

# Introduction to HPC Using the New Cluster at GACRC

---

Georgia Advanced Computing Resource Center

University of Georgia

Zhuofei Hou, HPC Trainer

[zhuofei@uga.edu](mailto:zhuofei@uga.edu)

# Outline

---

- What is GACRC?
- What is the new cluster at GACRC?
- How does it operate?
- How to work with it?

# What is GACRC?

---

## Who Are We?

- Georgia **A**dvanced **C**omputing **R**esource **C**enter
- Collaboration between the Office of Vice President for Research (**OVPR**) and the Office of the Vice President for Information Technology (**OVPI**T)
- Guided by a faculty advisory committee (GACRC-AC)

## Why Are We Here?

- To provide computing hardware and network infrastructure in support of high-performance computing (**HPC**) at UGA

## Where Are We?

- <http://gacrc.uga.edu> (Web)      <http://wiki.gacrc.uga.edu> (Wiki)
- [https://wiki.gacrc.uga.edu/wiki/Getting\\_Help](https://wiki.gacrc.uga.edu/wiki/Getting_Help) (Support)
- <https://blog.gacrc.uga.edu> (Blog)      <http://forums.gacrc.uga.edu> (Forums)

# What is the new cluster at GACRC?

---

- Cluster Structural Diagram
- General Information
- Computing Resources

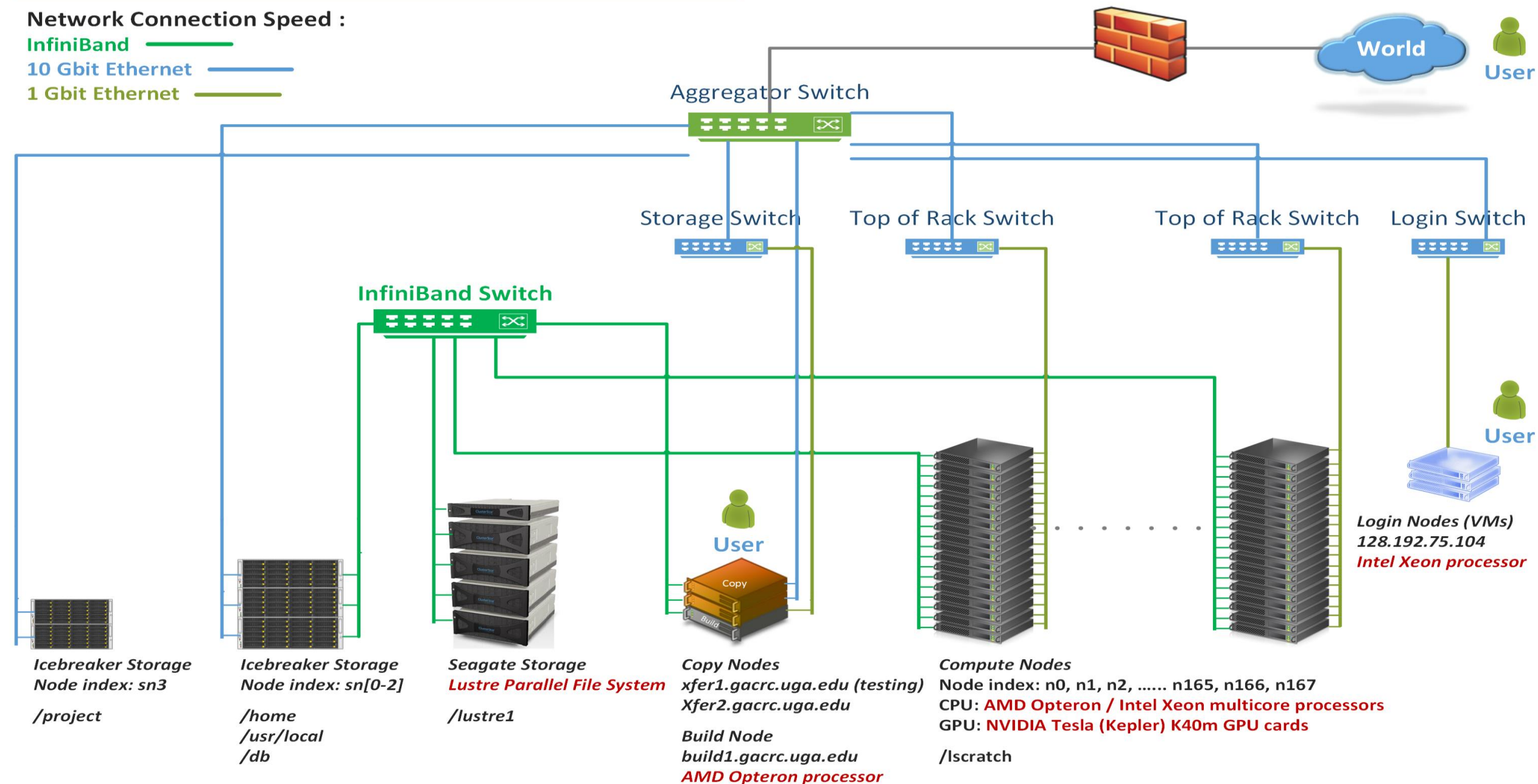
# The New GACRC Linux HPC Cluster Structural Diagram

