Georgia Advanced Computing Resource Center
UNIVERSITY OF GEORGIA

Introduction to HPC Using Sapelo Cluster at GACRC

Georgia Advanced Computing Resource Center

EITS/University of Georgia

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Outline

- GACRC
- Sapelo Cluster
- Job Submission Workflow
- Work with Sapelo
- Guideline and Practical Tips

GACRC

Who Are We?

- Georgia Advanced Computing Resource Center
- 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)

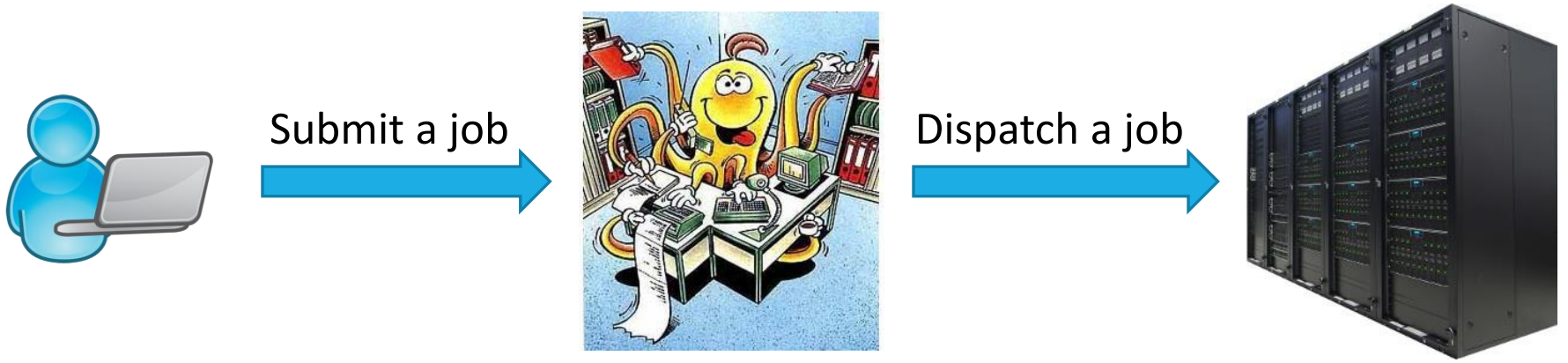
Sapelo Cluster

- Cluster Diagrams
- Cluster Overview
- Computing Resources
- Storage Environment

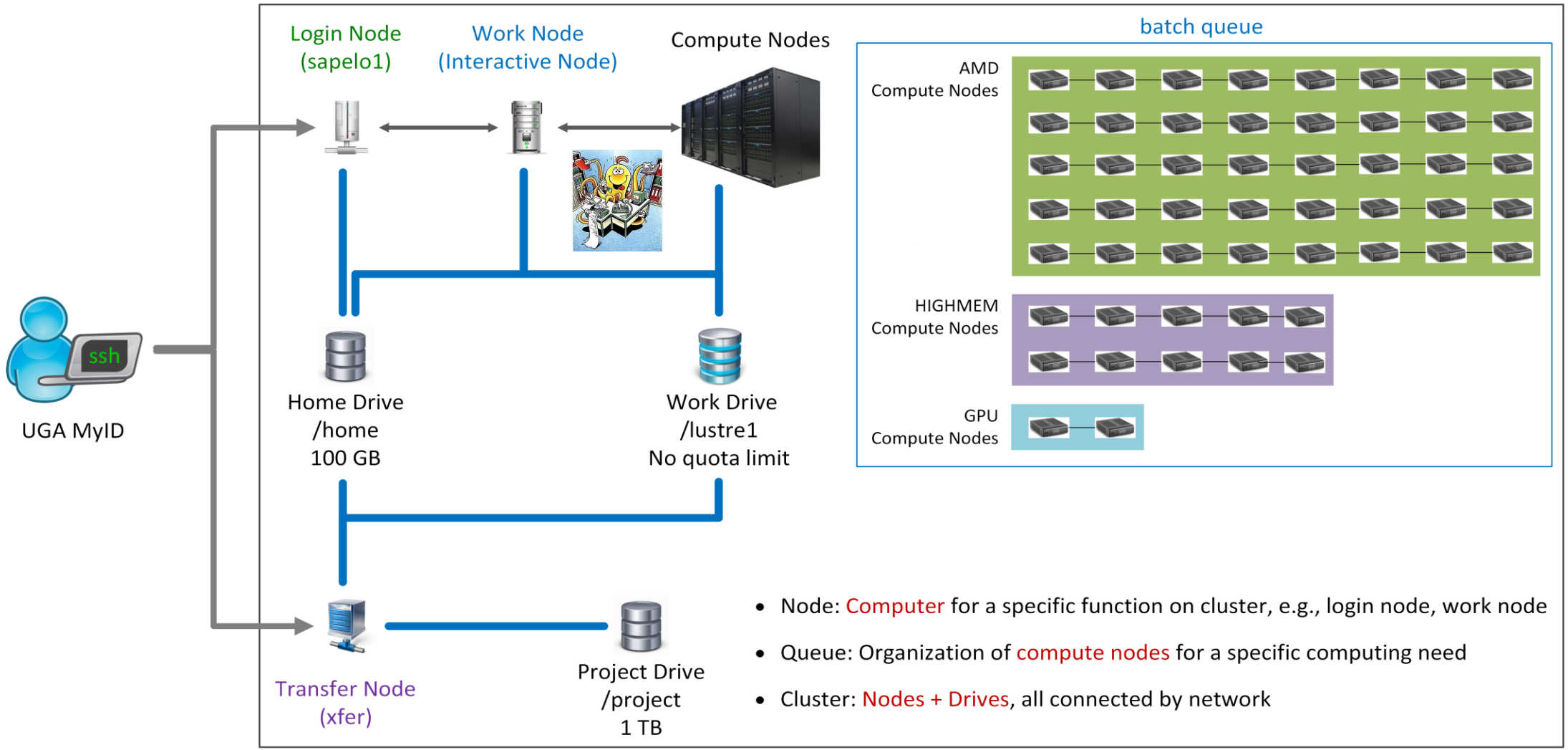
What is a Cluster?

