Introduction to the HPC Cluster

Rollins School of Public Health, BIOS 780
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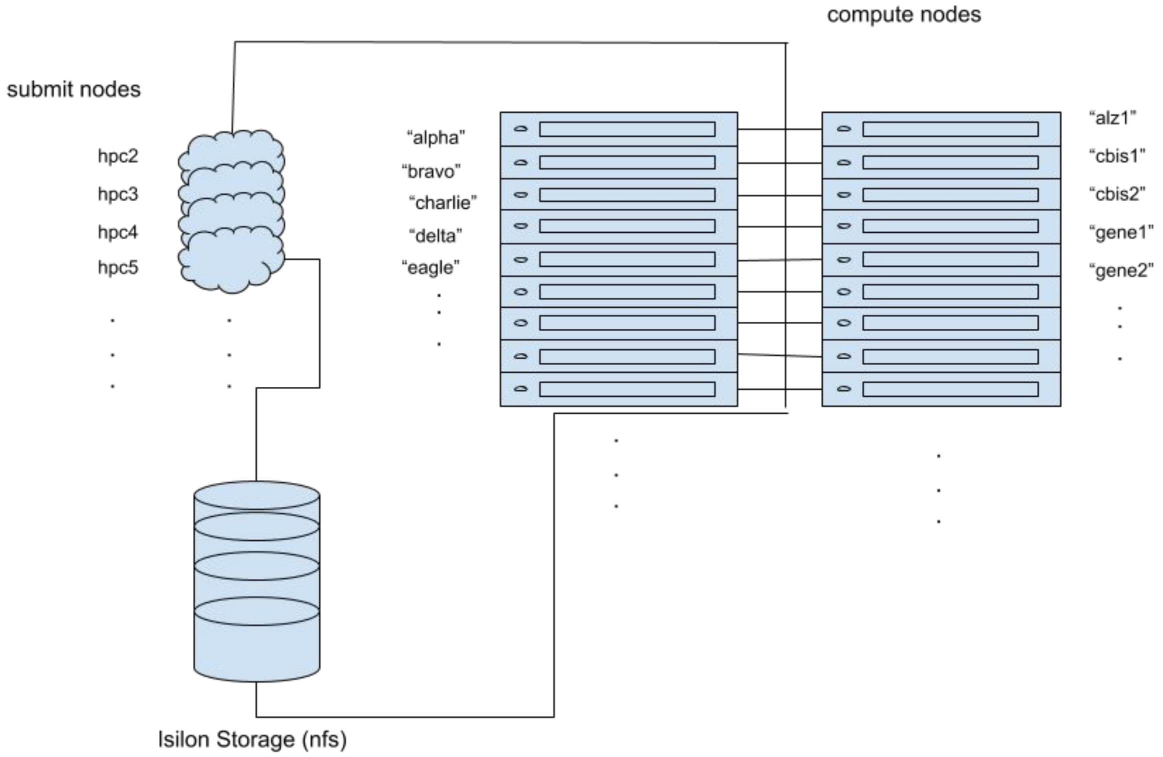
The HPC Cluster

The High Performance Computing (HPC) Cluster is a collection of computers dedicated to (scientific) computation and connected via a dedicated network and storage facility. It runs an operating system called *Linux* (Lee-nuks).

Our Layout:

- Compute nodes
- Submit hosts
- Storage service
- Scheduler
- License Manager

compute nodes
submit nodes
hpc2
hpc3
hpc4
hpc5
“alpha”
“bravo”
“charlie”
“delta”
“eagle”
“alz1”
“cbis1”
“cbis2”
“gene1”
“gene2”
Isilon Storage (nfs)

Submit hosts and Compute Nodes

Login/Submit hosts:

- Your “login host”. You **ssh**-in to this machine: *ssh <userid>@<submit_host>*
- You most likely will need VPN access to reach these (some campus wired connections are accepted)
- Firewall timeout: 15 minutes
- You copy data onto these systems, which have your home and project directories available (which are mounted everywhere)
- Limited application availability - don’t run jobs on these systems
- Named “hpc3”, “hpc4”, “hpc5”, etc.

Compute nodes:

- These are where the jobs are run
- Applications readily available here
- No direct login access
- Many cores, large amounts of RAM
- Physical servers (not VMs)
- Named after fruit (“apple”, “banana”, “cherry”) or research group (“gene1”, “gene2”, etc.) or randomly (“dynareg1”)
- There are 32 compute nodes
- 664 cores -> 1328 threads total
- Running RHEL 7

Logging in to the Cluster

- We use the Secure Shell (**ssh**) program to log into the submit hosts
- The easiest operating systems: Linux and Mac OS X clients.   Use the provided **Terminal** program, and **ssh** is already included.