Network Connection Speed :

**InfiniBand** ———

**10 Gbit Ethernet** ———

**1 Gbit Ethernet** ———



# What is the new cluster – General Information

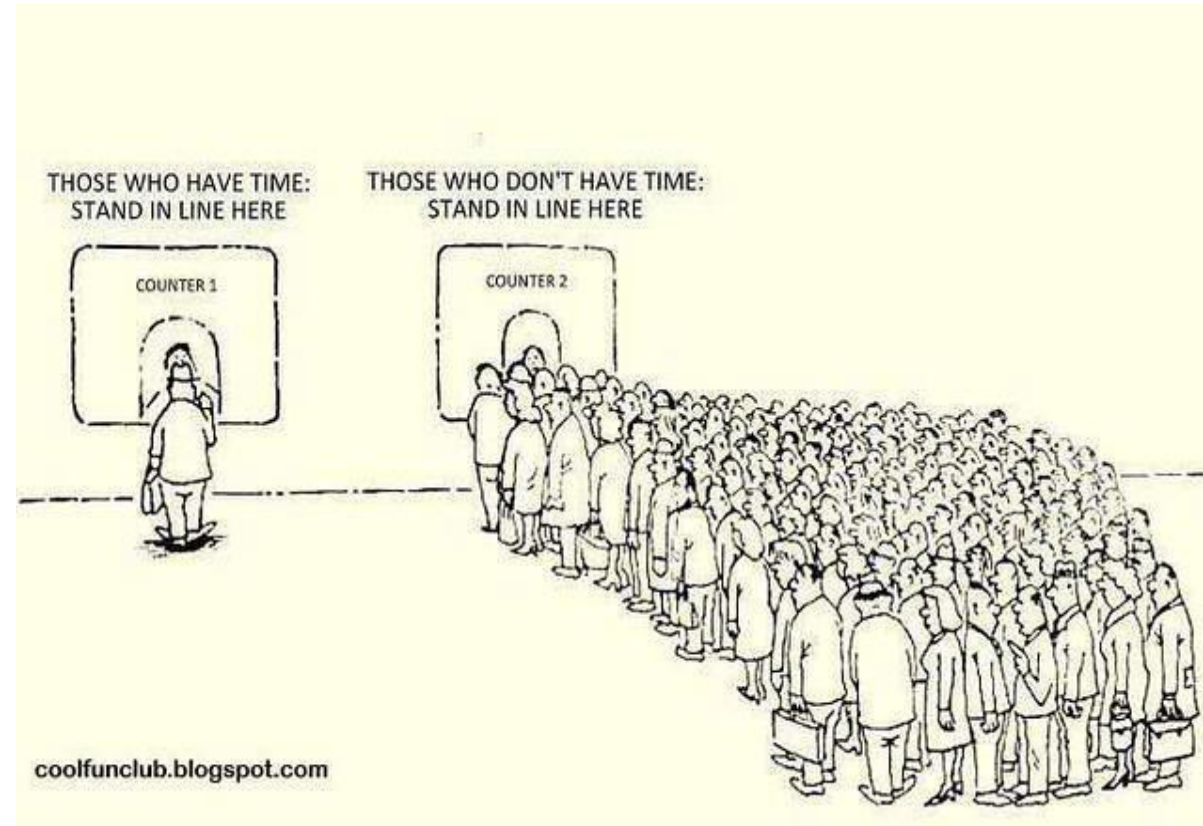
---

The new cluster is a Linux high performance computing (HPC) cluster:

- 64-bit CentOS 6.5 operating system
- Login node has Intel Xeon processors
- InfiniBand network provides internodal communication:
  - compute nodes ↔ compute nodes
  - compute nodes ↔ storage systems, e.g., /home and /scratch

# What is the new cluster – General Information

- Batch-queueing System:
  - Jobs can be started (submitted), monitored, and controlled
  - Determine which compute node is the best place to run a job
  - Determine appropriate execution priority for a job to run
- On new cluster:
  - Torque** Resource Manager
  - Moab** Workload Manager



# What is the new cluster – Computing Resources

Queue	Node Type	Total Nodes	Processor	Cores / Node	RAM (GB) / Node	GPU	GPU Cards / Node	InfiniBand
Batch	AMD	120	AMD Opteron	48	128	N/A	N/A	Yes
	HIGHMEM	3	AMD Opteron	48	512 (2)	N/A	N/A	Yes
					1024 (1)			
	GPU	2	Intel Xeon	16	128	NVIDIA K40m	8	Yes

**Peak Performance per Node: 500 Gflops/Node**

Home directory has a quota of **100 GB**

Scratch directory on /lutre1 has **NO** quota limit, auto-deleted in **30** days!



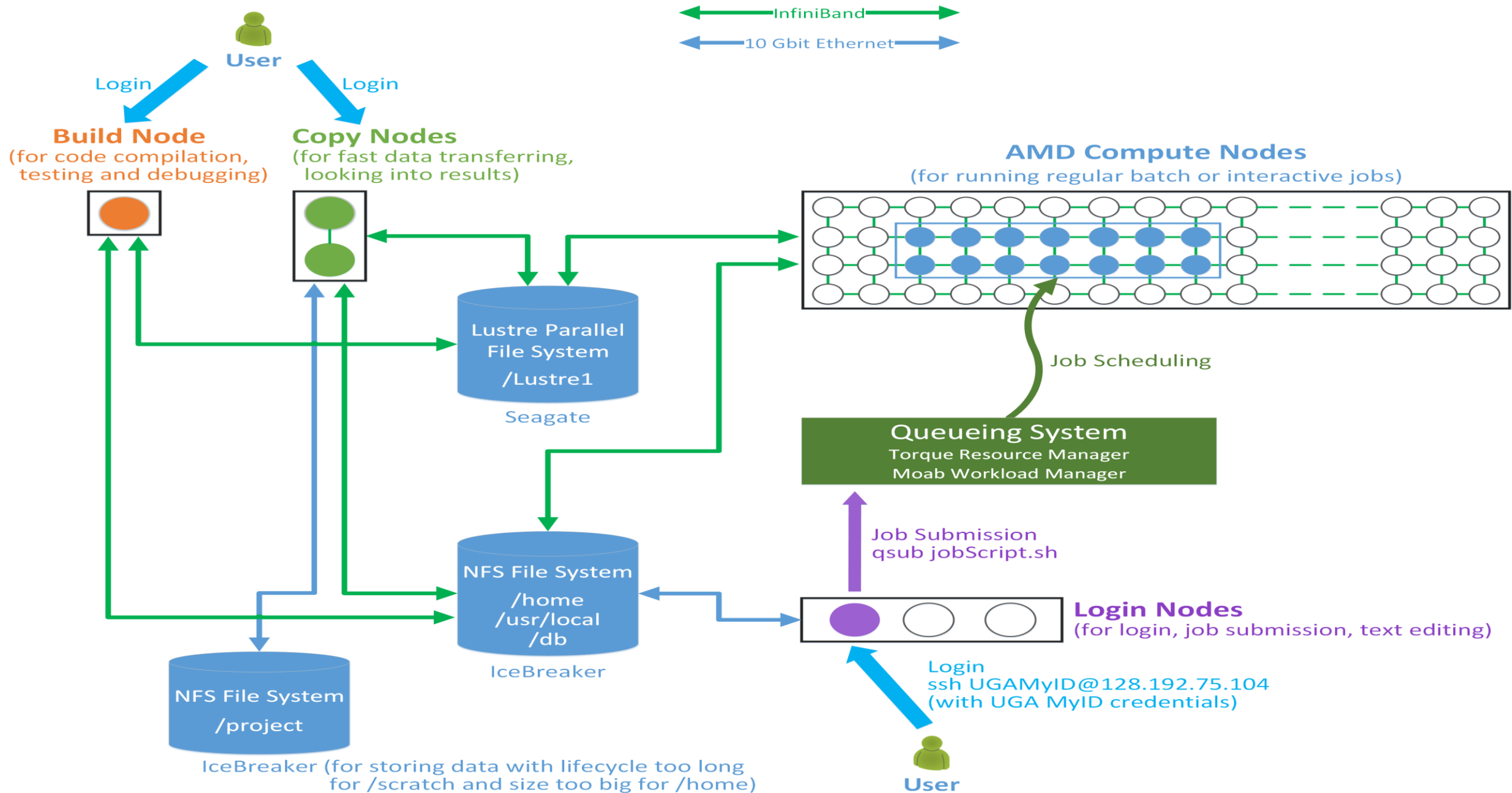
# How does it operate?