When you work on cluster, 3 roles are working:

- User: to submit a job
- Queueing System: to dispatch a job to run on cluster
- Cluster: to run a job

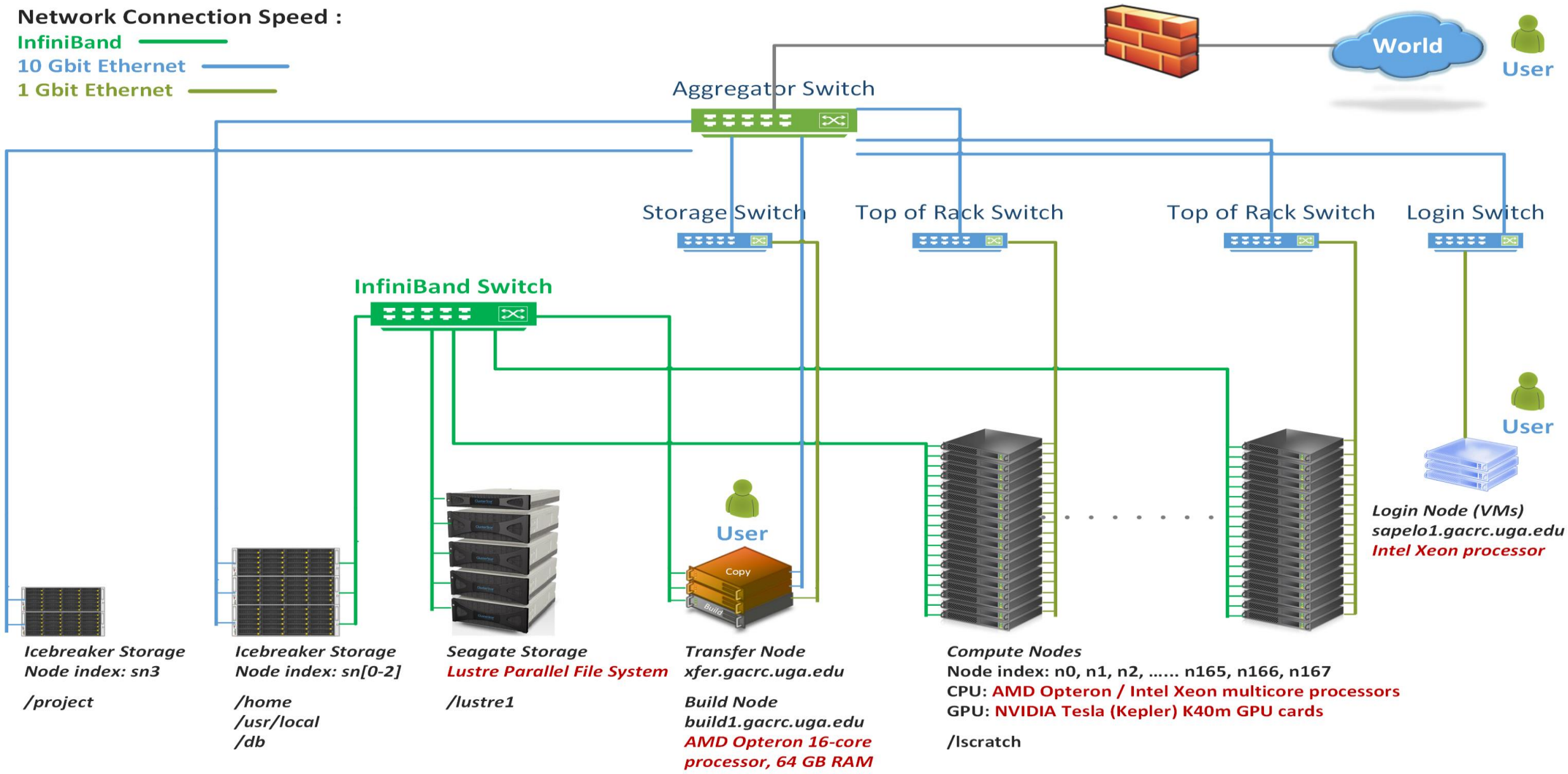


Sapelo Cluster Diagram



- Node: Computer for a specific function on cluster, e.g., login node, work node
- Queue: Organization of compute nodes for a specific computing need
- Cluster: Nodes + Drives, all connected by network

The New GACRC Linux HPC Cluster Structural Diagram



Cluster Overview

Sapelo is a Linux high-performance computing (HPC) cluster:

- OS: 64-bit CentOS Linux 6.5
- You can log on to:

  Login (username@sapelo1.gacrc.uga.edu) : edit script, submit batch job

  Transfer (username@xfer.gacrc.uga.edu) : transfer, compress, package data

  Build (username@build1.gacrc.uga.edu) : compile, test

- Login → (qlogin) → Work Node : edit script, submit batch job, run interactive job
- Internodal Communication: **InfiniBand network**