Preliminaries: Getting an SSH client for Windows

- Connecting to the cluster from Windows is more complicated. You'll need to add/install an **ssh** client. There are at least three options:
  - Install **Putty**.   Go to putty.org, download 64-bit .msi file and install. It works on older Windows systems
  - On Windows 10, use **Windows Subsystem for Linux**. Download Ubuntu from Windows store
  - Install **Linux** via a virtual machine: e.g., VirtualBox or VMWare.
  - Excellent how-to video, *Learning Linux Command Line* at
  - https://www.linkedin.com/learning-login/ (use Emory email)
  - HelpDesk: installation of Putty

Preliminaries: Changing your unix $SHELL

- A legacy “feature” of central IT at Emory: everyone’s Unix shell is set to ‘ksh’ in LDAP directory service.
- No one uses **ksh** anymore (the default shell on Linux is **bash,** Mac OS X now uses **zsh)**. The **bash** shell is preferred and supported on the cluster.
- All new Emory users have to change it themselves: https://mynetid.emory.edu/IDMProv/portal/cn/DefaultContainerPage/WelcometoMyNetID
- Call 7-7777 (Central IT help line) for assistance.

More Preliminaries: VPN access

- If you connect to the cluster from an off-site location, including Emory Unplugged (Emory's wireless network), you'll need access to the Emory VPN.
- This is granted by individual request by central IT (*LITS*): https://it.emory.edu/security/vpn.html
- You shouldn't need to request anything other than having VPN access "activated" for your Emory NetID.
- You need to install Emory's VPN client on your computer.
- Call 7-7777 (Central IT help line) for assistance.

Using SSH

- Use command *ssh <username>@<submit_host>.sph.emory.edu*, e.g., “`ssh fred@hpc6.sph.emory.edu`”
- Accept new key the first time you login
- Best practice: password-less key exchange and ssh-agent
- **ssh-copy-id** works well from any Linux/Mac OS X terminal.
- **.ssh/config** can be used to save aliases to further reduce typing.

Staying Connecting to the Cluster: **screen**

- Once logged in, both the VPN and the network firewall settings can “time out”.
- As a work-around, use the Unix command **screen.**
- After logging in, simply type ‘screen’. It will return a prompt to you, as if nothing happened. Type “<ctrl>-a d”, to exit a screen.
- If your connection gets dropped (while in a screen), you can “reattach” to the session via **screen -r**. (Type ‘<ctrl>-a ?’ in **screen**, for command list.)

