



RAYMOND NICHOLS HALL

Welcome

KU Community Cluster Introduction



Quick Recap



Reference:
<https://crc.ku.edu/using-hpc>



Account Creation

- You get access to what you (or your group) paid for
- We want to have accurate record keeping for everyone
- Fill out the form at the link below

Reference:

<https://crc.ku.edu/access>



Storage and shortcuts

- \$HOME - a linux standard (100 GB quota)
- \$SCRATCH - large space, short term (pseudo-unlimited, 60 day purge policy)
- \$WORK - smaller space, longer term (size varies per group, good for group collaboration)
- Usage is displayed on login, and with `mystats` command

Reference:

<https://crc.ku.edu/storage>



Shortcuts cont'd.

- `$PBS_O_WORKDIR` Shortcut to the directory you submitted from
- `$PBS_JOBID` ID of your job
- `$PBS_O_HOST` Hostname of the machine you submitted from (submit1 or submit2)
- `$PBS_NODEFILE` List of hostnames your job was assigned to

Reference:

<https://crc.ku.edu/storage>



Modules

- All old software is located under the "legacy" module
 - `module load legacy`
- As time goes on we will build new software that doesn't require the legacy step
- New modules will also "chain load" the compiler and MPI libraries they were built with so you don't have to load any module except the one for the program you'd like to work with

Reference:

<https://crc.ku.edu/software>



Modules cont'd.

- When you first login you get a default set of modules pre-loaded for you
 - `compiler/gcc/6.3`, `python/3.6`, `anaconda/4.3`, `openmpi/2.0`, `StdEnv`
- If you don't like this behavior, feel free to unload the modules in your `.bashrc`
 - `module unload <module_name>`
- Loading a different module of the same type (`python/2.7` for example), the `python/3.6` module will automatically be unloaded in favor of the new one

Reference:

<https://crc.ku.edu/software>



MPI Enhancements

- mpicc MYCODE.c or mpif90 MYCODE.f90 still works
- mpirun ./program (no need for -np XX, --machinefile=\$PBS_NODEFILE).
- The new MPI libraries are compiled with the scheduler so it is aware of the nodes and number of processes.

Reference:

<https://crc.ku.edu/software>



Running a job - what stayed the same

- You can still use the #PBS directives you know and love in your submit script
- All directives still work the way you'd expect:
 - -q specifies a queue
 - -l specifies node features
 - -N specifies a job name
 - etc...

Reference:

<https://crc.ku.edu/using-hpc#Flags>



Running a job - things that changed

- To gain some new functionality, qsub has been replaced with msub
- Instead of #PBS, use #MSUB
- Instead of having highmem, gpu, and phi queues; each research group now has it's own queue
 - If you need a gpu/phi or higher memory requirements specify them with the -l command
 - ex) #MSUB -l gpus=1
- Requesting nodes and memory is the same/different

Reference:

<https://crc.ku.edu/using-hpc#Flags>



Requesting nodes and processors

- As you're used to, `nodes=x:ppn=y` still works, but is probably more specific than you need
- `-l procs=x` is a good option
- `-l nodes=x` also works, in this case nodes doesn't mean what you think though



Requesting memory

- -l mem=xxm works, but is interpreted differently for single node versus multi-node jobs.
 - Maximum amount of physical memory used by the job.
 - The mem resource will only work for single-node jobs. If your job requires multiple nodes, use pmem instead.
- -l pmem=XXm (or XXmb or XXg or XXgb). This is good for multi-node jobs
 - XXm=total mem required/number of cores requested
- There are other options, but these are the best and most commonly used

Reference:

<http://docs.adaptivecomputing.com/torque/6-1-0/adminGuide/help.htm#topics/torque/2-jobs/requestingRes.htm>



More on queues

- Each group that purchased hardware gets at least one queue
- Queue covers all hardware your group purchased, requesting specialty nodes done with flags in submit script
- Special 'sixhour' queue exists for submitting jobs to anywhere on the cluster. Runs at a lower priority and can only run for ≤ 6 hours.
 - `#MSUB -q sixhour`
- `showq -w class=<queue_name>` will show you all the jobs running in a given queue
- Your default queue is shown on login and by running `mystats`