  compute nodes ⇔ compute nodes ⇔ storage systems, e.g., /home and /lustre1

Cluster Overview

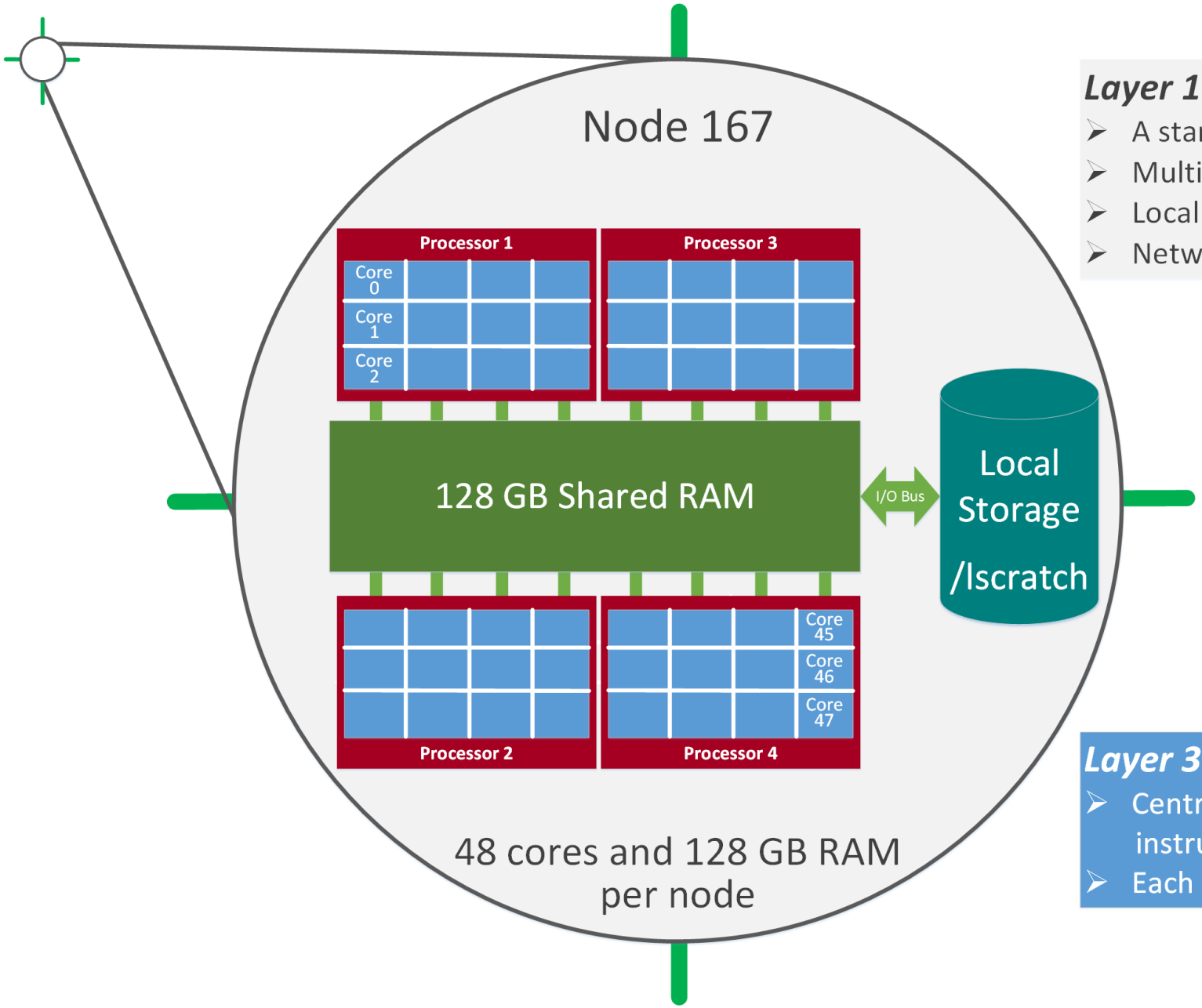
- Batch-queueing System:
  - Jobs can be started (submitted), monitored, and controlled
  - Determine which compute node is the best place to run a job
  - Determine appropriate execution priority for a job to run
- On Sapelo:
  - Torque Resource Manager + Moab Workload Manager
  - Queueing commands: `qsub`, `qstat`, `qdel` `showjobs`, `showq`

Computing Resources

Queue	Node Feature	Total	Processor	Cores /Node	RAM (GB) /Node	Max RAM (GB) /Single-node Job	GPU	GPU Cards /Node	InfiniBand
batch	AMD	112	AMD Opteron	48	128	126	N/A	N/A	Yes
		4			256	252			
	HIGHMEM	7			512 (6)	504			
					1024 (1)	997			
	GPU	2	Intel Xeon	16	128	126	NVIDIA K40m	8	
	abcnode (buy-in)	2	AMD Opteron	48	256	252	N/A	N/A	

Home: /home/username: 100GB

Global scratch: /lustre1/username: NO quota limit, auto-moved to /project if no modification in 30 days!



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

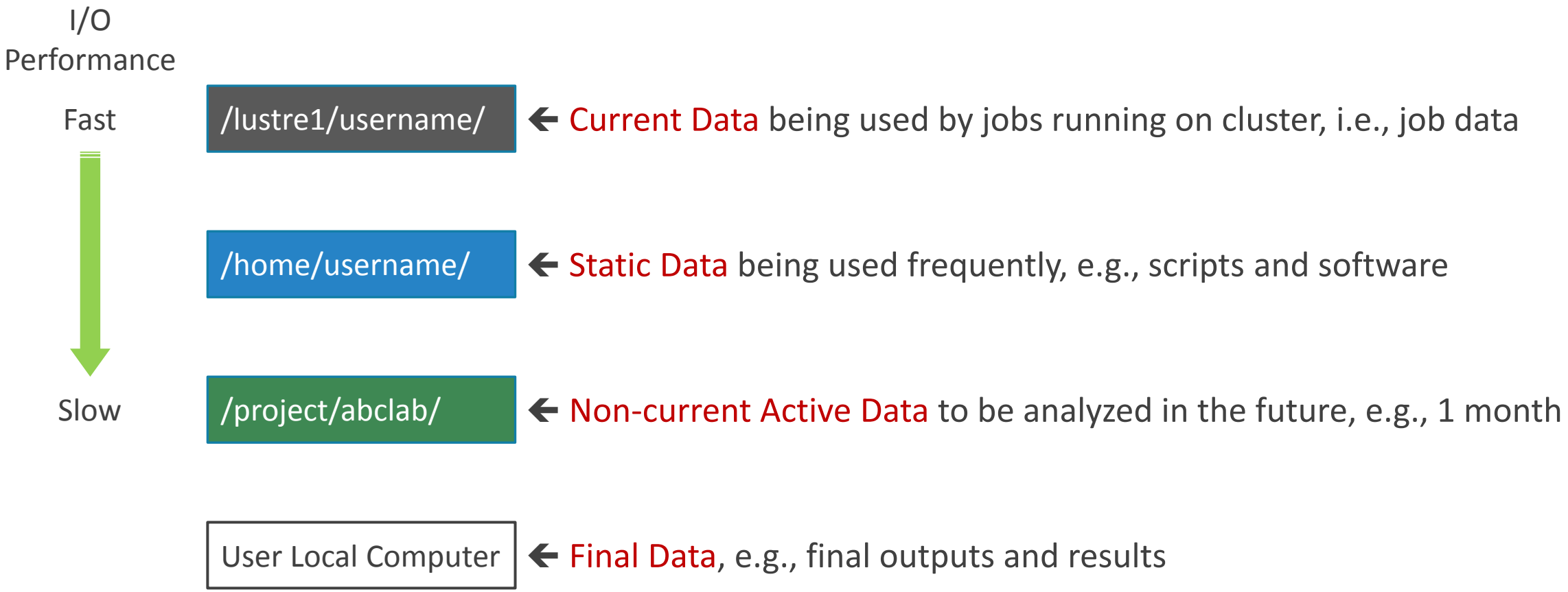
- Central processing unit (CPU) reading and executing instructions independently
- Each core is assigned to a software thread

