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?

- **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)

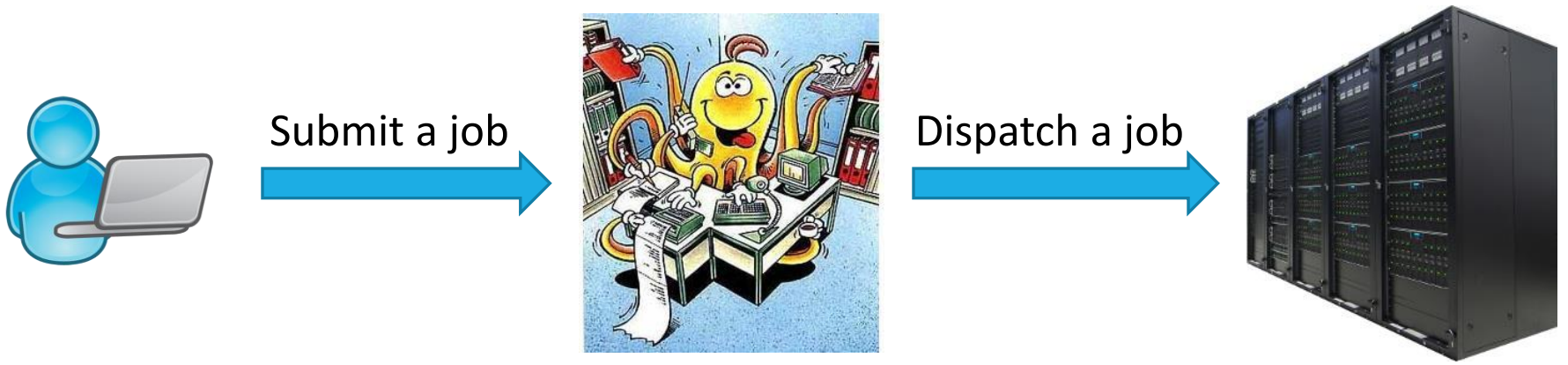
Sapelo Cluster

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

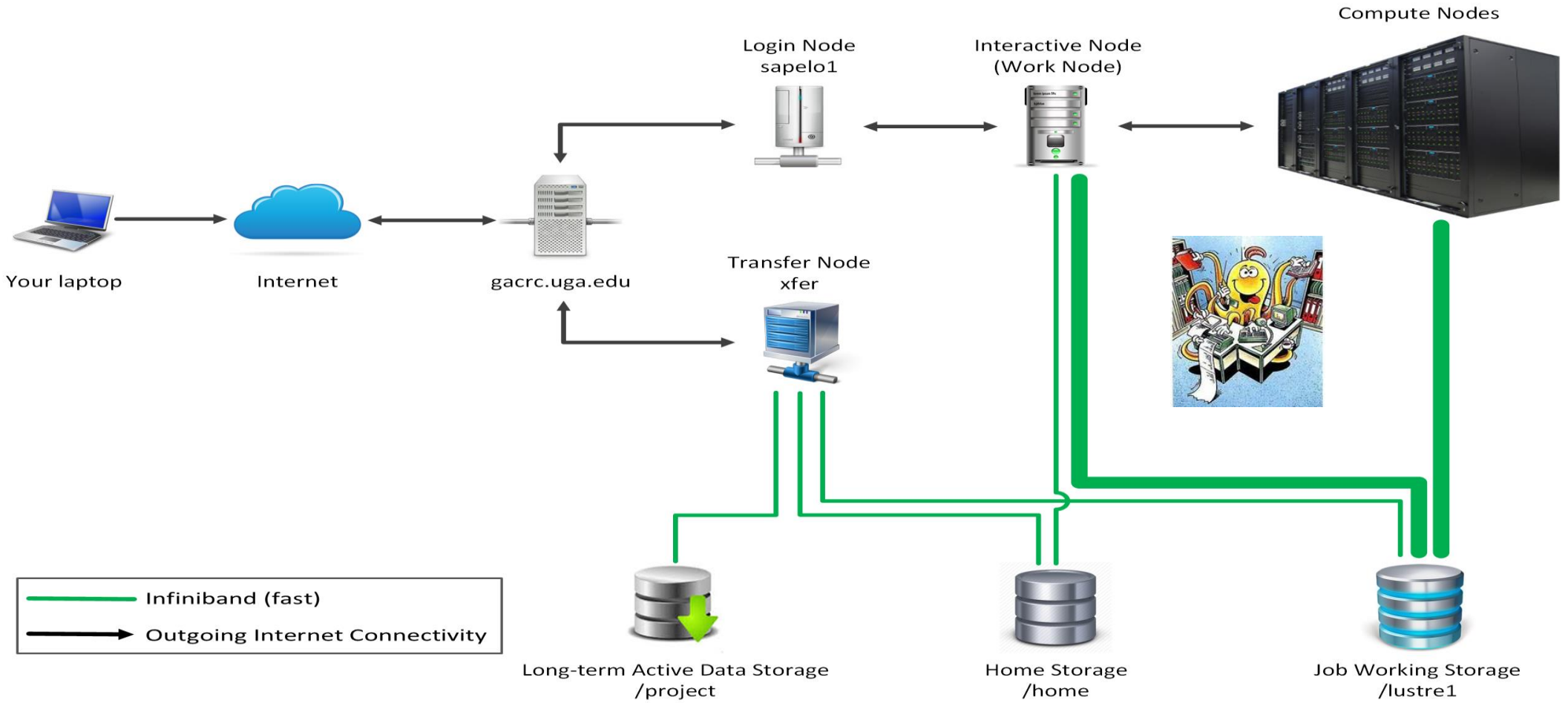
What is a Cluster?

