0      0      0
lh05g06            ok              -     64     11     11      0      0      0
lh05g07            ok              -     64      0      0      0      0      0
lh05g08            ok              -     64      2      2      0      0      0
lh05g09            ok              -     64      4      4      0      0      0
lh05g10            ok              -     64      3      3      0      0      0
```

bjobs : status of jobs

Check your job: $ **bjobs** *JobID*

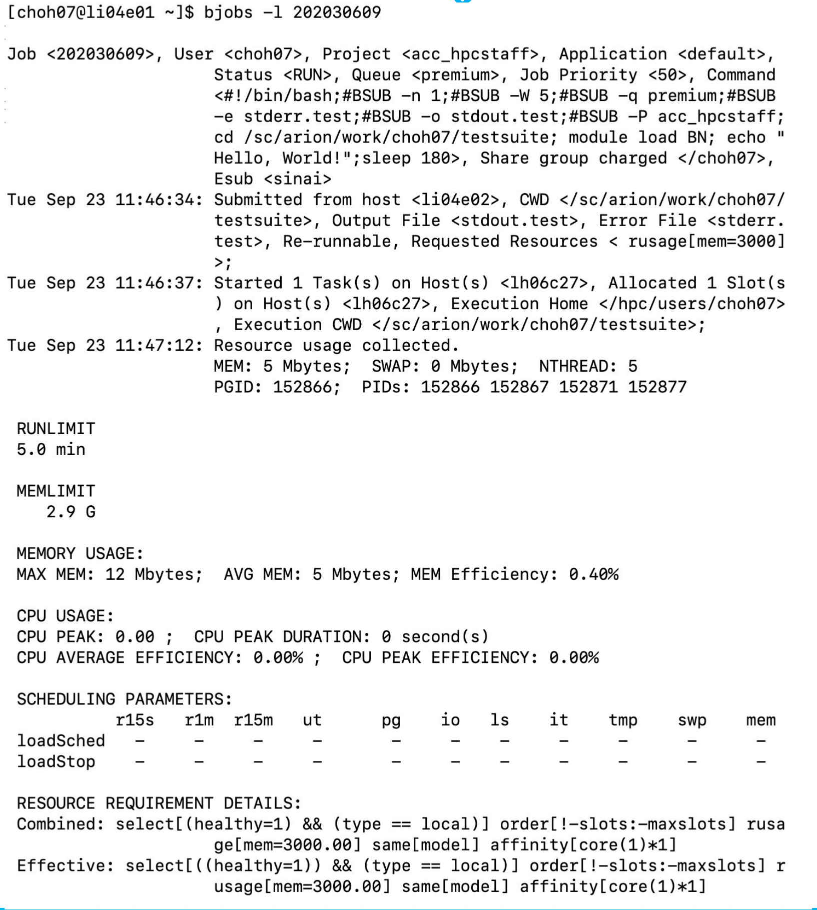
```
   JOBID      USER    JOB_NAME   STAT    QUEUE  FROM_HOST   EXEC_HOST   SUBMIT_TIME    START_TIME  TIME_LEFT
87426883    choh07   myfirstjob   PEND    premium    li03c03      -        Mar 27 14:38      -          -
```

Pending reasons: $ **bjobs** -p *JobID*

```
   JOBID      USER    JOB_NAME   STAT    QUEUE  FROM_HOST   EXEC_HOST   SUBMIT_TIME    START_TIME  TIME_LEFT
87426883    choh07   myfirstjob   PEND    premium    li03c03      -        Mar 27 14:38      -          -
New job is waiting for scheduling;
```

Show full details about the job: **bjobs** -ℓ *JobID*

bjobs : status of jobs