Storage Environment

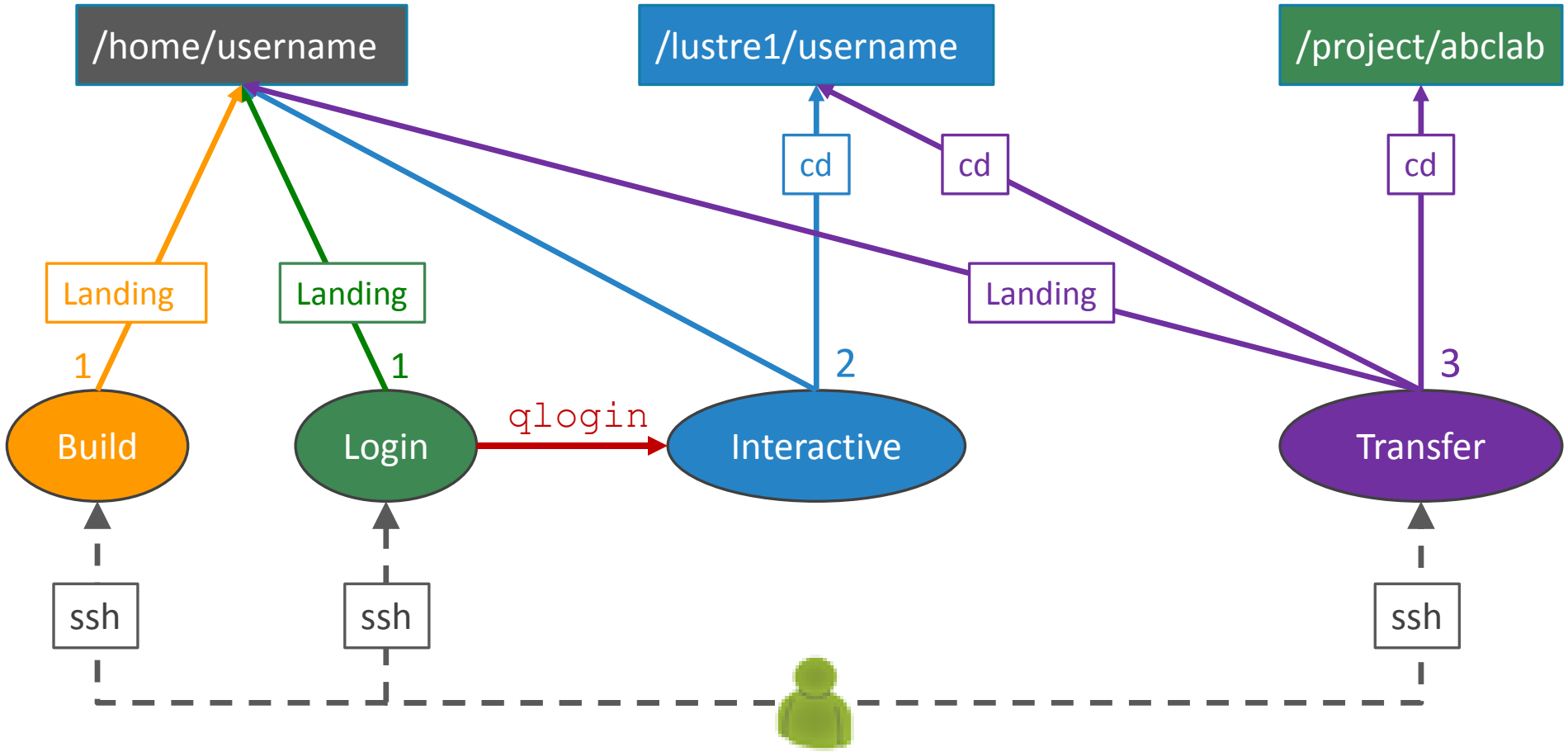
4 Filesystems	Role	Quota	Accessible from	Intended Use	Notes
/home/username/	Home	100GB	sapelo1.gacrc.uga.edu (Login) Interactive nodes (Interactive) xfer.gacrc.uga.edu (Transfer) build1.gacrc.uga.edu (Build) compute nodes (Compute)	Highly static data being used frequently, e.g., scripts, local software	Snapshots
/lustre1/username/	Global Scratch	No Limit	Interactive nodes (Interactive) xfer.gacrc.uga.edu (Transfer) compute nodes (Compute)	Temporarily storing large data being used by jobs	User to clean up
/lscratch/username/*	Local Scratch	250GB	Individual compute node	Jobs with heavy disk I/O	User to clean up
/project/abclab/	Storage	1TB (Initial)	xfer.gacrc.uga.edu (Transfer)	Long-term active data storage	Group sharing possible

Note: /usr/local/apps : Software installation directory ; /db : Bioinformatics database installation directory
* denotes component or policy to be implemented in the future

Storage Environment - *Data Storing Rule*



Storage Environment - *Accessing Rule of 123*



Storage Environment

7 Main Functions	On/From-Node	Related Filesystem
Login Landing	Login or Transfer or Build	/home/username (Home) (Always!)
Batch Job Submitting	Login	/home/username (Home)
	Interactive	/lustre1/username (Scratch) (Suggested!) /home/username (Home)
Interactive Job Running		/lustre1/username (Scratch) /home/username (Home)
Data Transferring, Archiving , Compressing	Transfer	/lustre1/username (Scratch) /home/username (Home)
Long-term Active Data Storing		/project/abclab
Code Compilation, Test	Build	/home/username (Home)
Job Data Temporarily Storing	Compute	/lustre1/username (Scratch) /lscratch/username (Local Scratch)*

Note: * denotes component or policy to be implemented in the future

Job Submission Workflow

Job Working Space is Global Scratch: /lustre1/username/

- Why?

  No quota limit + The I/O fastest filesystem

- How to access?

  From Interactive Node, `cd /lustre1/username/`

- What need to pay attention?