Reference:

<https://crc.ku.edu/using-hpc#Queues>



Sample Submit Script

```
#!/bin/bash
#MSUB -N MyJob
#MSUB -l procs=48,pmem=48m,walltime=05:00
#MSUB -m abe
#MSUB -M crchelp@ku.edu
#MSUB -j oe
#MSUB -q sixhour
```

```
module load compiler/gcc/6.3
module load openmpi/2.0
```

```
mpirun $HOME/myprogram.out
```

Reference:

<https://crc.ku.edu/using-hpc#Script>



Viewpoint and RemoteViz

Moab VIEWPOINT



Moab VIEWPOINT

Welcome, n227e821 [Sign Out](#)

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[Q](#)

Workload [Refresh](#) Refresh Interval: 15s [CREATE JOB](#)

Job ID	Job Name	Submitter ID	Start Date	Submit Date	Queue Status	Cores	Nodes	Wall Clock
7237	STDIN	n227e821	2017-03-06 17:15:33	2017-03-06 17:15:33	COMPLETED	128	2	00:06:00.00
7233	STDIN	n227e821	2017-03-06 17:11:05	2017-03-06 17:10:39	COMPLETED	48	7	00:06:00.00
7231	STDIN	n227e821	2017-03-06 17:10:00	2017-03-06 17:10:00	COMPLETED	48	7	00:06:00.00
7229	STDIN	n227e821	2017-03-06 17:06:43	2017-03-06 17:06:38	COMPLETED	48	6	00:06:00.00
7228	STDIN	n227e821	2017-03-06 17:05:35	2017-03-06 17:05:32	COMPLETED	48	6	00:06:00.00
7226	STDIN	n227e821	2017-03-06 17:04:39	2017-03-06 17:04:39	COMPLETED	1	1	00:06:00.00
7225	testnem	n227e821	2017-03-06 17:03:03	2017-03-06 17:02:57	COMPLETED	48	4	00:06:00.00
7223	testnem	n227e821	2017-03-06 17:00:38	2017-03-06 17:00:36	COMPLETED	48	4	00:06:00.00
7206	testnem	n227e821	2017-03-06 16:55:27	2017-03-06 16:55:25	COMPLETED	2	1	00:06:00.00
7190	testnem	n227e821	2017-03-06 16:52:50	2017-03-06 16:52:45	COMPLETED	1	1	00:06:00.00
7162	hostname-test	n227e821	2017-03-06 16:42:08	2017-03-06 16:42:05	COMPLETED	1	1	00:06:00.00
6842	wh21n-rexopln	n227e821	2017-03-06 15:33:46	2017-03-06 15:33:44	COMPLETED	320	20	04:04:00.00
5193	Remote_viz_job	n227e821	2017-03-03 11:18:11	2017-03-03 11:18:10	COMPLETED	1	1	99:23:59:59
4512	STDIN	n227e821	2017-03-02 11:35:59	2017-03-02 11:35:59	COMPLETED	1	1	00:06:00.00
2861	STDIN	n227e821	2017-03-01 10:09:07	2017-03-01 10:09:07	COMPLETED	1	1	00:06:00.00
2618	mpiTest	n227e821	2017-02-28 21:49:26	2017-02-28 21:49:25	COMPLETED	4	1	00:00:00.30
2617	mpiTest	n227e821	2017-02-28 21:49:26	2017-02-28 21:49:22	COMPLETED	1	1	00:00:00.30
2259	mpiTest	n227e821	2017-02-28 20:30:52	2017-02-28 20:30:51	COMPLETED	1	1	00:00:00.30
2247	mpiTest	n227e821	2017-02-28	2017-02-28	COMPLETED	1	1	00:00:00.30

Dedicated System Resources
CPU **MEMORY**

24h... Current

Node Summary
322 NODES

[View All Nodes](#)

