Introduction to HPC Using the New Cluster at GACRC

Georgia Advanced Computing Resource Center
University of Georgia
Zhuofei Hou, HPC Trainer
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?

- **G**eorgia **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 (**OVPIT**)
- 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)
- http://gacrc.uga.edu/help/ (Web Help)
- https://wiki.gacrc.uga.edu/wiki/Getting_Help (Wiki Help)

GACRC Users September 2015

Colleges & Schools	Depts	PIs	Users
Franklin College of Arts and Sciences	14	117	661
College of Agricultural & Environmental Sciences	9	29	128
College of Engineering	1	12	33
School of Forestry & Natural Resources	1	12	31
College of Veterinary Medicine	4	12	29
College of Public Health	2	8	28
College of Education	2	5	20
Terry College of Business	3	5	10
School of Ecology	1	8	22
School of Public and International Affairs	1	3	3
College of Pharmacy	2	3	5
	40	214	970
Centers & Institutes	9	19	59
TOTALS:	49	233	1029

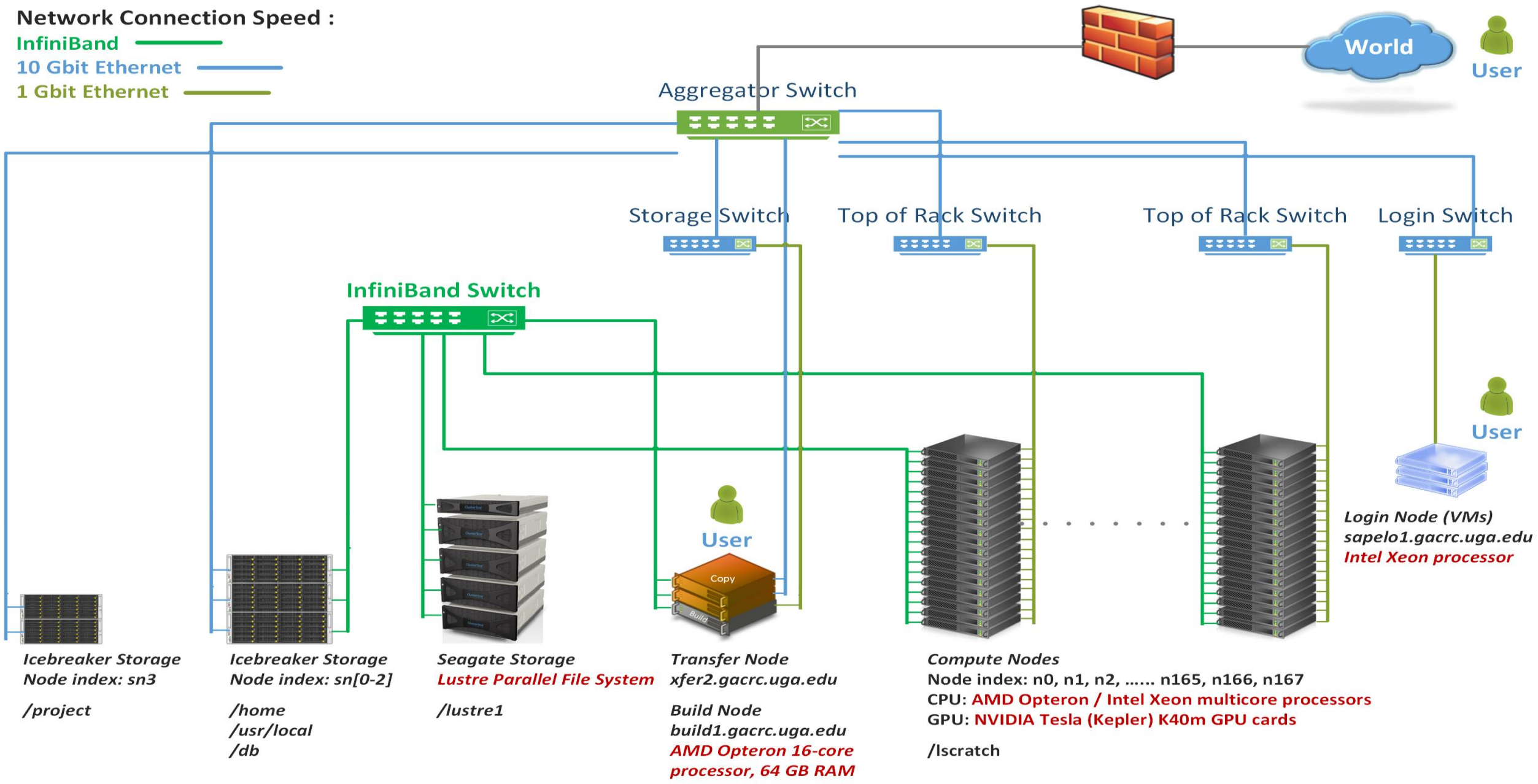
GACRC Users September 2015

Centers & Institutes	PIs	Users
Center for Applied Isotope Study	1	1
Center for Computational Quantum Chemistry	3	10
Complex Carbohydrate Research Center	6	28
Georgia Genomics Facility	1	5
Institute of Bioinformatics	1	1
Savannah River Ecology Laboratory	3	9
Skidaway Institute of Oceanography	2	2
Center for Family Research	1	1
Carl Vinson Institute of Government	1	2
	19	**59**

What is the new cluster at GACRC?

- Cluster Structural Diagram
- General Information
- Computing Resources

The New GACRC Linux HPC Cluster Structural Diagram



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
- User can login to:

  Login node: sapelo1.gacrc.uga.edu (for login & job submission)

  Transfer mode: xfer2.gacrc.uga.edu (for data transferring & compression)

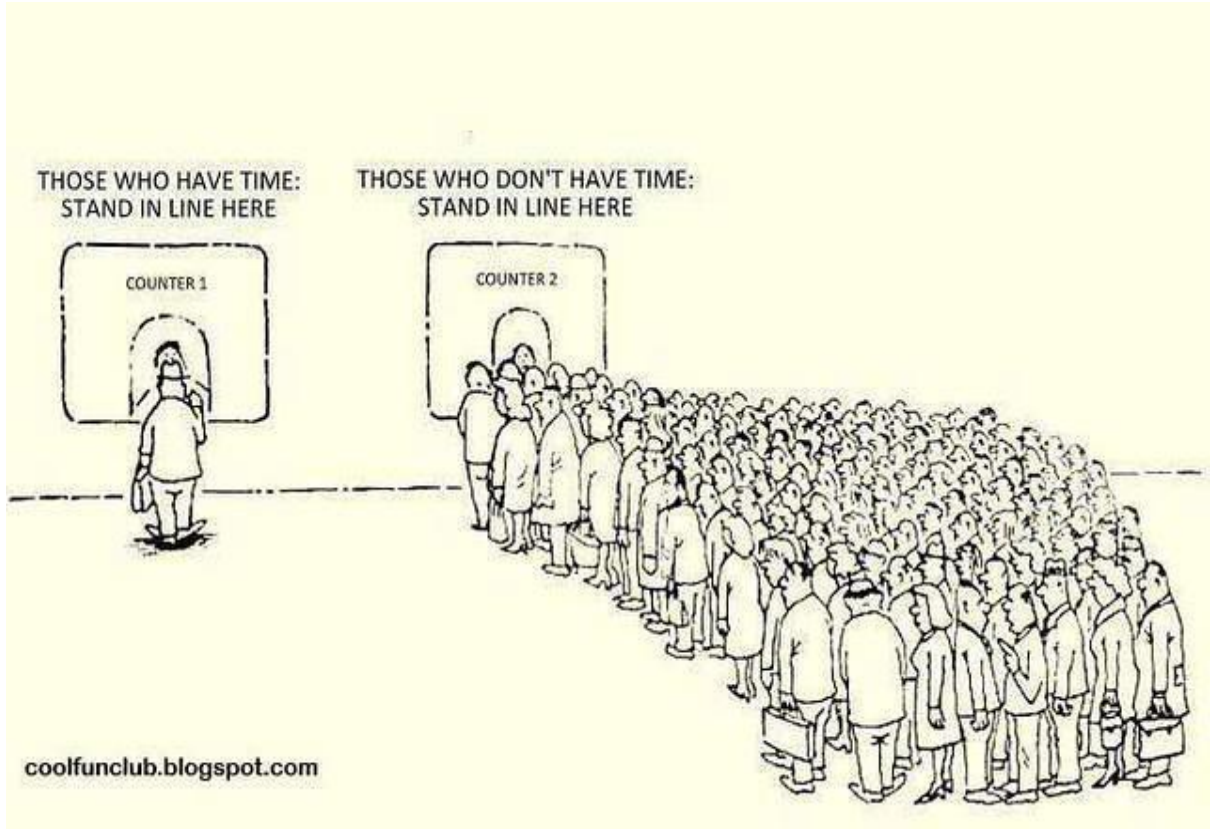
  Build node: build1.gacrc.uga.edu (for code compilation)
- **InfiniBand network** provides internodal communication:

  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	Max RAM can be Request /Single-node Job	GPU	GPU Cards /Node	InfiniBand
batch	AMD	120	AMD Opteron	48	128	126	N/A	N/A	Yes
	HIGHMEM	3	AMD Opteron	48	512 (2)	504	N/A	N/A	Yes
					1024 (1)	997			
	GPU	2	Intel Xeon	16	128	126	NVIDIA K40m	8	Yes
	abcnode (buy-in)	2	AMD Opteron	48	256	252	N/A	N/A	Yes

Peak Performance per Node: 500Gflops/Node

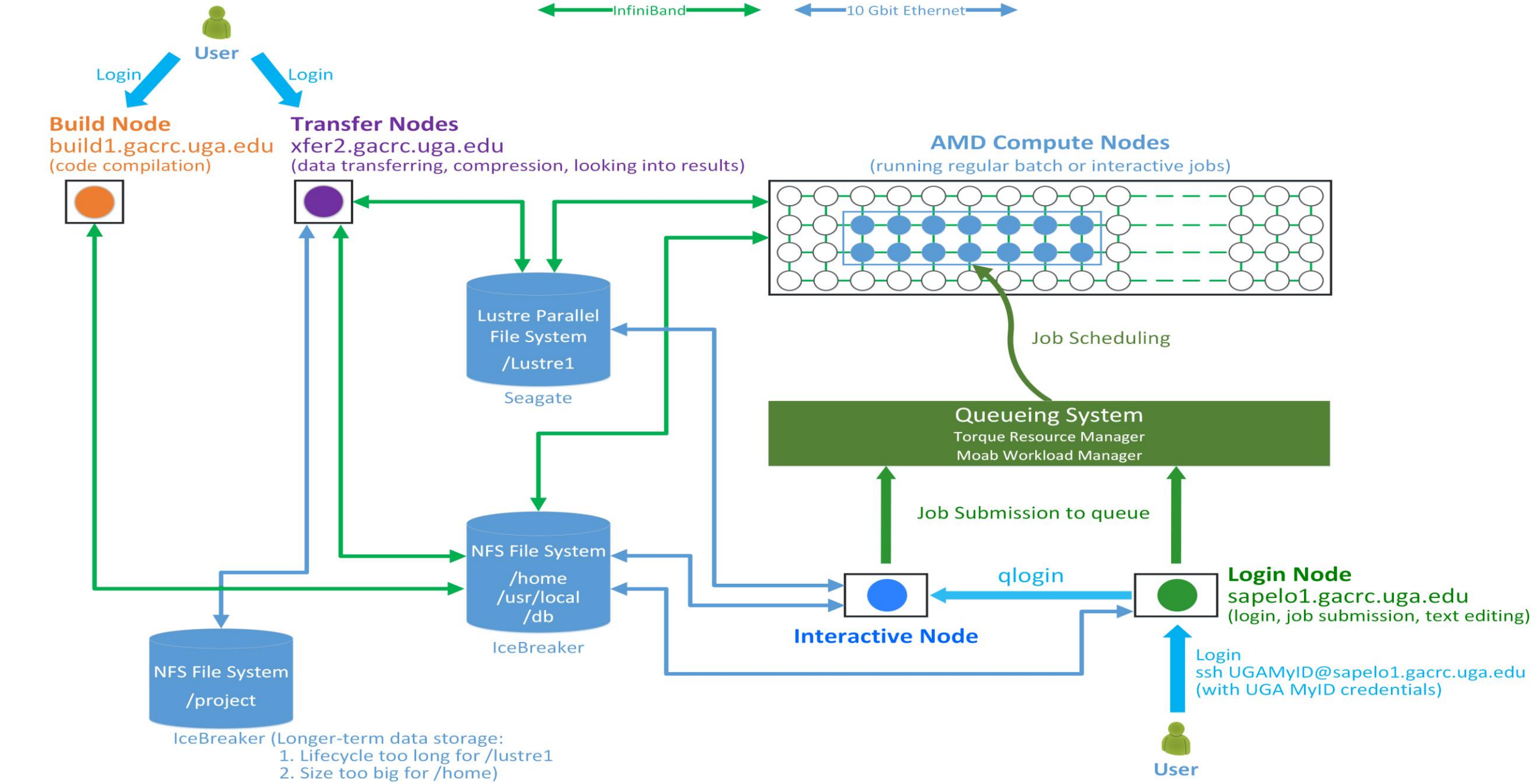
Home directory: 100GB

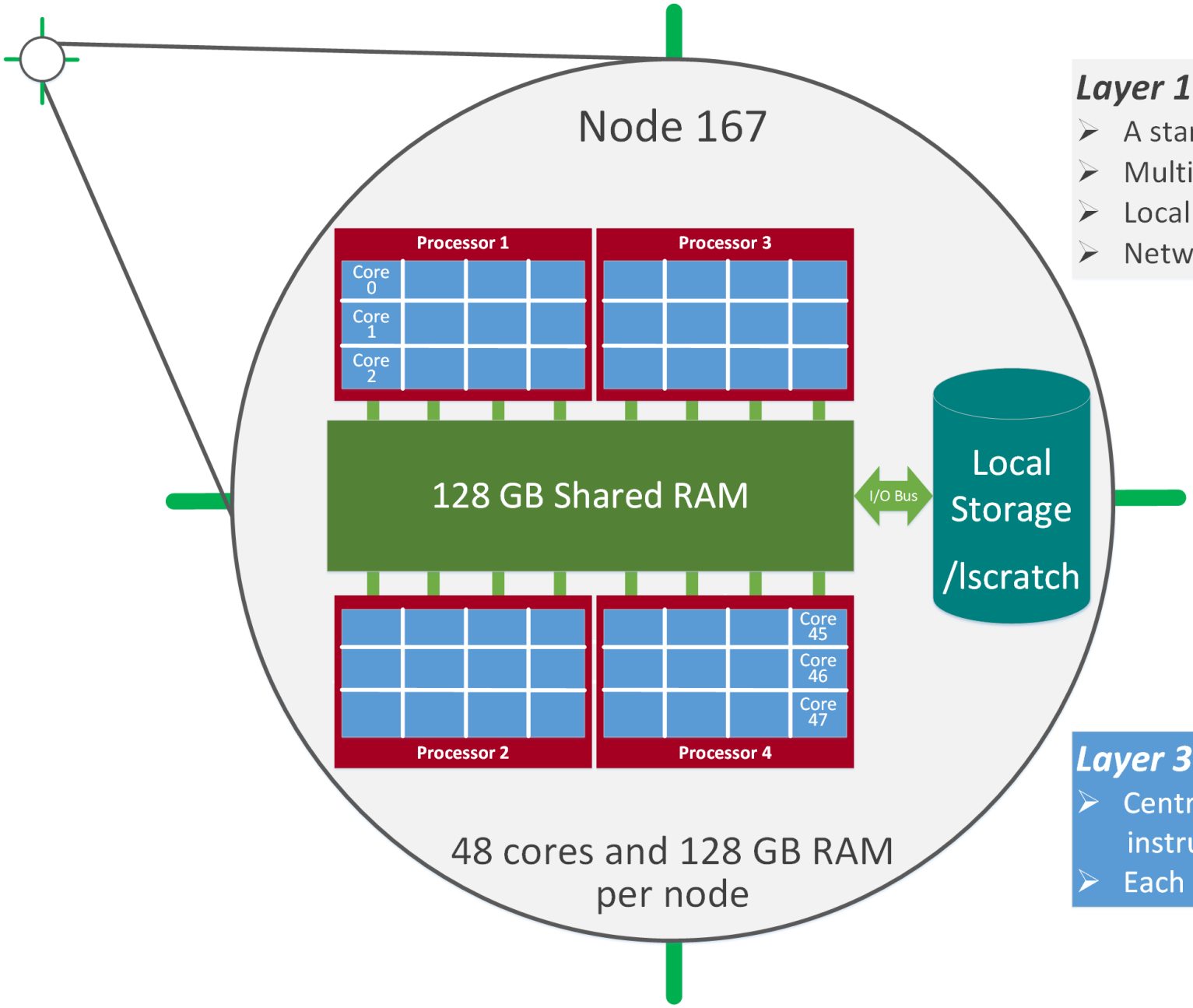
Scratch directory on /lustre1: NO quota limit, auto-moved to /project if no modification in 30 days!