```
[choh07@li04e01 ~]$ bjobs -l 202030609

Job <202030609>, User <choh07>, Project <acc_hpcstaff>, Application <default>,
                     Status <RUN>, Queue <premium>, Job Priority <50>, Command
                     <#!/bin/bash;#BSUB -n 1;#BSUB -W 5;#BSUB -q premium;#BSUB
                     -e stderr.test;#BSUB -o stdout.test;#BSUB -P acc_hpcstaff;
                     cd /sc/arion/work/choh07/testsuite; module load BN; echo "
                     Hello, World!";sleep 180>, Share group charged </choh07>,
                     Esub <sinai>
Tue Sep 23 11:46:34: Submitted from host <li04e02>, CWD </sc/arion/work/choh07/
                     testsuite>, Output File <stdout.test>, Error File <stderr.
                     test>, Re-runnable, Requested Resources < rusage[mem=3000]
                     >;
Tue Sep 23 11:46:37: Started 1 Task(s) on Host(s) <lh06c27>, Allocated 1 Slot(s
                     ) on Host(s) <lh06c27>, Execution Home </hpc/users/choh07>
                     , Execution CWD </sc/arion/work/choh07/testsuite>;
Tue Sep 23 11:47:12: Resource usage collected.
                     MEM: 5 Mbytes;  SWAP: 0 Mbytes;  NTHREAD: 5
                     PGID: 152866;  PIDs: 152866 152867 152871 152877

 RUNLIMIT
 5.0 min

 MEMLIMIT
    2.9 G

 MEMORY USAGE:
 MAX MEM: 12 Mbytes;  AVG MEM: 5 Mbytes; MEM Efficiency: 0.40%

 CPU USAGE:
 CPU PEAK: 0.00 ;  CPU PEAK DURATION: 0 second(s)
 CPU AVERAGE EFFICIENCY: 0.00% ;  CPU PEAK EFFICIENCY: 0.00%

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

 RESOURCE REQUIREMENT DETAILS:
 Combined: select[(healthy=1) && (type == local)] order[!-slots:-maxslots] rusa
                     ge[mem=3000.00] same[model] affinity[core(1)*1]
 Effective: select[((healthy=1)) && (type == local)] order[!-slots:-maxslots] r
                     usage[mem=3000.00] same[model] affinity[core(1)*1]
```

bkill : terminate jobs in the queue

Lots of ways to get away with murder

Kill by JobID	**bkill** 87426883
Kill by JobName	**bkill** -J myjob
Kill a bunch of jobs	**bkill** -J myjob_*
Kill all your jobs	**bkill** 0

bpeek: display output of the job produced so far

```
$ bpeek 2937044
<< output from stdout >>
"Hello Minerva"


<< output from stderr >>
```

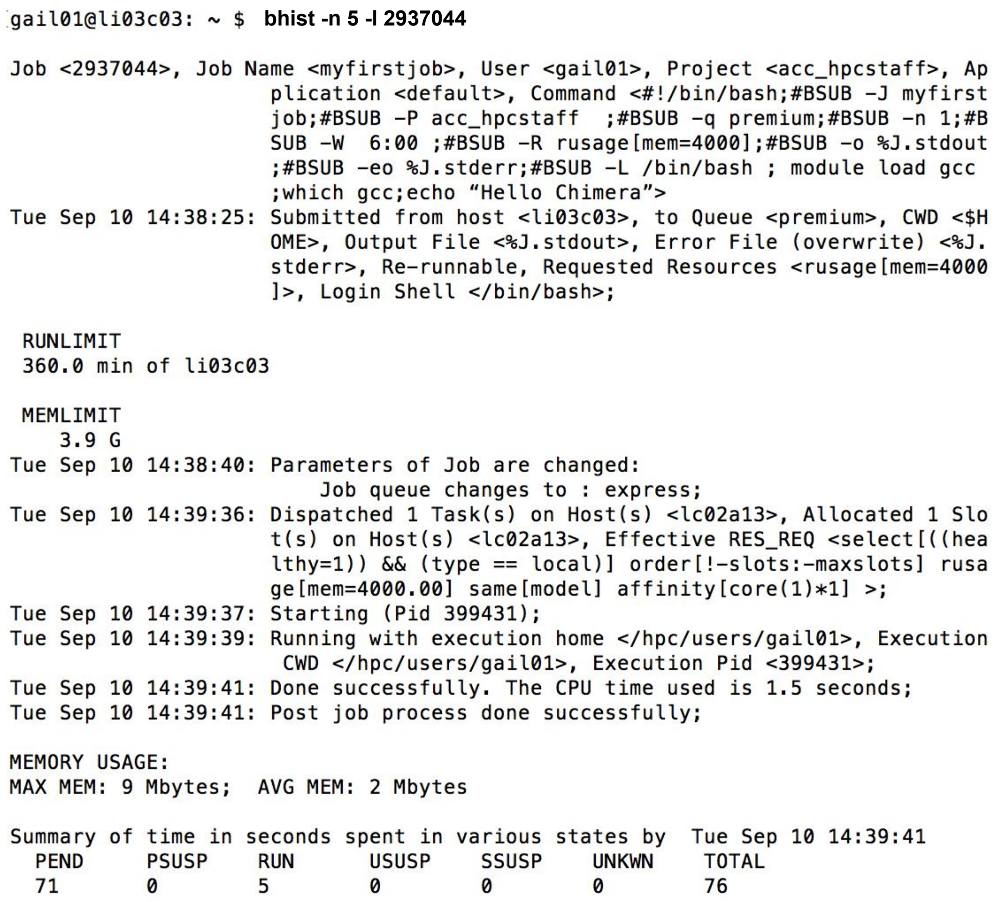
bmod: modify submission options of "pending" jobs

bmod takes similar options to **bsub**

- **bmod** -R rusage[mem=20000] *JobID*
  - -R replaces **ALL** R fields not just the one you specify
- **bmod** -q express *JobID*