---

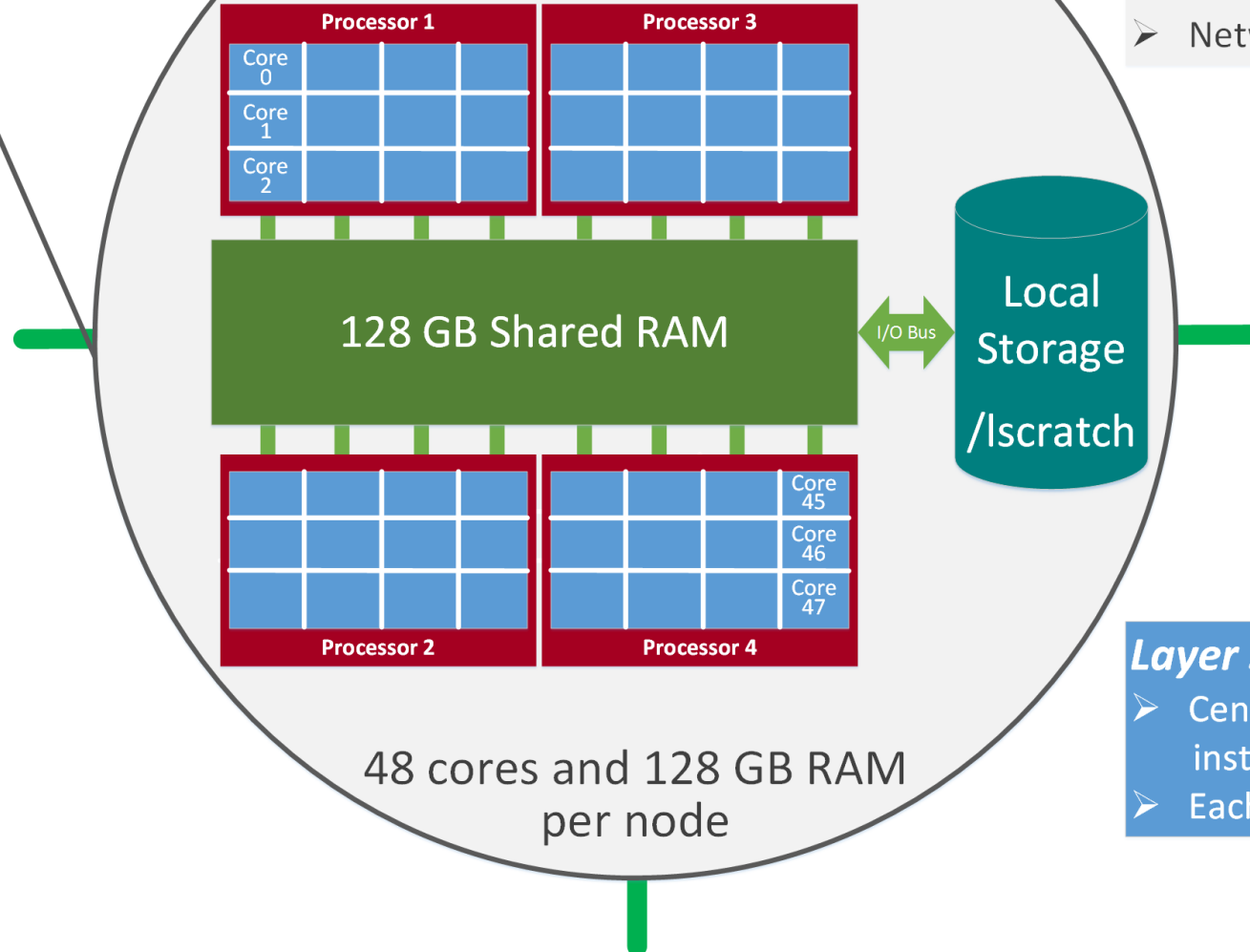
Next Page



# The New GACRC Linux HPC Cluster Operational Diagram



## Node 167



### Layer 1: Node

- A standalone “computer in a box”
- Multiple processors, e.g. 4, sharing memory
- Local disk storage, network interface, etc.
- Networked into a cluster

### Layer 2: Processor

- A single computing component
- Multicore processor, e.g. 12 cores

### Layer 3: Core

- Central processing unit (CPU) reading and executing instructions independently
- Each core is assigned to a software thread

# How to work with it?

---

*Before we start:*

- To get the new cluster to be your best HPC buddy, go to  
**GACRC Wiki** (<http://wiki.gacrc.uga.edu>)  
**GACRC Web** (<http://gacrc.uga.edu>)
- To get the most effective and qualified support from us, go to  
**GACRC Support** ([https://wiki.gacrc.uga.edu/wiki/Getting\\_Help](https://wiki.gacrc.uga.edu/wiki/Getting_Help))
- To work happily and productively, follow the new cluster's  
Community Code of Conduct (**CCOC**)

# How to work with it?

---

- Cluster's CCOC:

On cluster, you are not alone..... Each user is sharing finite resources, e.g., CPU cycles, RAM, disk storage, network bandwidth, with other researchers.

*What you do may affect other researchers on the cluster.*

6 rules of thumb to remember:

- NO jobs running on login node
- NO multi-threaded job running with only 1 core requested
- NO large memory job running on regular nodes