  Clean up! Non-current Active Data ➔ /project/abclab/
  Non-active Data ➔ local storage

  } using Transfer Node

Job Submission Workflow

1. Linux/Mac user:

```
ssh username@sapelo1.gacrc.uga.edu
```

Windows user:

Login

2. `qlogin`

Interactive

3. `cd /lustre1/username`
4. `mkdir ./workDir`
5. `cd ./workDir`

lustre1

7. `nano ./sub.sh`

```
#PBS -S /bin/bash
#PBS -q batch
#PBS -N testBlast
#PBS -l nodes=1:ppn=1:AMD
#PBS -l mem=20gb
#PBS -l walltime=48:00:00
cd $PBS_O_WORKDIR
module load ncbiblast+/2.2.29
blastn [options] > outputfile
```

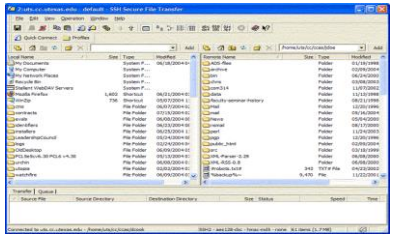
8.

```
$ qsub sub.sh
```

6. Linux/Mac user:

```
scp file username@xfer.gacrc.uga.edu:/lustre1/username/workDir
```

Windows user:



Note: `-r` option of scp command will recursively copy a directory

Useful PBS headers:

```
#PBS mem=200gb : use 256GB AMD nodes
ppn=24 : request 24 cores for 24 threads
```

Job Submission Workflow

1. Log on to Sapelo Login node: `ssh username@sapelo1.gacrc.uga.edu`
2. From Sapelo Login node, transfer to Interactive node by issuing the command: `qlogin`
3. From Interactive node: Change directory to global scratch: `cd /lustre1/username`
4. Create a working subdirectory on global scratch: `mkdir ./workDir`
5. Change directory to `workDir`: `cd ./workDir`
6. Transfer data to `workDir` using `scp` or SSH Client File Transfer (with `tar` or `gzip`)
7. Make a Sapelo job submission script: `nano ./sub.sh`
8. Submit job: `qsub ./sub.sh`

Useful PBS headers: `#PBS -l mem=200gb` : use 256GB high-RAM AMD nodes
`#PBS -l nodes=1:ppn=24:AMD` : request 24 cores for 24 threads, max 48!

Work on Sapelo

Before we start:

GACRC Wiki: http://wiki.gacrc.uga.edu

GACRC Support: https://wiki.gacrc.uga.edu/wiki/Getting_Help

Work on Sapelo

To submit a ticket to us?

- **Job Troubleshooting:**

  Please tell us details of your question or problem, including but not limited to:

  - ✓ Your user name
  - ✓ Your job ID
  - ✓ Your working directory
  - ✓ The queue name and command you used to submit the job

- **Software Installation:**

  - ✓ Specific name and version of the software
  - ✓ Download website
  - ✓ Supporting package information if have

Note:
It's USER's responsibility to make sure the correctness of datasets being used by jobs!

Work on Sapelo

- User Account
- Connect and Login
- Transfer Files Using Transfer Node
- Software Packages
- Run Interactive Jobs
- Run Batch Jobs
  - ✓ Submit Batch Jobs
  - ✓ ***Serial***, ***Threaded***, and ***MPI*** Batch Job Submission Scripts
  - ✓ Check Job Status and Cancel a Job
  - ✓ Check Computing Resources Used by a Job

User Account

- User Account: UGAMyID@sapelo1.gacrc.uga.edu
  A valid official UGA MyID is a MUST to create a user account! 

- To get a user account:

1. Computing Lab Registration: http://help.gacrc.uga.edu/labAcct.php (for PI of a new group)
2. User Account Request: http://help.gacrc.uga.edu/userAcct.php (for PI of an existing group)
3. New User Training: http://gacrc.uga.edu/help/training/
4. Welcome letter with whole package of information about your Sapelo user account

Connect and Login

- On Linux/Mac: use Terminal utility 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 with its UGI to be forwarded to local

[2] On Windows, use a *SSH client* to open the connection (next page))

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

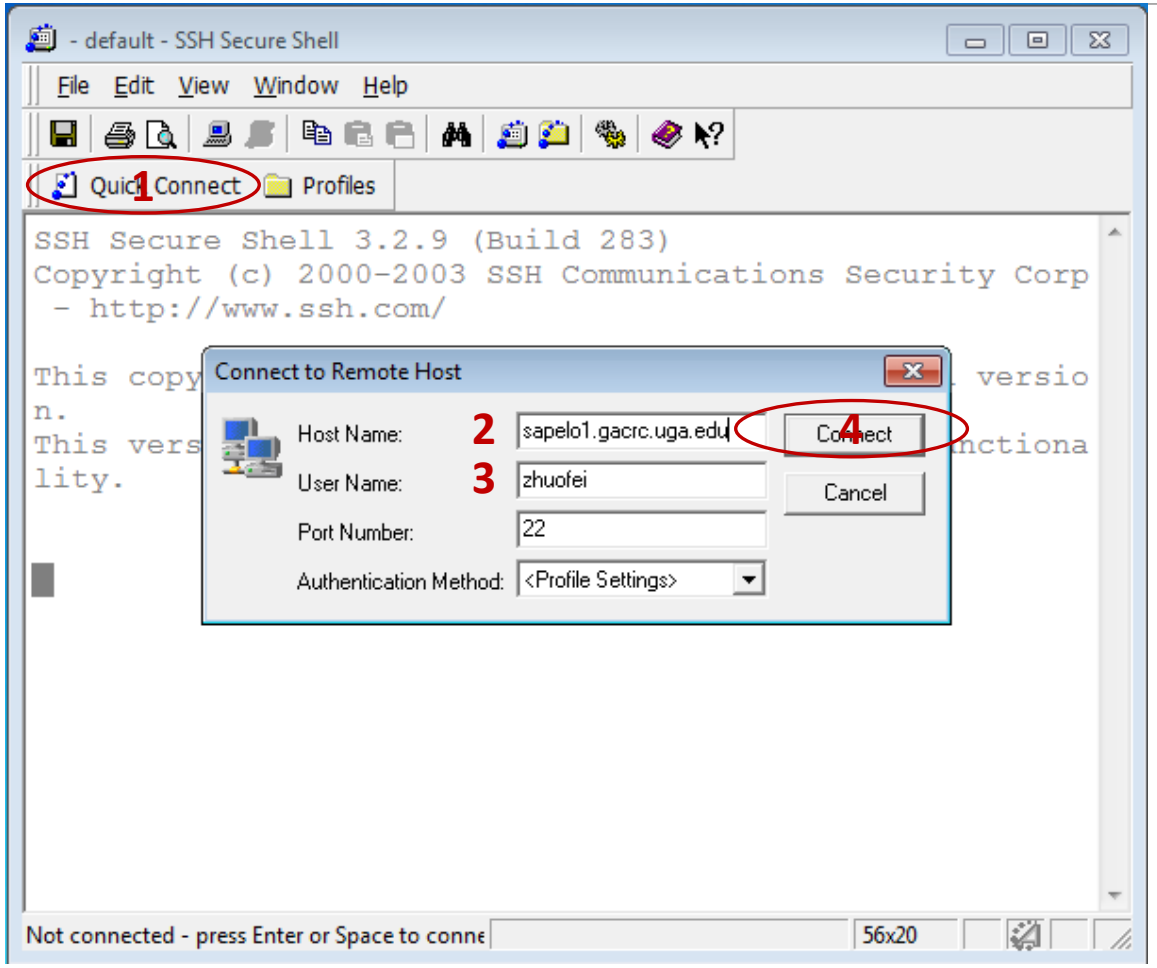
```
zhuofei@sapelo1.gacrc.uga.edu's password:
```