Unix: a few helpful commands

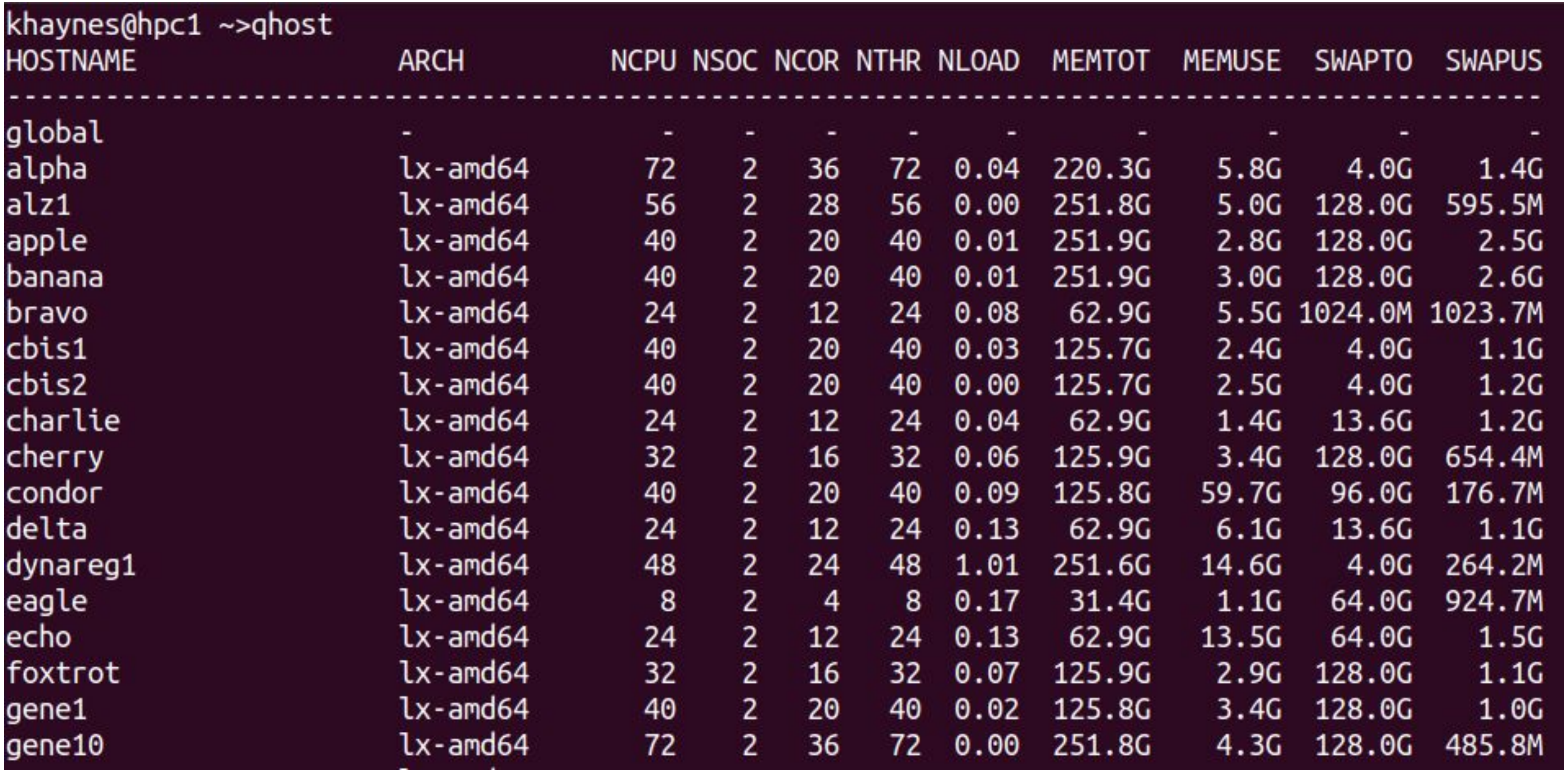
- **du :** shows disk usage. Ex: **du -hs /home/<*netid*>** shows how large your home directory is (in gigabytes). (*This command may take a few minutes to complete.*)
- **ls** : list files in current working directory
- **pwd** : print working directory
- **more** : read contents of a text file, with paging
- **chown** : change user or group ownership of a file
- **vim** : a lightweight text file editor (worth learning)
- **man** : read manual pages. Ex. **man chown**
- **scp :** secure copy, part of **ssh**
- Free course! *Learning Linux Command Line* via Emory
- Go to https://www.linkedin.com/learning-login/

Using the Cluster: Grid Engine q-commands

Work on the cluster is submitted in the form of “jobs”, or programming tasks, that are sent to the compute nodes from the submit nodes. The *q-commands* are Grid Engine commands that perform various job functions:

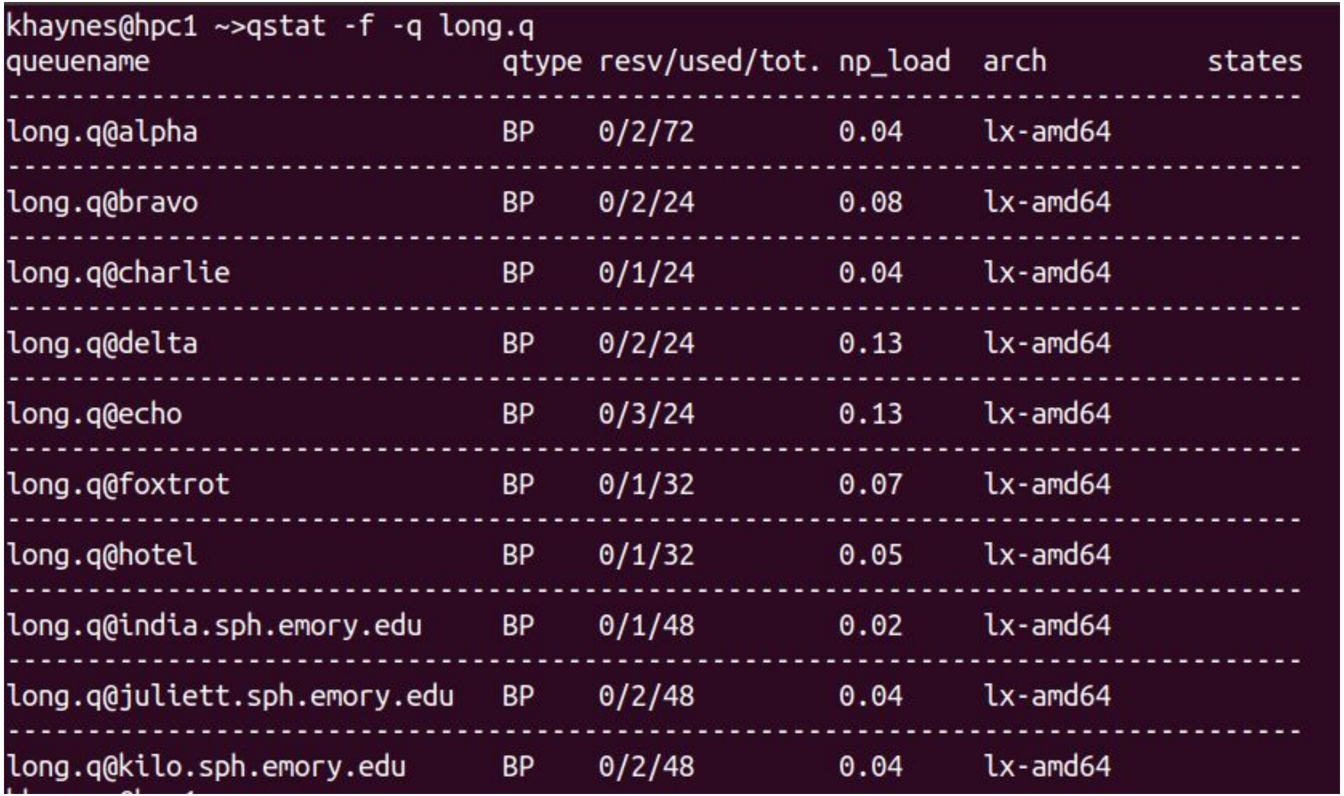
Submit jobs	**qsub**, **qlogin**
Check job status	**qstat**
Delete jobs	**qdel**
Cluster/queue state	**qhost, qstat**