```
$ bmod -q express 2937044
Parameters of job <2937044> are being changed
```

bhist : historical information



```
gail01@li03c03: ~ $  bhist -n 5 -l 2937044

Job <2937044>, Job Name <myfirstjob>, User <gail01>, Project <acc_hpcstaff>, Ap
                     plication <default>, Command <#!/bin/bash;#BSUB -J myfirst
                     job;#BSUB -P acc_hpcstaff  ;#BSUB -q premium;#BSUB -n 1;#B
                     SUB -W  6:00 ;#BSUB -R rusage[mem=4000];#BSUB -o %J.stdout
                     ;#BSUB -eo %J.stderr;#BSUB -L /bin/bash ; module load gcc
                     ;which gcc;echo “Hello Chimera”>
Tue Sep 10 14:38:25: Submitted from host <li03c03>, to Queue <premium>, CWD <$H
                     OME>, Output File <%J.stdout>, Error File (overwrite) <%J.
                     stderr>, Re-runnable, Requested Resources <rusage[mem=4000
                     ]>, Login Shell </bin/bash>;

 RUNLIMIT
 360.0 min of li03c03

 MEMLIMIT
    3.9 G
Tue Sep 10 14:38:40: Parameters of Job are changed:
                         Job queue changes to : express;
Tue Sep 10 14:39:36: Dispatched 1 Task(s) on Host(s) <lc02a13>, Allocated 1 Slo
                     t(s) on Host(s) <lc02a13>, Effective RES_REQ <select[((hea
                     lthy=1)) && (type == local)] order[!-slots:-maxslots] rusa
                     ge[mem=4000.00] same[model] affinity[core(1)*1] >;
Tue Sep 10 14:39:37: Starting (Pid 399431);
Tue Sep 10 14:39:39: Running with execution home </hpc/users/gail01>, Execution
                      CWD </hpc/users/gail01>, Execution Pid <399431>;
Tue Sep 10 14:39:41: Done successfully. The CPU time used is 1.5 seconds;
Tue Sep 10 14:39:41: Post job process done successfully;

MEMORY USAGE:
MAX MEM: 9 Mbytes;  AVG MEM: 2 Mbytes

Summary of time in seconds spent in various states by  Tue Sep 10 14:39:41
  PEND     PSUSP    RUN      USUSP    SSUSP    UNKWN    TOTAL
  71       0        5        0        0        0        76
```

Interactive access to compute resources

- Set up an interactive environment on compute nodes with **internet access**
- Useful for testing and debugging jobs
- **Interactive GPU** is available for job testing

```
bsub -P acc_hpcstaff -q interactive -n 4 -W 2:00 -R rusage[mem=4000] -R span[hosts=1] -XF -Is /bin/bash
```

- -Is: Interactive terminal/shell
- -XF: X11 forwarding
- /bin/bash : the shell to use

```
$ bsub -P acc_hpcstaff -q interactive -n 4 -W 2:00 -R rusage[mem=4000] -R span[hosts=1]
-XF -Is /bin/bash
Job <2916837> is submitted to queue <interactive>.
<<ssh X11 forwarding job>>
<<Waiting for dispatch ...>>
<<Starting on lc02a29>>
```

Dependent Job

Any job can be dependent on other LSF jobs.

Syntax

bsub -w 'dependency_expression**'**

usually based on the job states of preceding jobs.