When you work on cluster, 3 roles are working:

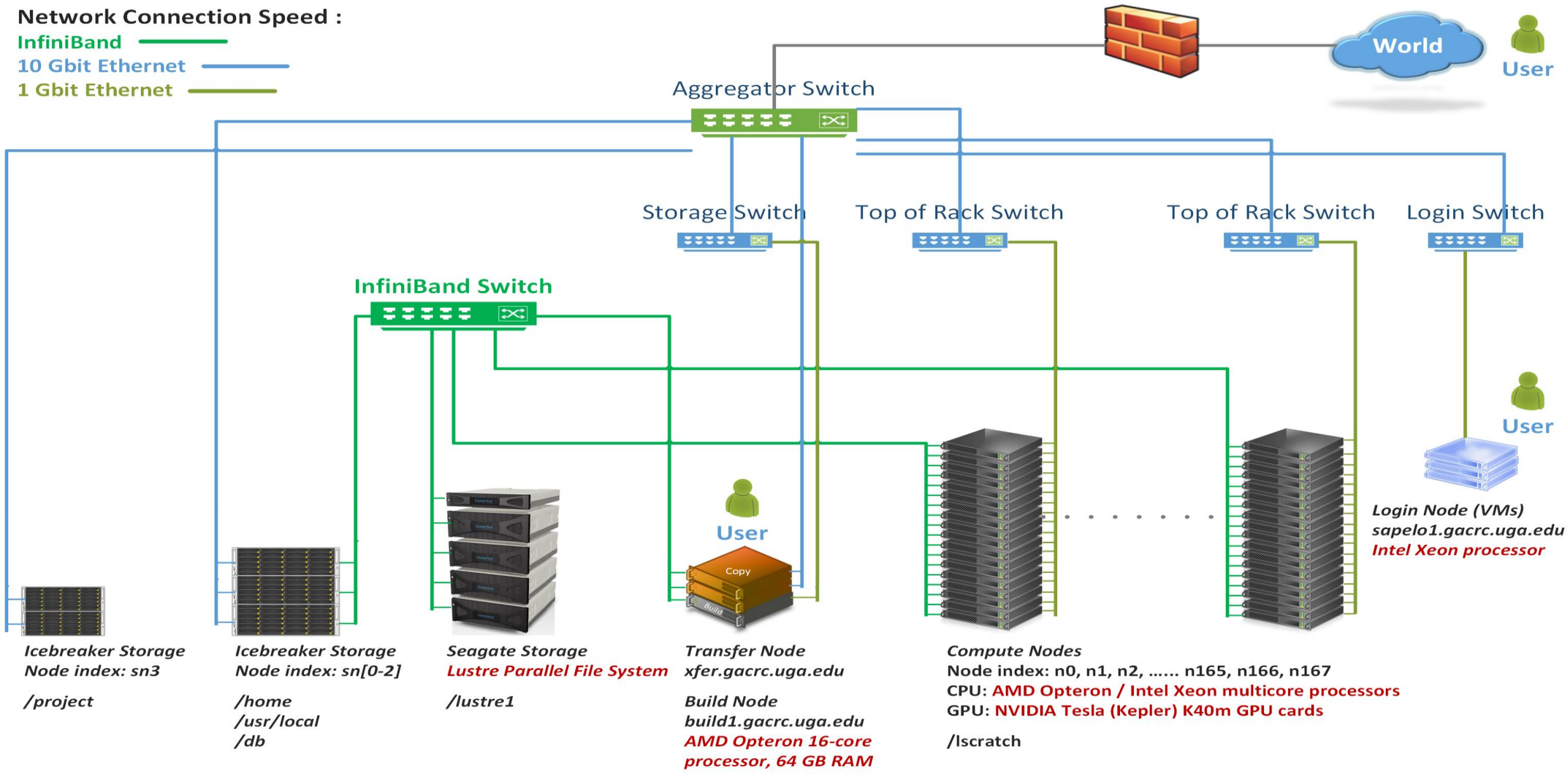
- You: Who submit a job
- Queueing System: Who dispatch your job to run on cluster
- Cluster: Who run your job