Cluster status: **qhost** - show available hosts



```
khaynes@hpc1 ~>qhost
HOSTNAME                ARCH         NCPU NSOC NCOR NTHR  NLOAD  MEMTOT  MEMUSE  SWAPTO  SWAPUS
----------------------------------------------------------------------------------------------
global                  -               -    -    -    -      -       -       -       -       -
alpha                   lx-amd64       72    2   36   72   0.04  220.3G    5.8G    4.0G    1.4G
alz1                    lx-amd64       56    2   28   56   0.00  251.8G    5.0G  128.0G  595.5M
apple                   lx-amd64       40    2   20   40   0.01  251.9G    2.8G  128.0G    2.5G
banana                  lx-amd64       40    2   20   40   0.01  251.9G    3.0G  128.0G    2.6G
bravo                   lx-amd64       24    2   12   24   0.08   62.9G    5.5G 1024.0M 1023.7M
cbis1                   lx-amd64       40    2   20   40   0.03  125.7G    2.4G    4.0G    1.1G
cbis2                   lx-amd64       40    2   20   40   0.00  125.7G    2.5G    4.0G    1.2G
charlie                 lx-amd64       24    2   12   24   0.04   62.9G    1.4G   13.6G    1.2G
cherry                  lx-amd64       32    2   16   32   0.06  125.9G    3.4G  128.0G  654.4M
condor                  lx-amd64       40    2   20   40   0.09  125.8G   59.7G   96.0G  176.7M
delta                   lx-amd64       24    2   12   24   0.13   62.9G    6.1G   13.6G    1.1G
dynareg1                lx-amd64       48    2   24   48   1.01  251.6G   14.6G    4.0G  264.2M
eagle                   lx-amd64        8    2    4    8   0.17   31.4G    1.1G   64.0G  924.7M
echo                    lx-amd64       24    2   12   24   0.13   62.9G   13.5G   64.0G    1.5G
foxtrot                 lx-amd64       32    2   16   32   0.07  125.9G    2.9G  128.0G    1.1G
gene1                   lx-amd64       40    2   20   40   0.02  125.8G    3.4G  128.0G    1.0G
gene10                  lx-amd64       72    2   36   72   0.00  251.8G    4.3G  128.0G  485.8M
```