([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
```

Connect and Login



1. To download:

http://eits.uga.edu/hardware_and_software/software/

with your UGA MyID and password

2. After connection is built, working environment is Linux, same as Linux/Mac users'

Transfer Files Using Transfer Node xfer.gacrc.uga.edu

- ✓ `ssh username@xfer.gacrc.uga.edu` with your UGA MyID password
- ✓ Landing directory: `/home/username` (Sapelo home)
- ✓ Move data into/out of Sapelo (`scp`, `sftp`, `rsync`, SSH Secure Shell File Transfer, FileZilla)
- ✓ Compress or package data on Sapelo (`tar`, `gzip`)
- ✓ Transfer data between Sapelo and zcluster (`cp`, `mv`)
- ✓ Filesystems you can access:
  - /home/username/ : Sapelo home (landing spot)
  - /lustre1/username/ : Sapelo global scratch
  - /project/abclab/ : long-term active data storage
  - /panfs/pstor.storage/home/abclab/username/ : zcluster home
  - /escratch4/username/ : zcluster scratch
- ✓ Most file systems on Transfer are *auto-mounted* upon *the first time full-path access*, e.g., `cd /project/abclab/`

Transfer Files Using Transfer Node xfer.gacrc.uga.edu

User's local  

 Transfer (xfer.gacrc.uga.edu)

- On Linux, Mac or cygwin on Windows : `scp (-r) [Source] [Target]`

E.g. 1: working on local machine, from Local ➔ Sapelo global scratch

```
scp ./file zhuofei@xfer.gacrc.uga.edu:/lustre1/zhuofei/workDir/
```

```
scp -r ./folder/ zhuofei@xfer.gacrc.uga.edu:/lustre1/zhuofei/workDir/
```

E.g. 2: working on local machine, from Sapelo global scratch ➔ Local

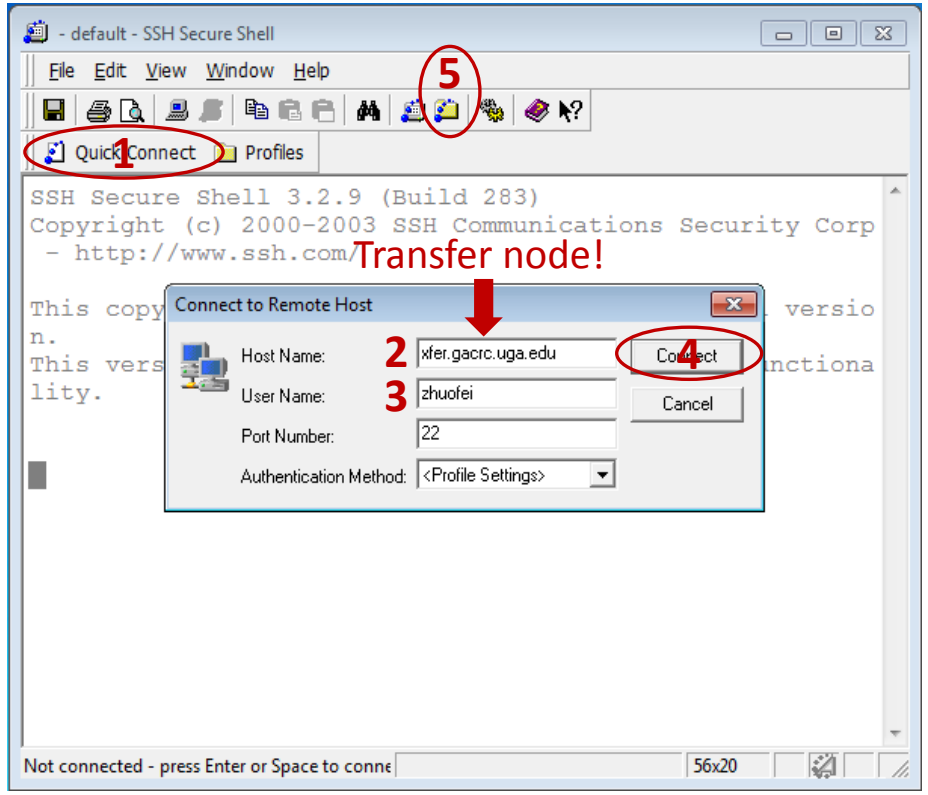
```
scp zhuofei@xfer.gacrc.uga.edu:/lustre1/zhuofei/workDir/file ./
```

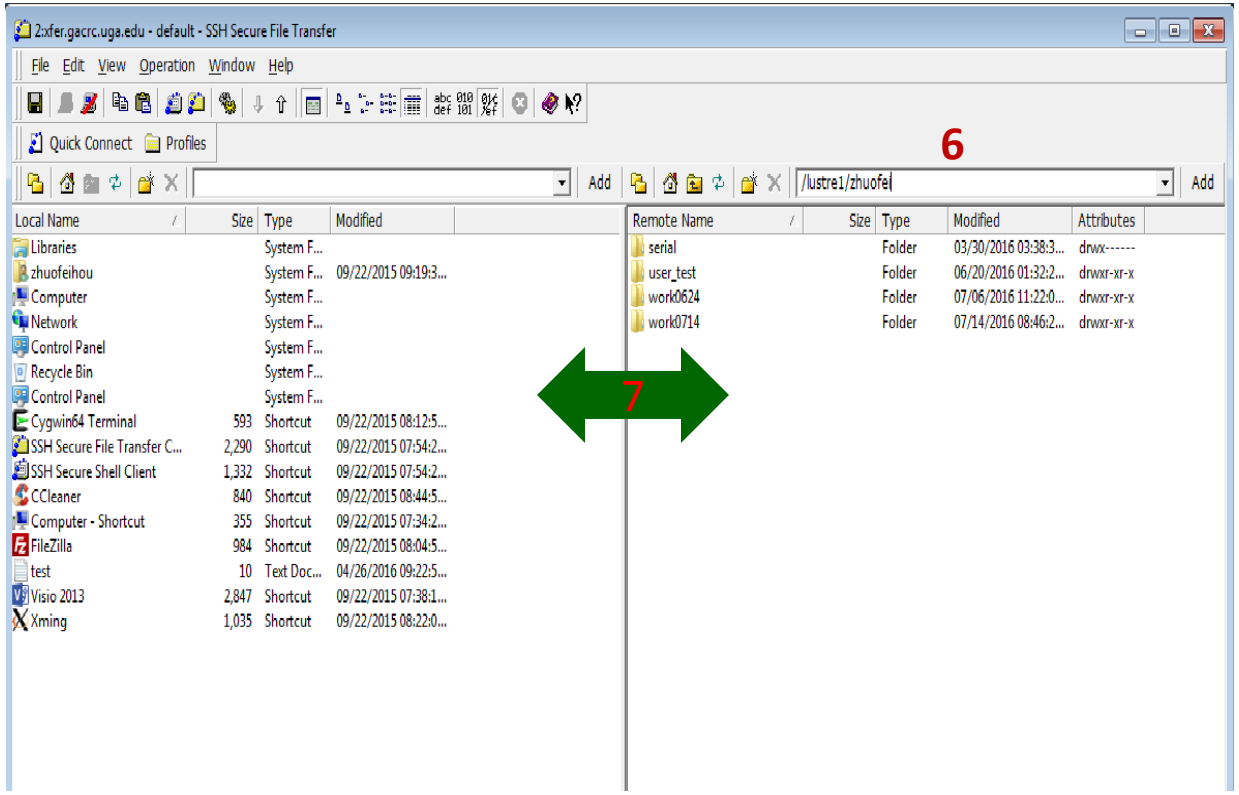
```
scp -r zhuofei@xfer.gacrc.uga.edu:/lustre1/zhuofei/workDir/folder/ ./
```

- On Window: SSH Secure Shell File Transfer, FileZilla, WinSCP (next page)

Transfer Files Using Transfer Node xfer.gacrc.uga.edu

User's local  SSH client  Transfer (xfer.gacrc.uga.edu)





Software Packages

- The cluster uses environment modules to define the various paths for software packages
- Current number of modules installed is ~300 and expanding daily!
- `module avail` to list all available modules (centralized installation):