How does it operate?

Next Page

The New GACRC Linux HPC Cluster Operational Diagram





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)
- 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:

- 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@sapelo1.gacrc.uga.edu

  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 4 steps:

1. New user training (http://gacrc.uga.edu/help/training/)
2. Tell us your Name, UGA MyID, Lab name and PI's name, via GACRC Support (https://wiki.gacrc.uga.edu/wiki/Getting_Help)
3. We send you an invitation letter with instructions to start account initialization
4. With Step 3 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@sapelo1.gacrc.uga.edu
```

or

```
ssh -X zhuofei@sapelo1.gacrc.uga.edu
```

([1] `-X` is for X windows application running on the cluster to be forwarded to your local machine

[2] 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@sapelo1.gacrc.uga.edu's password:
```

([3] 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)     gsl/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, qdel
  - qstat -f, showjobs, showq 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 *sub.sh* running NCBI Blast +

```
#PBS -S /bin/bash                    → Linux shell (bash)
#PBS -q batch                        → Queue name (batch)
#PBS -N testBlast                    → Name of the job (testBlast)
#PBS -l nodes=1:ppn=1:AMD            → Number of nodes (1), number of cores/node (1), node type (AMD)
#PBS -l mem=20gb                     → Maximum amount of physical memory (20 GB) used by the job
#PBS -l walltime=48:00:00            → Maximum wall clock time (48 hours) for the job, default 6 minutes

cd $PBS_O_WORKDIR                    → Use the directory from which the job is submitted as the working directory

module load ncbiblast+/2.2.29        → Load the module of ncbiblast+, version 2.2.29

time blastn [options] > outputfile   → 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 *sub.sh* 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 ae
#PBS -j oe

cd $PBS_O_WORKDIR

module load ncbiblast+/2.2.29

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

➔ 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 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 *sub.sh* running RAxML with 50 MPI processes

```
#PBS -S /bin/bash
#PBS -q batch
#PBS -N testRAxML
#PBS -l nodes=2:ppn=48:AMD
#PBS -l walltime=480:00:00
#PBS -l mem=20gb
#PBS -j oe

cd $PBS_O_WORKDIR

module load raxml/8.1.20
module load intel/15.0.2
module load openmpi/1.8.3/intel/15.0.2

mpirun –np 50 raxmlHPC-MPI-AVX [options] > outputfile
```

➔ Number of nodes (2), number of cores/node (48), node type (AMD)
Total cores requested = 2 × 48 = 96
We suggest, Number of MPI Processes (50) ≤ Number of cores requested (96)

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

➔ Run raxmlHPC-MPI-AVX with 50 MPI processes (–np 50)

```
#PBS -S /bin/bash
#PBS -q batch
#PBS -N testRAxML
#PBS -l nodes=2:ppn=27:AMD
#PBS -l walltime=480:00:00
#PBS -l mem=20gb
#PBS -j oe

cd $PBS_O_WORKDIR

# Context Sharing
CONTEXTS=$(/usr/local/bin/set_contexts.sh $PBS_NUM_PPN)
if [[ "$?" -eq "0" ]] ; then
  export PSM_SHAREDCONTEXTS_MAX=$CONTEXTS
fi

module load raxml/8.1.20
module load intel/15.0.2
module load openmpi/1.8.3/intel/15.0.2

mpirun –np 50 raxmlHPC-MPI-AVX [options] > outputfile
```

➔ ppn number (27) fewer than 48 MUST be a multiplier of 3!

New lines copied from GACRC Wiki

➔ 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 1h
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
```

← Stay on list 1 hr

How to work with it – Run Jobs

- How to check computing resources? ***qstat -f JobID*** for a *running job* or a *finished job in 1 hour)*

```
[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
```

How to work with it – Run Jobs

- How to check computing resources? ***showjobs JobID*** for a *finished job over 1 hour, but no longer than 7 days)*

```
[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
```

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            QUEUETIME

0 blocked jobs

Total jobs:  158
```

Thank You!