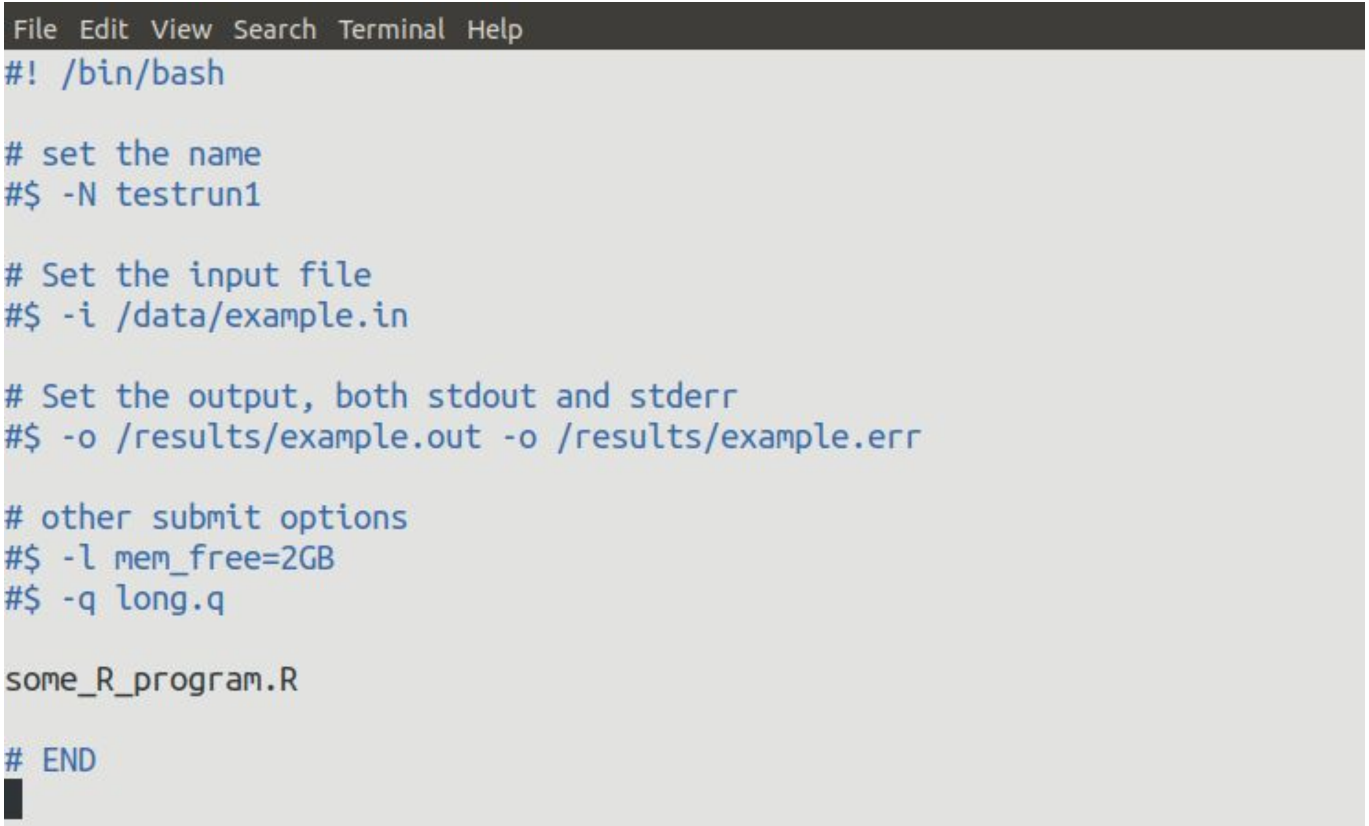
Cluster status: qstat -f



```
khaynes@hpc1 ~>qstat -f -q long.q
queuename                      qtype resv/used/tot. np_load  arch          states
---------------------------------------------------------------------------------
long.q@alpha                   BP    0/2/72         0.04     lx-amd64
---------------------------------------------------------------------------------
long.q@bravo                   BP    0/2/24         0.08     lx-amd64
---------------------------------------------------------------------------------
long.q@charlie                 BP    0/1/24         0.04     lx-amd64
---------------------------------------------------------------------------------
long.q@delta                   BP    0/2/24         0.13     lx-amd64
---------------------------------------------------------------------------------
long.q@echo                    BP    0/3/24         0.13     lx-amd64
---------------------------------------------------------------------------------
long.q@foxtrot                 BP    0/1/32         0.07     lx-amd64
---------------------------------------------------------------------------------
long.q@hotel                   BP    0/1/32         0.05     lx-amd64
---------------------------------------------------------------------------------
long.q@india.sph.emory.edu     BP    0/1/48         0.02     lx-amd64
---------------------------------------------------------------------------------
long.q@juliett.sph.emory.edu   BP    0/2/48         0.04     lx-amd64
---------------------------------------------------------------------------------
long.q@kilo.sph.emory.edu      BP    0/2/48         0.04     lx-amd64
```