- NO long job running on interactive node
- NO small memory job running on large memory nodes
- Use the copy node for file transfer and compression



# How to work with it?

---

- Start with the Cluster
- Connect & Login
- Software Packages
- Run Jobs
  - How to submit a job
  - How to make a job submission script
  - How to check job status, cancel a job, etc.

# How to work with it – Start with the Cluster

---

- You need a **User Account**: [UGAMyID@128.192.75.104](mailto:UGAMyID@128.192.75.104)

To create your account correctly, you must provide us with your **official UGA MyID**, not a UGA MyID alias! 

- To get a user account, follow 3 steps:

1. Tell us your **Name**, **UGA MyID**, **Lab name** and **PI's name**, via **GACRC Support** ([https://wiki.gacrc.uga.edu/wiki/Getting\\_Help](https://wiki.gacrc.uga.edu/wiki/Getting_Help))
2. We send you an **invitation letter** with instructions to start account initialization
3. With Step 2 finished successfully, we send you a **welcome letter** with whole package of information about your account created successfully

# How to work with it – Connect & Login

---

- Open a connection: Open a terminal and `ssh` to your account

```
ssh zhuofei@128.192.75.104
```

or

```
ssh -X zhuofei@128.192.75.104
```

<sup>(1)</sup> `-X` is for X windows application running on the cluster to be forwarded to your local machine

<sup>(2)</sup> If using Windows, use `SSH client` to open connection, get from UGA download software page)