```
bsub -J myJ < myjob.lsf
bsub -w 'done(myJ)' < dependent.lsf
```

For more details about the dependency_expression:

https://www.ibm.com/docs/en/spectrum-lsf/10.1.0?topic=scheduling-dependency-conditions

Parallel Jobs

- **Distributed memory program**: Message passing between processes (e.g. MPI) Map-reduce(e.g. Spark)
  - Processes execute across multiple CPU cores or nodes

- **Shared memory program** (SMP): multi-threaded execution (e.g. OpenMP)
  - Running across multiple CPU cores **on same node**

- **GPU programs**: offloading to the device via CUDA

- **Array job**: Parallel analysis for multiple instances of the same program
  - Execute on multiple data files simultaneously
  - Each instance running independently

Message Passing Interface (MPI) Jobs

- This example requests 48 cores and 2 hours in the "express” queue.
    - Those 48 cores are dispatched **across multiple nodes**

```
#!/bin/bash
#BSUB -J myjobMPI
#BSUB -P acc_hpcstaff
#BSUB -q express
#BSUB -n 48
#BSUB -R span[ptile=8]

#BSUB -W 02:00
#BSUB -o %J.stdout
#BSUB -eo %J.stderr
#BSUB -L /bin/bash

cd $LS_SUBCWD
module load openmpi
mpirun -np 48 /my/bin/executable < my_data.in
```

Multithreaded Jobs - OpenMP

- Multiple CPU cores within one node using shared memory
    - In general, a multithreaded application uses a single process which then spawns multiple threads of execution
    - It’s highly recommended the number of threads is set to the number of compute cores
- Your program has to be written to use multi-threading

```
#!/bin/bash
#BSUB -J myjob
#BSUB -P YourAllocationAccount
#BSUB -q express
#BSUB -n 4
#BSUB -R "span[hosts=1]”
#BSUB -R rusage[mem=12GB]
#BSUB -W 01:00
#BSUB -o %J.stdout
#BSUB -eo %J.stderr
#BSUB -L /bin/bash

cd $LS_SUBCWD
export OMP_NUM_THREADS=4            #sets the number of threads
/my/bin/executable < my_data.in
```

Specifying a resource - OpenMP job

Span: define the shape of the slots you ask for:

-n 12 -R span[hosts=1]	- allocate all 12 cores to one host
-n 12 -R span[ptile=12]	- all 12 slots/cores must be on 1 node
-n 24 -R span[ptile=12]	- allocate 12 cores per node = 2 nodes

OMP_NUM_THREADS must be set in script:

- **bsub -n 12 -R span[hosts=1] < my_parallel_job**
  export OMP_NUM_THREADS=12
- **bsub -n 12 -R span[ptile=12] -a openmp < my_parallel_job**
  LSF sets it for you as number of procs per node
- **bsub -n 1 -R “affinity[core(12)]” -R “rusage[mem=12000]” -a openmp < my_parallel_job**
  - 1 job slot with 12 cores, 12000MB memory to that job slot...not per core
  - Advantage: Can vary number of cores and/or memory without making any other changes or calculations

A Bravura Submission - Mixing it all together

Suppose you want to run a combined MPI-openMP job. One mpi process per node, openMP in each MPI Rank:

```
bsub -n 20 -R span[ptile=1] -R affinity[core(8)] -a openmp < my_awsome_job
```

ptile=1 - one slot on each node

core(8) - 8 cores per job slot

openmp - will set OMP_NUM_THREADS on each node to 8

GPGPU (General Purpose Graphics Processor Unit)

- GPGPU resources on Minerva
  - interactive queue (1 GPU node)
  - gpu/gpuexpress queue for batch
- GPU option specification:

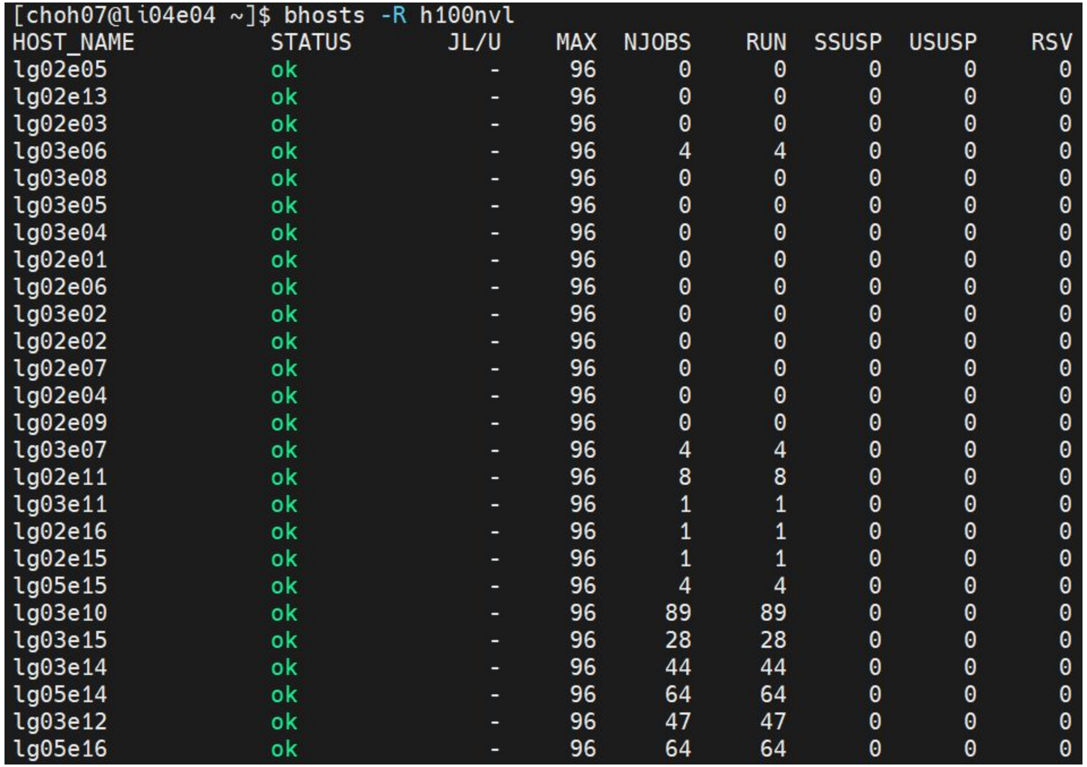
-gpu num=*Ngpus* **-R** *GPU_Model*

e.g. **-gpu num**=4 **-R** h100nvl

GPU_Model	
v100	TeslaV100_PCIE_16GB
a100	NVIDIAA100_PCIE_40GB
a10080g	NVIDIAA100_SXM4_80GB
h10080g	NVIDIAH100_PCIE_80GB
h100nvl	NVIDIAH100_SXM5_80GB
l40s	NVIDIAL40S_PCIE_48GB
b200	NVIDIAB200

Ngpus : Number of GPU cards requested **PER NODE**.
To request GPU cards on the same node, "**-R span[hosts=1]**" MUST be added.

GPGPU (continue)



```
[choh07@li04e04 ~]$ bhosts -R h100nvl
HOST_NAME              STATUS       JL/U    MAX  NJOBS    RUN  SSUSP  USUSP    RSV
lg02e05                ok              -     96      0      0      0      0      0
lg02e13                ok              -     96      0      0      0      0      0
lg02e03                ok              -     96      0      0      0      0      0
lg03e06                ok              -     96      4      4      0      0      0
lg03e08                ok              -     96      0      0      0      0      0
lg03e05                ok              -     96      0      0      0      0      0
lg03e04                ok              -     96      0      0      0      0      0
lg02e01                ok              -     96      0      0      0      0      0
lg02e06                ok              -     96      0      0      0      0      0
lg03e02                ok              -     96      0      0      0      0      0
lg02e02                ok              -     96      0      0      0      0      0
lg02e07                ok              -     96      0      0      0      0      0
lg02e04                ok              -     96      0      0      0      0      0
lg02e09                ok              -     96      0      0      0      0      0
lg03e07                ok              -     96      4      4      0      0      0
lg02e11                ok              -     96      8      8      0      0      0
lg03e11                ok              -     96      1      1      0      0      0
lg02e16                ok              -     96      1      1      0      0      0
lg02e15                ok              -     96      1      1      0      0      0
lg05e15                ok              -     96      4      4      0      0      0
lg03e10                ok              -     96     89     89      0      0      0
lg03e15                ok              -     96     28     28      0      0      0
lg03e14                ok              -     96     44     44      0      0      0
lg05e14                ok              -     96     64     64      0      0      0
lg03e12                ok              -     96     47     47      0      0      0
lg05e16                ok              -     96     64     64      0      0      0
```

GPGPU (continue)