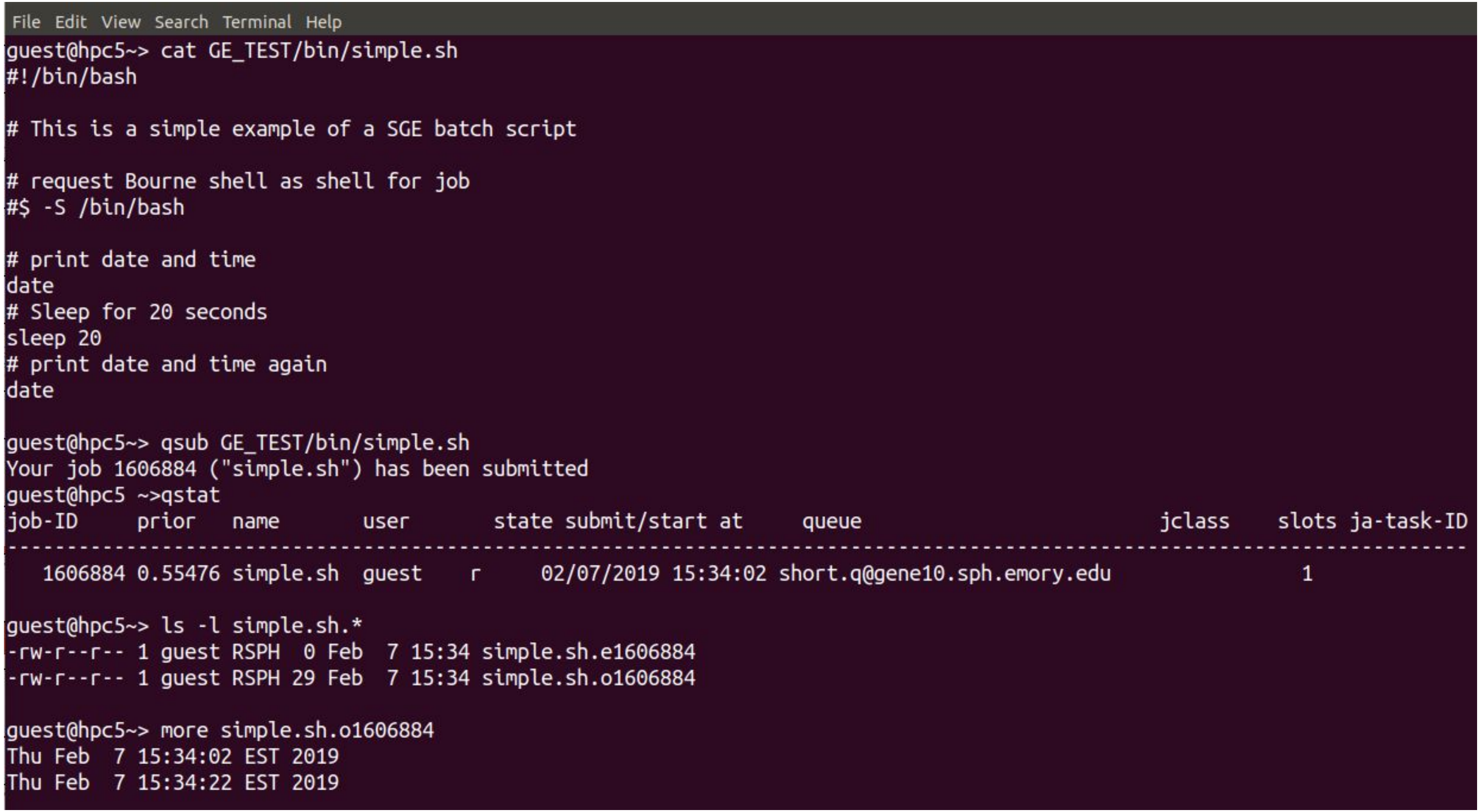
Submitting jobs: **qsub**

- Batch job submission is done via **qsub**
- **qsub *<program_name>*** submits a job running <program_name> with default attributes, after which the job will appear in the output of **qstat**
- Many attributes can be specified, such as run queue, input, output, job name, memory usage, etc.
- Ex. **qsub -cwd -i /data/example.in -o /results/example.out -N testrun1 -q long.q -l mem_free=2GB R_wrapper_script.sh**
- That's a lot of typing! Most people put those attributes in a job submission script.



```
#! /bin/bash

# set the name
#$ -N testrun1

# Set the input file
#$ -i /data/example.in

# Set the output, both stdout and stderr
#$ -o /results/example.out -o /results/example.err

# other submit options
#$ -l mem_free=2GB
#$ -q long.q

some_R_program.R

# END
```

A sample job submission script.



```
guest@hpc5~> cat GE_TEST/bin/simple.sh
#!/bin/bash

# This is a simple example of a SGE batch script

# request Bourne shell as shell for job
#$ -S /bin/bash

# print date and time
date
# Sleep for 20 seconds
sleep 20
# print date and time again
date

guest@hpc5~> qsub GE_TEST/bin/simple.sh
Your job 1606884 ("simple.sh") has been submitted
guest@hpc5 ~>qstat
job-ID     prior   name       user       state submit/start at     queue                          jclass     slots ja-task-ID
------------------------------------------------------------------------------------------------------------------------------
   1606884 0.55476 simple.sh  guest    r     02/07/2019 15:34:02 short.q@gene10.sph.emory.edu                    1

guest@hpc5~> ls -l simple.sh.*
-rw-r--r-- 1 guest RSPH  0 Feb  7 15:34 simple.sh.e1606884
-rw-r--r-- 1 guest RSPH 29 Feb  7 15:34 simple.sh.o1606884

guest@hpc5~> more simple.sh.o1606884
Thu Feb  7 15:34:02 EST 2019
Thu Feb  7 15:34:22 EST 2019
```