- Logging in: You will be prompted for your **UGA MyID password**

```
zhuofei@128.192.75.104's password: █
```

<sup>(3)</sup> On Linux/Mac, when you type in the password, the prompt blinks and does not move)

- Logging out: `exit` to leave the system

```
[zhuofei@75-104 ~]$ exit
```



# How to work with it – Software Packages

- The cluster uses **environment modules** to define the various paths for software packages
- Current number of modules installed is ~70 and expanding daily!
- **module avail** to list all modules available on the cluster:

```
[zhuofei@75-104 ~]$ module avail
```

----- /usr/local/modulefiles -----				
Core/StdEnv	exabayes/1.4.1	java/jdk1.8.0_20	openmpi/1.6.5/gcc/4.4.7	rsem/latest
Data/cache/moduleT.new	examl/3.0.11	java/latest (D)	openmpi/1.6.5/pgi/14.9	rsem/1.2.20 (D)
Data/cache/moduleT (D)	expat/latest	lammps/5Sep14	openmpi/1.8.3/gcc/4.4.7	samtools/latest
Data/system.txt	expat/2.0.1 (D)	lammps/16Aug13 (D)	openmpi/1.8.3/gcc/4.7.4	samtools/0.1.19
R/3.1.2	fastqc/latest	moab/7.2.10	openmpi/1.8.3/gcc/4.8.0 (D)	samtools/1.1
bedops/latest	fastqc/0.11.3 (D)	moab/8.1.1 (D)	openmpi/1.8.3/intel/14.0	samtools/1.2 (D)
bedops/2.4.14 (D)	gcc/4.7.4	moabs/1.3.2	openmpi/1.8.3/intel/15.0.2 (D)	scripture/latest
boost/1.47.0/gcc447	gcc/4.8.0 (D)	mvapich2/2.0.0/gcc/4.4.7	openmpi/1.8.3/pgi/14.9	scripture/03202015 (D)
boost/1.57.0/gcc447	gmap-gsnap/latest	mvapich2/2.0.0/pgi/14.9	orca/3.0.3	sparsehash/latest
boost/1.57.0_thread/gcc447	gmap-gsnap/2014-12-24 (D)	ncbiblast+/2.2.29	perl/latest	sparsehash/2.0.2 (D)
bowtie/latest	gnuplot/5.0.0	netcdf/3.6.3/gcc/4.4.7	perl/5.20.1	tophat/latest
bowtie/1.1.1 (D)	gs/1.16/gcc/4.4.7	netcdf/3.6.3/intel/14.0	perl/5.20.2 (D)	tophat/2.0.13 (D)
bowtie2/latest	hdf5/1.8.14/gcc/4.4.7	netcdf/3.6.3/intel/15.0.2 (D)	pgi/14.9	trinity/latest
bowtie2/2.2.4 (D)	hdf5/1.8.14/intel/15.0.2	netcdf/4.1.3/gcc/4.4.7	pgi/14.10 (D)	trinity/r20140717
cuda/5.0.35/gcc/4.4.7	hdf5/1.8.14/pgi/14.9	netcdf/4.1.3/intel/15.0.2	python/2.7.8-ucs4	trinity/2.0.6 (D)
cuda/6.5.14/gcc/4.4.7	imb/3.2	netcdf/4.1.3/pgi/14.10	python/2.7.8	zlib/gcc447/1.2.8
cufflinks/latest	intel/14.0	netcdf/4.3.2/gcc/4.4.7	python/3.4.3 (D)	
cufflinks/2.2.1 (D)	intel/15.0.2 (D)	netcdf/4.3.2/pgi/14.9	raxml/8.1.20	

# How to work with it – Software Packages

- `module list` to list which modules currently loaded:

```
[zhuofei@75-104 ~]$ module list  
  
Currently Loaded Modules:  
  1) StdEnv   2) moab/7.2.10
```

- `module load` to load the needed modules:

```
[zhuofei@75-104 ~]$ module load ncbiblast+/2.2.29  
[zhuofei@75-104 ~]$ module load python/2.7.8  
[zhuofei@75-104 ~]$ module load R/3.1.2  
[zhuofei@75-104 ~]$ module list  
  
Currently Loaded Modules:  
  1) StdEnv   2) moab/7.2.10   3) ncbiblast+/2.2.29   4) python/2.7.8   5) R/3.1.2
```