```
#BSUB -q gpu                          # submit to gpu queue
#BSUB -n 4                            # number of CPU cores on the node

#BSUB -gpu num=2                      # 2 GPUs on V100 node
#BSUB -R v100
#BSUB -R span[hosts=1]                # all CPU cores and GPU cards on the same node

module purge
module load anaconda3 ( or 2)
module load cuda
source activate tfGPU

python -c "import tensorflow as tf"
```

Array Job

- Groups of jobs with the same executable and resource requirements, but different input files that can be indexed by numbers.
  - -J “Jobname[index | start-end:increment]”
  - Range of job index is **1**~ 10,000
  - **LSB_JOBINDEX** is set to array index

```
#!/bin/bash
#BSUB -P acc_hpcstaff
#BSUB -n 1
#BSUB -W 02:00
#BSUB -q express
#BSUB -J "jobarraytest[1-10]"
#BSUB -o logs/out.%J.%I
#BSUB -e logs/err.%J.%I
echo “Working on file.$LSB_JOBINDEX”
```

Array Job (continue)

```
$ bsub < myarrayjob.sh
Job <2946012> is submitted to queue <express>.

$ bjobs
    JOBID      USER     JOB_NAME   STAT      QUEUE  FROM_HOST    EXEC_HOST
SUBMIT_TIME    START_TIME  TIME_LEFT
   2946012    gail01 *rraytest[1]   PEND    express    li03c03     -       Sep 10 14:50      -          -
   2946012    gail01 *rraytest[2]   PEND    express    li03c03     -       Sep 10 14:50      -          -
   2946012    gail01 *rraytest[3]   PEND    express    li03c03     -       Sep 10 14:50      -          -
   2946012    gail01 *rraytest[4]   PEND    express    li03c03     -       Sep 10 14:50      -          -
   2946012    gail01 *rraytest[5]   PEND    express    li03c03     -       Sep 10 14:50      -          -
   2946012    gail01 *rraytest[6]   PEND    express    li03c03     -       Sep 10 14:50      -          -
   2946012    gail01 *rraytest[7]   PEND    express    li03c03     -       Sep 10 14:50      -          -
   2946012    gail01 *rraytest[8]   PEND    express    li03c03     -       Sep 10 14:50      -          -
   2946012    gail01 *rraytest[9]   PEND    express    li03c03     -       Sep 10 14:50      -          -
   2946012    gail01 *raytest[10]   PEND    express    li03c03     -       Sep 10 14:50      -          -
```

Self-scheduler

- Submit large numbers of independent short **serial** jobs as a single batch

```
#!/bin/bash
#BSUB -q express
#BSUB -W 1:00
#BSUB -n 12
#BSUB -R span[ptile=2]
#BSUB -J selfsched
#BSUB -o test01
module load selfsched                    # load the selfsched module
mpirun -np 12 selfsched < test.inp       # 12 cores, with one master process
```

`$cat test.inp` (test.inp: input for Self-Scheduler; a series of job commands)

```
/path/to/bin/program_to_run < input_jason > output_jason
/path/to/bin/program_to_run < input_tom > output_tom
. . .
/path/to/bin/program_to_run < input_jane > output_jane
```

Common errors of batch jobs

1. Valid allocation account needed in the submission script

```
-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-
    Project acc_project is not valid for user gail01
-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-
Request aborted by esub. Job not submitted.
```

- Use ***mybalance*** to see accessible accounts.

2. Reach memory limit