```
[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
```

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
```

Run Interactive Jobs

- To run an interactive job, using `qlogin` command from Login node:

```
[zhuofei@75-104 ~]$ qlogin
qsub: waiting for job 1058157.pbs.scm to start
qsub: job 1058157.pbs.scm ready
[zhuofei@n14 ~]
[zhuofei@n14 ~]$ module load R/3.2.3
[zhuofei@n14 ~]$ R

R version 3.2.3 (2015-12-10) -- "Wooden Christmas-Tree"
Copyright (C) 2015 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)

...
[Previously saved workspace restored]

>
```

← Now I am on n14, which is an interactive node

- When you are done, remember to `exit` the session

Run Batch Jobs

- Components you need to run a job:
  - Software already loaded. If not, used `module load`
  - Job submission script to run the software, and specify 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

Submit Batch Jobs

```
[zhuofei@n15 workDir]$ pwd          ← n15: interactive node
/lustre1/zhuofei/workDir            ← /lustre1/zhuofei/: global scratch
[zhuofei@n15 workDir]$
[zhuofei@n15 workDir]$ qsub sub.sh
1165617.pbs.scm
```

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.

Example 1: Serial job script *sub.sh* running NCBI Blast +

```
#PBS -S /bin/bash
#PBS -q batch
#PBS -N testBlast
#PBS -l nodes=1:ppn=1:AMD
#PBS -l mem=20gb
#PBS -l walltime=48:00:00

cd $PBS_O_WORKDIR

module load ncbiblast+/2.2.29

time blastn [options] >outputfile 2>&1
```

- → Linux shell (bash)
- → Queue name (batch)
- → Name of the job (testBlast)
- → Number of nodes (1), number of cores/node (1), node type (AMD)
- → Maximum amount of physical memory (20 GB) used by the job
- → Maximum wall clock time (48 hours) for the job, default 6 minutes
- → Use the directory from which the job is submitted as the working directory
- → Load the module of ncbiblast+, version 2.2.29
- → Run blastn with 'time' command to measure the amount of time it takes to run the application

Example 1: Serial job script *sub.sh* running NCBI Blast +

```
#PBS -S /bin/bash
#PBS -q batch
#PBS -N testBlast
#PBS -l nodes=1:ppn=1:AMD
#PBS -l mem=200gb
#PBS -l walltime=48:00:00

cd $PBS_O_WORKDIR


module load ncbiblast+/2.2.29

time blastn [options] >outputfile 2>&1
```

➔ Job will be dispatched to run on AMD 256GB node

Example 2: Threaded job script *sub.sh* running NCBI Blast+

```
#PBS -S /bin/bash
#PBS -q batch
#PBS -N testBlast
#PBS -l nodes=1:ppn=24:AMD
#PBS -l mem=200gb
#PBS -l walltime=480:00:00

#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 24 [options] >outputfile 2>&1
```

➔ Number of nodes (1), number of cores/node (24), node type (AMD)
Number of threads (24) = Number of cores requested (24)

➔ Email address to receive a notification for computing resources
➔ Send email notification when job aborts (a) or terminates (e)
➔ Standard error file (testBlast.e1234) will be merged into standard out file (testBlast.o1234)