- `module unload` to remove the specific module:

```
[zhuofei@75-104 ~]$ module unload R/3.1.2  
[zhuofei@75-104 ~]$ module list  
  
Currently Loaded Modules:  
  1) StdEnv   2) moab/7.2.10   3) ncbiblast+/2.2.29   4) python/2.7.8
```

# How to work with it – Run Jobs

---

- Components you need to run a job:
  - **Software** already loaded. If not, used `module load`
  - **Job submission script** to run the software, specifying computing resources:
    - ✓ Number of nodes and cores
    - ✓ Amount of memory
    - ✓ Type of nodes
    - ✓ Maximum wallclock time, etc.
- Common commands you need:
  - `qsub`, `qstat`, `qdel`
  - `showq`, `checkjob`, etc.

# How to work with it – Run Jobs

- How to submit a job? **Easy!**

```
[zhuofei@75-104 MPIs]$ qsub sub.sh
```

**qsub** is to  
submit a job

**sub.sh** is your **job submission script**  
specifying:

- ✓ Number of nodes and cores
- ✓ Amount of memory
- ✓ Type of nodes
- ✓ Maximum wallclock time, etc.

- How to make a job submission script? **Next Page!**

# How to work with it – Run Jobs

- Example 1: **Serial job script** running NCBI Blast +

<code>#PBS -S /bin/bash</code>	→ Linux shell ( <b>bash</b> )
<code>#PBS -q batch</code>	→ Queue name ( <b>batch</b> )
<code>#PBS -N testBlast</code>	→ Name of the job ( <b>testBlast</b> )
<code>#PBS -l nodes=1:ppn=1:AMD</code>	→ Number of nodes ( <b>1</b> ), number of cores/node ( <b>1</b> ), node type ( <b>AMD</b> )
<code>#PBS -l mem=20gb</code>	→ Maximum amount of physical memory ( <b>20 GB</b> ) used by the job
<code>#PBS -l walltime=48:00:00</code>	→ Maximum wall clock time ( <b>48 hours</b> ) for the job, default 6 minutes
 <code>cd \$PBS_O_WORKDIR</code>	 → Use the directory from which the job is submitted as the working directory
 <code>module load ncbiblast+/2.2.29</code>	 → Load the module of ncbiblast+, version 2.2.29
 <code>time blastn [options]</code>	 → Run blastn with 'time' command to measure the amount of time it takes to run the application

# How to work with it – Run Jobs

- Example 2: **Threaded job script** running NCBI Blast + with **4** threads

```
#PBS -S /bin/bash
```

```
#PBS -q batch
```

```
#PBS -N testBlast
```

```
#PBS -l nodes=1:ppn=4:AMD
```

```
#PBS -l walltime=480:00:00
```

```
#PBS -l mem=20gb
```

```
#PBS -M jSmith@uga.edu
```

```
#PBS -m abe
```

```
#PBS -j oe
```

```
cd $PBS_O_WORKDIR
```

```
module load ncbiblast+/2.2.29
```

```
time blastn -num_threads 4 [options]
```

→ Number of nodes (1), number of cores/node (4), node type (AMD)  
Number of threads (4) = Number of cores requested (4)

→ Email to receive a summary of computing resources used by the job

→ Receive an email when the job begins (b) and finishes (e)

→ Standard error file (testBlast.e1234) will be merged into standard out file (testBlast.o1234)

→ Run blastn with 4 threads (-num\_threads 4)

# How to work with it – Run Jobs

- Example 3: **MPI job script** running RAxML with **50** MPI processes

```
#PBS -S /bin/bash
```

```
#PBS -q batch
```

```
#PBS -N testRAxML
```

```
#PBS -l nodes=2:ppn=48:AMD
```

→ Number of nodes (**2**), number of cores/node (**48**), node type (AMD)

```
#PBS -l walltime=480:00:00
```