```
$ bhist -n 10 -l 107992756
Fri Jul 27 11:07:33: Completed <exit>; TERM_MEMLIMIT: job killed after
                             reaching LSF memory usage limit;
```

- memory based on one core, with 3 GB as default
- multithreaded applications need to be on the same node, such as STAR, BWA,...

3. No suitable hosts for the job

- Requested resource is non-exist : -n 256 -R span[hosts=1]

Tips for efficient usage of the queuing system

- Request reasonable resource
  - **Prior knowledge needed.** (Try short test runs before production to get a reasonable estimate)
  - User limit:

    Max running jobs per user: 4,000

    Max pending jobs per user: 20,000

    Max num. of GPUs per user: 50

    Global Memory limit: 30TB (20TB on CATS)

    Heavy users: depending on the resource requested

  - Monitor resource usage of a running job: "***bjobs -ℓ JobID***"

```
...
 MEMORY USAGE:
 MAX MEM: 68.1 Gbytes;  AVG MEM: 37.4 Gbytes; MEM Efficiency: 79.83%

 CPU USAGE:
 CPU PEAK: 19.89 ;  CPU Efficiency: 99.43%
```

Tips for efficient usage of the queuing system

- Find appropriate queue and nodes
  - use -q interactive: for debug (both CPU and GPU with internet access)
  - use -q express if walltime < 12h
- Memory request is **per core** in *MB, not per job.*
- You can open an interactive session on a regular compute node, too.

  bsub -q ***premium*** -n … -W … -P … … -Is /bin/bash
- Job not start after a long pending time
  - Whether the resource requested is non-exist:

    -R rusage[mem = 100GB] -n 256 -R span[hosts=1]
  - Run into PM:

```
NOTE: Because of PM reservations, job may not run
        until after Sat 21 Mar at  8:00PM
-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-
Job <6628109> is submitted to queue <premium>.
```

- /sc/arion/{projects,work,scratch} not backed up,
- Efficient use of limited resources.
- Job temporary dir configured to /local/JOBS instead of /tmp.

Final Friendly Reminder

All publications utilizing Minerva resources must include one of the following acknowledgements depending on your funding status:

- **If your *NIH-funded projects* use NIH-funded CPUs & B200 GPUs from both machines (AIMS & CATS described above) funded by NIH S10 on Minerva, you must include the following in all your publications:** "*This work was supported in part through the Minerva computational and data resources and staff expertise provided by Scientific Computing and Data at the Icahn School of Medicine at Mount Sinai and supported by the Clinical and Translational Science Awards (CTSA) grant UL1TR004419 from the National Center for Advancing Translational Sciences. Research reported in this publication was also supported by the Office of Research Infrastructure of the National Institutes of Health under award number **S10OD030463 and S10OD038231**. The content is solely the responsibility of the authors and does not necessarily represent the official views of the National Institutes of Health.*"

- **If your NIH-funded projects only use the AIMS B200 GPUs, you must include the following in all your publications:** "*This work was supported in part through the Minerva computational and data resources and staff expertise provided by Scientific Computing and Data at the Icahn School of Medicine at Mount Sinai and supported by the Clinical and Translational Science Awards (CTSA) grant UL1TR004419 from the National Center for Advancing Translational Sciences. Research reported in this publication was also supported by the Office of Research Infrastructure of the National Institutes of Health under award number **S10OD038231**. The content is solely the responsibility of the authors and does not necessarily represent the official views of the National Institutes of Health.*"

- **If your NIH-funded projects only use the CATS CPU nodes, you must include the following in all your publications:** "*This work was supported in part through the Minerva computational and data resources and staff expertise provided by Scientific Computing and Data at the Icahn School of Medicine at Mount Sinai and supported by the Clinical and Translational Science Awards (CTSA) grant UL1TR004419 from the National Center for Advancing Translational Sciences. Research reported in this publication was also supported by the Office of Research Infrastructure of the National Institutes of Health under award number **S10OD030463**. The content is solely the responsibility of the authors and does not necessarily represent the official views of the National Institutes of Health.*"

- **If you *DO NOT have NIH-funded projects* on Minerva, you MUST include the following in all your publications:** "*This work was supported in part through the Minerva computational and data resources and staff expertise provided by Scientific Computing and Data at the Icahn School of Medicine at Mount Sinai and supported by the Clinical and Translational Science Awards (CTSA) grant UL1TR004419 from the National Center for Advancing Translational Sciences.*"

Last but not Least

- Got a problem? Need a program installed? Send an email to:

hpchelp@hpc.mssm.edu

Follow us by visiting
https://labs.icahn.mssm.edu/minervalab

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CTSA Clinical & Translational Science Awards ®