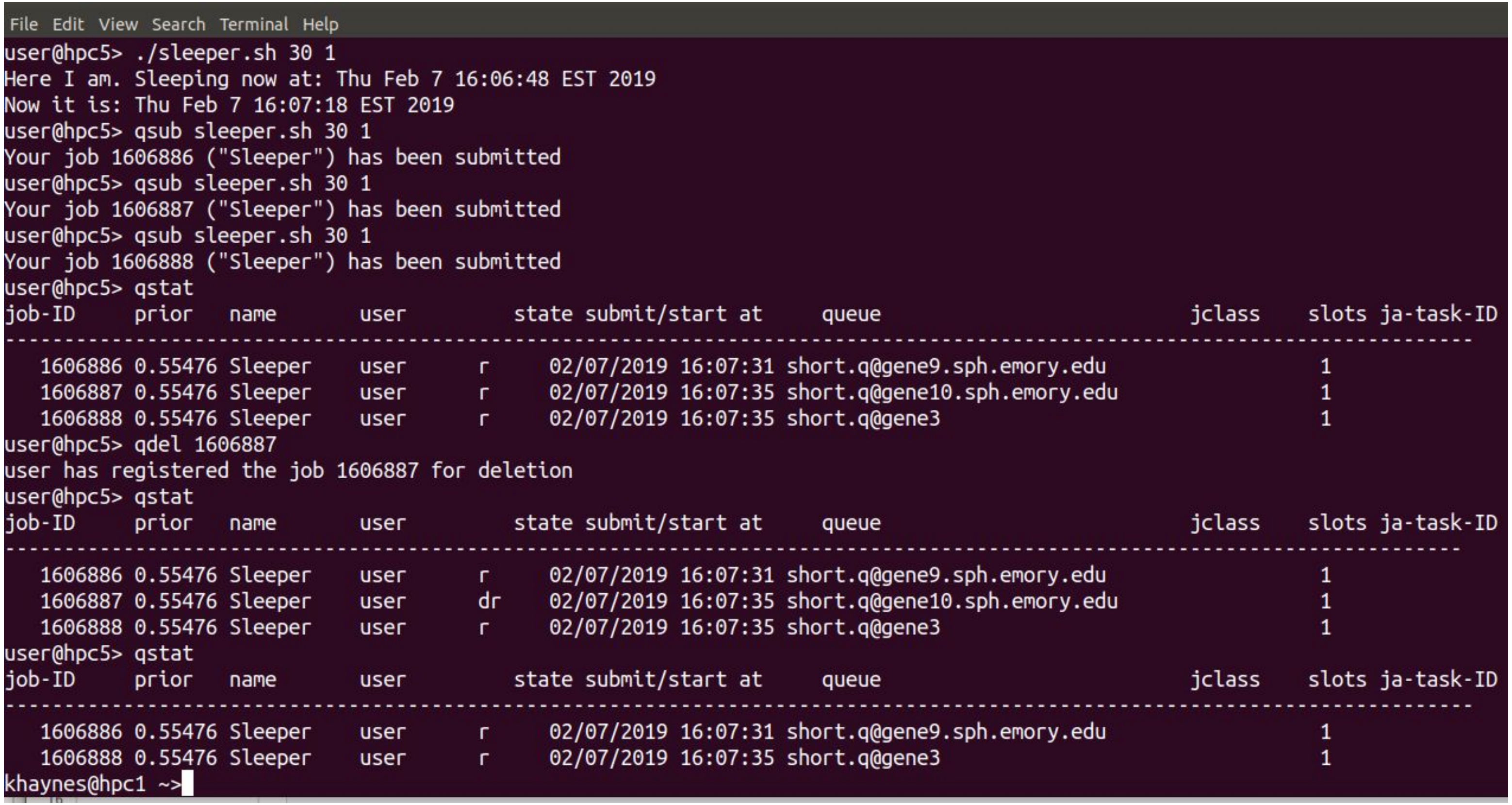
A **qsub** workflow example.