➔ Run blastn with 24 threads (-num_threads 24)

Example 3: MPI job script *sub.sh* running RAxML

```
#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

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 2>&1
```

➔ 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=20g

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 2>&1
```

➔ 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)

Check Job Status (`qstat`) and Cancel a Job (`qdel`)

```
[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

```
[jsmith@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
```

Check Computing Resources Used by a Job

Option 1: **`qstat -f JobID`** for ***running jobs*** or ***finished jobs in 1 hour***

Option 2: **`showjobs JobID`** for ***finished jobs over 1 hour, but ≤ 7 days***

Option 3: Email notification from ***finished jobs (completed, canceled, or crashed)***,

if using:

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

`qstat -f JobID` for running jobs or finished jobs in 1 hour

```
[zhuofei@75-104 MPIs]$ qstat -f 699847
Job Id: 699847.pbs.scm
    Job_Name = testJob
    Job_Owner = zhuofei@uga-2f0f976.scm
    resources_used.cput = 00:11:55
    resources_used.energy_used = 0
    resources_used.mem = 411572kb
    resources_used.vmem = 6548528kb
    resources_used.walltime = 07:01:36
    job_state = C
    queue = batch
     .
    Error_Path = uga-2f0f976.scm:/home/zhuofei/MPIs/testJob.e699847
    exec_host = n165/0-23
    Output_Path = uga-2f0f976.scm:/home/zhuofei/MPIs/testJob.o699847
     .
    Resource_List.mem = 5gb
    Resource_List.nodect = 1
    Resource_List.nodes = 1:ppn=24:AMD
    Resource_List.walltime = 10:00:00
     .
    Variable_List = PBS_O_QUEUE=batch,PBS_O_HOME=/home/zhuofei, …… ,
                    PBS_O_WORKDIR=/home/zhuofei/MPIs,
```

`showjobs JobID` for finished jobs over 1 hour, but ≤ 7 days

```
[zhuofei@75-104 MPIs]$ showjobs 699847
Job Id             : 699847.pbs.scm
Job Name           : testJob
Output File        : uga-2f0f976.scm:/home/zhuofei/MPIs/testJob.o699847
Error File         : uga-2f0f976.scm:/home/zhuofei/MPIs/testJob.e699847
Working Directory  : /home/zhuofei/MPIs
Home Directory     : /home/zhuofei
Submit Arguments   : sub.sh
User Name          : zhuofei
Group Name         : rccstaff
Queue Name         : batch
Wallclock Limit    : 10:00:00
Wallclock Duration: 07:01:36
CPUTime            : 00:11:55
Memory Used        : 401.9Mb
Memory Limit       : 5gb
vmem Used          : 6.2Gb
Submit Time        : Wed Nov  4 12:02:22 2015
Start Time         : Wed Nov  4 12:03:41 2015
End Time           : Wed Nov  4 12:04:45 2015
Exit Code          : 0
Master Host        : n165
```

Email notification from finished jobs

```
PBS Job Id: 700009.pbs.scm
Job Name:   testJob
Exec host:  n1/4-27
Execution terminated
Exit_status=0
resources_used.cput=00:05:12
resources_used.energy_used=0
resources_used.mem=410984kb
resources_used.vmem=6548516kb
resources_used.walltime=04:00:59
Error_Path: uga-
2f0f976.scm:/home/zhuofei/MPIs/testJob.o700009
Output_Path: uga-
2f0f976.scm:/home/zhuofei/MPIs/testJob.o700009
```

```
PBS Job Id: 700097.pbs.scm
Job Name:   testJob
Exec host:  n1/4-27
Execution terminated
Exit_status=271
resources_used.cput=00:11:22
resources_used.energy_used=0
resources_used.mem=412304kb
resources_used.vmem=6548524kb
resources_used.walltime=05:00:41
Error_Path: uga-
2f0f976.scm:/home/zhuofei/MPIs/testJob.o700097
Output_Path: uga-
2f0f976.scm:/home/zhuofei/MPIs/testJob.o700097
```

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
.
50 eligible jobs

blocked jobs-----------------------
JOBID              USERNAME      STATE PROCS     WCLIMIT            QUEUETIME

0 blocked jobs
Total jobs:  158
```

Guideline Tips

- Do NOT use Login Node to run jobs ➔ Interactive Node or the queue
- Do NOT use Login Node upload or download data to/from cluster
- Do NOT use Login Node to transfer data to the home dir

Transfer Node

- NO large memory job running on AMD nodes ➔ HIGHMEM nodes
- NO small memory job running on HIGHMEM nodes ➔ AMD nodes
- As a general rule, threads # = cores # requested

Practical Tips

- Each directory should not have too many files inside! A rule of thumb would be to try to keep no more than a few tens of thousands of files (<10000 would be even better) in any single directory which is accessed frequently.

All files are in ONE single dir!

Files are organized in subdirs!

Practical Tips

- Job name should have a specific computational meaning.

  Good Examples: `#PBS -N blastn_dataSet1_trail2 ; #PBS -N M-10-1121`

  Bad Examples: `#PBS -N job1 ; #PBS -N bowtie ; #PBS -N 20160930`

- Redirect standard output and error of the application to a file, instead of letting it be written in the stdout .o file and stderr .e file of the job, e.g.:

```
time application >file 2>&1
```

- Monitor job progress from time to time, to catch if a job gets stuck
- Batch job deletion to cancel all your running and waiting jobs from queue

```
qdel $(qstat | egrep '^[0-9]' | awk '$5!~/C/ {print $1}')
```

Useful Links

- GACRC Web: http://gacrc.uga.edu/
- GACRC Wiki: https://wiki.gacrc.uga.edu/wiki/Main_Page
- GACRC Help : http://gacrc.uga.edu/help/
- GACRC Training: https://wiki.gacrc.uga.edu/wiki/Training
- GACRC User Account: https://wiki.gacrc.uga.edu/wiki/User_Accounts
- GACRC Software: https://wiki.gacrc.uga.edu/wiki/Software

Georgia Advanced Computing Resource Center
4098C Stegeman Coliseum
University of Georgia
Athens, GA 30602

Telephone Support
EITS HELPDESK: 706-542-3106
MONDAY – THURSDAY: 8AM – 10PM
FRIDAY: 8AM – 6PM
SATURDAY – SUNDAY: 1PM – 7PM

Thank You!