Workload Summary
303 JOBS

[View All Workload](#)



Moab VIEWPOINT

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Nodes

Refresh Interval



Node ID	Status	Class	Feature	Cores Available/Consumed	Jobs	CPU Utilization	Memory Utilization
n004	IDLE	sixhour	r20c1n1.d...	20/20	0	0	0
n005	BUSY	shontz.sik...	ib.gpu.inte...	0/24	2	100	10.78
n006	BUSY	shontz.sik...	ib.gpu.inte...	0/24	2	100	10.78
n007	BUSY	shontz.sik...	ib.gpu.inte...	0/24	2	100	10.78
n008	BUSY	shontz.sik...	ib.gpu.inte...	0/24	2	100	10.78
n009	BUSY	shontz.sik...	ib.gpu.inte...	0/24	2	100	10.78
n010	BUSY	shontz.sik...	ib.gpu.inte...	0/24	2	100	10.78
n011	BUSY	shontz.sik...	ib.gpu.inte...	0/24	2	100	10.78
n012	BUSY	shontz.sik...	ib.gpu.inte...	0/24	2	100	10.78
n013	BUSY	shontz.sik...	ib.gpu.inte...	0/24	2	100	10.78
n014	BUSY	shontz.sik...	ib.gpu.inte...	0/24	2	100	10.78
n016	IDLE	shontz.sik...	ib.gpu.inte...	24/24	0	0	0
n017	IDLE	shontz.sik...	ib.gpu.inte...	2/24	0	0	0
h001	IDLE	sixhour	del_int_20...	20/20	0	0	0
h002	IDLE	shontz.sik...	ib.intel.av...	24/24	0	0	0
h003	IDLE	shontz.sik...	ib.intel.av...	24/24	0	0	0
h004	IDLE	shontz.sik...	ib.intel.av...	24/24	0	0	0
h005	IDLE	shontz.sik...	ib.intel.av...	0/24	0	0	0
h006	IDLE	shontz.sik...	ib.intel.av...	1/24	0	0	0
h007	BUSY	shontz.sik...	ib.intel.av...	0/24	2	100	22.68
h008	BUSY	shontz.sik...	ib.intel.av...	0/24	1	100	34.02
h009	IDLE	shontz.sik...	ib.intel.av...	0/24	0	0	0

Current Search: 322 results returned

- Select -

Narrow Search

Filters

Select Status

Processors To

Jobs To

CPU Utilization To

Memory Utilization To

RESET

FILTER



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HOMEWORKLOADTEMPLATESNODES**FILE MANAGER**SESSIONS

File Manager

Remote File System / home / n227e821

UploadNew Folder

Filter by Name

../gromacs-5.0.4

gromacs-5.0.4/

2017/03/06

test.job

67 Bytes2017/03/06

testmem.e7190

0 Bytes2017/03/06

testmem.e7206

0 Bytes2017/03/06

testmem.e7223

0 Bytes2017/03/06

testmem.e7225

0 Bytes2017/03/06

testmem.o7190

0 Bytes2017/03/06

testmem.o7206

0 Bytes2017/03/06

testmem.o7223

0 Bytes2017/03/06

testmem.o7225

0 Bytes2017/03/06

wh21n-rexoplsn

487 Bytes2017/03/06

Show64entries

Select All

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COMPUTING

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Recap & useful links

<https://crc.ku.edu/>

<https://crc.ku.edu/using-hpc>

<https://crc.ku.edu/access>

<https://crc.ku.edu/storage>

<https://crc.ku.edu/software>

<https://crc.ku.edu/using-hpc#Flags>

<http://docs.adaptivecomputing.com/torque/6-1-0/adminGuide/help.htm#topics/torque/2-jobs/requestingRes.htm>

<https://crc.ku.edu/using-hpc#Queues>

<https://crc.ku.edu/using-hpc#Script>



Questions?

Email us at crchelp@ku.edu and we'll get back to you as quickly as we can

Thank you for your patience

See these slides at: <https://goo.gl/W8oLCz>

Thank you!