Total cores requested =  $2 \times 48 = 96$

```
#PBS -l mem=20gb
```

We suggest, Number of MPI Processes (50)  $\leq$  Number of cores requested (96)

```
#PBS -j oe
```

```
cd $PBS_O_WORKDIR
```

```
module load raxml/8.1.20
```

→ To run raxmlHPC-MPI-AVX, MPI version using OpenMPI 1.8.3/Intel 15.0.2

```
module load intel/15.0.2
```

```
module load openmpi/1.8.3/intel/15.0.2
```



```
mpirun -np 50 raxmlHPC-MPI-AVX [options]
```

→ Run raxmlHPC-MPI-AVX with 50 MPI processes (**-np 50**)

# How to work with it – Run Jobs

- How to check job status? ***qstat!***

```
[jSmith@75-104 MPIs]$ qstat
```

Job ID	Name	User	Time Use	S	Queue
481929.pbs	testJob1	jSmith	900:58:0	C	batch
481931.pbs	testJob2	jSmith	04:00:03	R	batch
481934.pbs	testJob3	jSmith	0	Q	batch

Job status:  
 R : job is running  
 C : job completed (or crashed) and is not longer running. Jobs stay in this state for 24h  
 Q : job is pending, waiting for resources to become available

- How to cancel *testJob3* with jobID 481934? ***qdel!***

```
[zhuofei@75-104 MPIs]$ qdel 481934
```

```
[jSmith@75-104 MPIs]$ qstat
```

Job ID	Name	User	Time Use	S	Queue
481929.pbs	testJob1	jSmith	900:58:0	C	batch
481931.pbs	testJob2	jSmith	04:00:03	R	batch
481934.pbs	testJob3	jSmith	0	C	batch



# How to work with it – Run Jobs

- How to check resource utilization of a job? ***qstat -f*** or ***checkjob!***

```
[zhuofei@75-104 MPIs]$ qstat -f 481939
Job Id: 481939.pbs.scm
  Job_Name = testJob
  Job_Owner = zhuofei@uga-2f0f976.scm
  job_state = Q
  queue = batch
.
Error_Path = uga-2f0f976.scm:/home/zhuofei/MPIs/testJob.e481939
.
Join_Path = oe
.
Mail_Points = abe
Mail_Users = zhuofei@uga.edu
.
Output_Path = uga-2f0f976.scm:/home/zhuofei/MPIs/testJob.o481939
.
Resource_List.mem = 20gb
.
Resource_List.nodes = 1:ppn=48:AMD
Resource_List.walltime = 48:00:00
Shell_Path_List = /bin/bash
Variable_List = PBS_O_QUEUE=batch, PBS_O_HOME=/home/zhuofei, . . .
euser = zhuofei
egroup = rccstaff
.
submit_args = sub.sh
```

# How to work with it – Run Jobs

- How to check queue status?  
*showq!*

```
[zhuofei@75-104 MPIs]$ showq
active jobs-----
JOBID                USERNAME            STATE  PROCS    REMAINING            STARTTIME
481914                brant               Running    1      20:46:21    Fri Jun 12 11:32:23
481915                brant               Running    1      20:48:56    Fri Jun 12 11:34:58
481567                becton              Running   288     2:04:15:48    Wed Jun 10 15:01:50
481857                kkim                Running    48     9:18:21:41    Fri Jun 12 09:07:43
481859                kkim                Running    48     9:18:42:21    Fri Jun 12 09:28:23
.
108 active jobs          5141 of 5740 processors in use by local jobs (89.56%)
                        121 of 122 nodes active          (99.18%)
eligible jobs-----
481821                joykai              Idle      48     50:00:00:00    Thu Jun 11 13:41:20
481813                joykai              Idle      48     50:00:00:00    Thu Jun 11 13:41:19
481811                joykai              Idle      48     50:00:00:00    Thu Jun 11 13:41:19
481825                joykai              Idle      48     50:00:00:00    Thu Jun 11 13:41:20
.
50 eligible jobs
blocked jobs-----
JOBID                USERNAME            STATE  PROCS    WCLIMIT            QUEUE TIME
0 blocked jobs
Total jobs: 158
```

Thank You for Your Attention!

A solid blue horizontal bar spans the entire width of the slide at the bottom.