Checking on Jobs: **qstat** and **qacct**

- **qstat** (without arguments) shows the status all of your currently queued jobs
- Jobs usually have status of **r** (“running”), **qw** (“queue wait” or pending), or **Eqw** (in and “error” state)
- Use **qacct -j *<job_id>*** to get detailed information about any job.

Killing jobs: **qdel**

- Use **qdel *<job_id>*** to kill a submitted job



```
user@hpc5> ./sleeper.sh 30 1
Here I am. Sleeping now at: Thu Feb 7 16:06:48 EST 2019
Now it is: Thu Feb 7 16:07:18 EST 2019
user@hpc5> qsub sleeper.sh 30 1
Your job 1606886 ("Sleeper") has been submitted
user@hpc5> qsub sleeper.sh 30 1
Your job 1606887 ("Sleeper") has been submitted
user@hpc5> qsub sleeper.sh 30 1
Your job 1606888 ("Sleeper") has been submitted
user@hpc5> qstat
job-ID     prior   name       user         state submit/start at     queue                          jclass    slots ja-task-ID
----------------------------------------------------------------------------------------------------------------------------
   1606886 0.55476 Sleeper    user      r     02/07/2019 16:07:31 short.q@gene9.sph.emory.edu                  1
   1606887 0.55476 Sleeper    user      r     02/07/2019 16:07:35 short.q@gene10.sph.emory.edu                 1
   1606888 0.55476 Sleeper    user      r     02/07/2019 16:07:35 short.q@gene3                                1
user@hpc5> qdel 1606887
user has registered the job 1606887 for deletion
user@hpc5> qstat
job-ID     prior   name       user         state submit/start at     queue                          jclass    slots ja-task-ID
----------------------------------------------------------------------------------------------------------------------------
   1606886 0.55476 Sleeper    user      r     02/07/2019 16:07:31 short.q@gene9.sph.emory.edu                  1
   1606887 0.55476 Sleeper    user      dr    02/07/2019 16:07:35 short.q@gene10.sph.emory.edu                 1
   1606888 0.55476 Sleeper    user      r     02/07/2019 16:07:35 short.q@gene3                                1
user@hpc5> qstat
job-ID     prior   name       user         state submit/start at     queue                          jclass    slots ja-task-ID
----------------------------------------------------------------------------------------------------------------------------
   1606886 0.55476 Sleeper    user      r     02/07/2019 16:07:31 short.q@gene9.sph.emory.edu                  1
   1606888 0.55476 Sleeper    user      r     02/07/2019 16:07:35 short.q@gene3                                1
khaynes@hpc1 ~>
```

A **qdel** workflow example.

Cluster queues

- *qlogin.q* - interactive sessions; dedicated 64 cores; timeout after 24 hours
- *long.q* - general use; no time limit; 14 jobs/user max.
- *short.q* - general use subordinate queue; 72 hour limit; 240 cores; limited to 40 jobs/user
- Restricted queues: *fruit.q, gene.q, sunlab.q, cbis.q, alz.q, mh.q*
- Restricted queues have priority on owned systems, and have no per user job limit or run-time limit
- All queues have corresponding parallel queue (*long, short, gene*, etc.)
- Ex. **qsub -pe long 4 <*program_name*>** requests a parallel environment with four processors

Available Software

- C/C++, Fortran compilers
- Python*
- R**
- MATLAB
- SAS
- Openmpi
- Others, including user-installed

Look in /usr/local/ for the latest installed versions!

(E.g., use /usr/local/R-3.6.0/bin/R)

Storage on Cluster

- Each account is granted a home directory in /home/<NetID>, which is mounted across all nodes of the cluster (i.e., software installed there is available everywhere).
- Initial quota is set to 16 GB.   Quota can be increased once, no questions asked. Users are responsible for deleting/off-loading and compressing files.
- For large data installations, request a project directory. There is a cost associated with project directories, depending on type.

Getting Help

- If you need help with the HPC Cluster, you should open a help ticket with RSPH IT.
- Send email to “help@sph.emory.edu” and CC: keven.haynes@emory.edu, and include the following:
  - Your Emory NetID
  - **State in both the Subject and the body of the ticket that you your request concerns the HPC Cluster.**
  - The particular issue you are having. (“It is broken” is not an issue.)
  - The name of the system you were logged into, or the particular software package.
- We can help with systems-related issues.

More info

- Excellent how-to videos are available to Emory community (free!) via https://www.linkedin.com/learning-login/. Click on sign in, then enter your Emory email address, and you will be redirected to Emory for sign in. Search for *Learning Linux Command Lin*e for video instructions on how to install Windows Subsystem for Linux or Linux in a virtual machine (plus, basic Linux usage).
- The old HPC Cluster documentation is still here: https://intranet.sph.emory.edu/services/it/environment/cluster/index.html

  (It is in need of updating!)