Sapelo Cluster Diagram



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

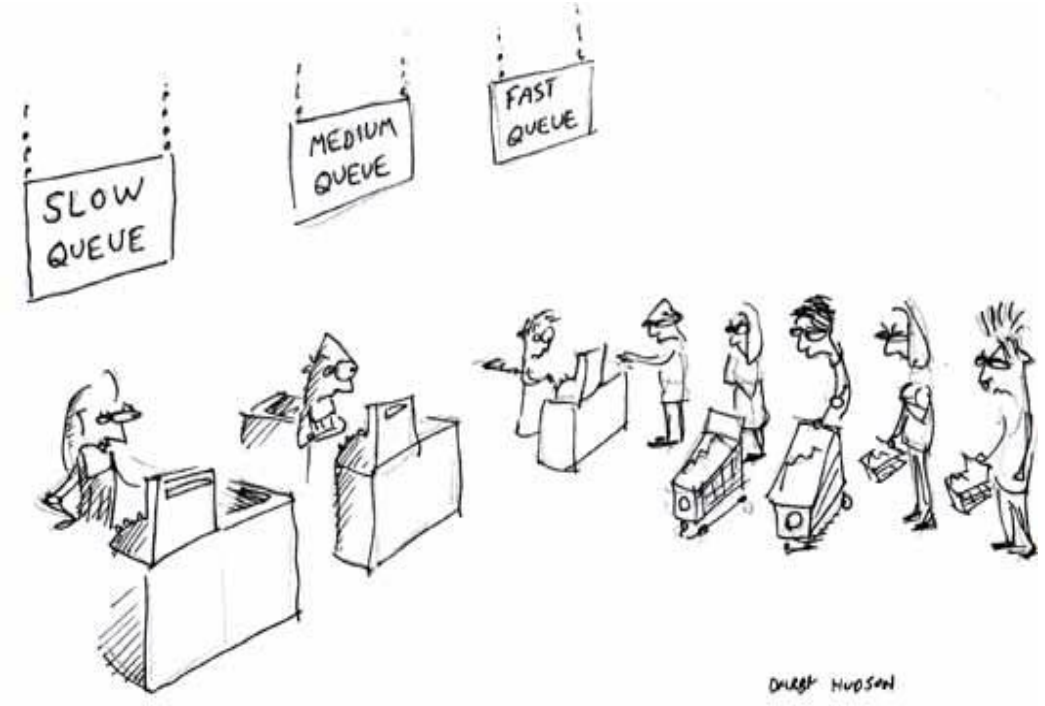
- Login → (qlogin) Interactive Node : edit script, submit batch job, run interactive job
- Internodal Communication: **InfiniBand network**

  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`

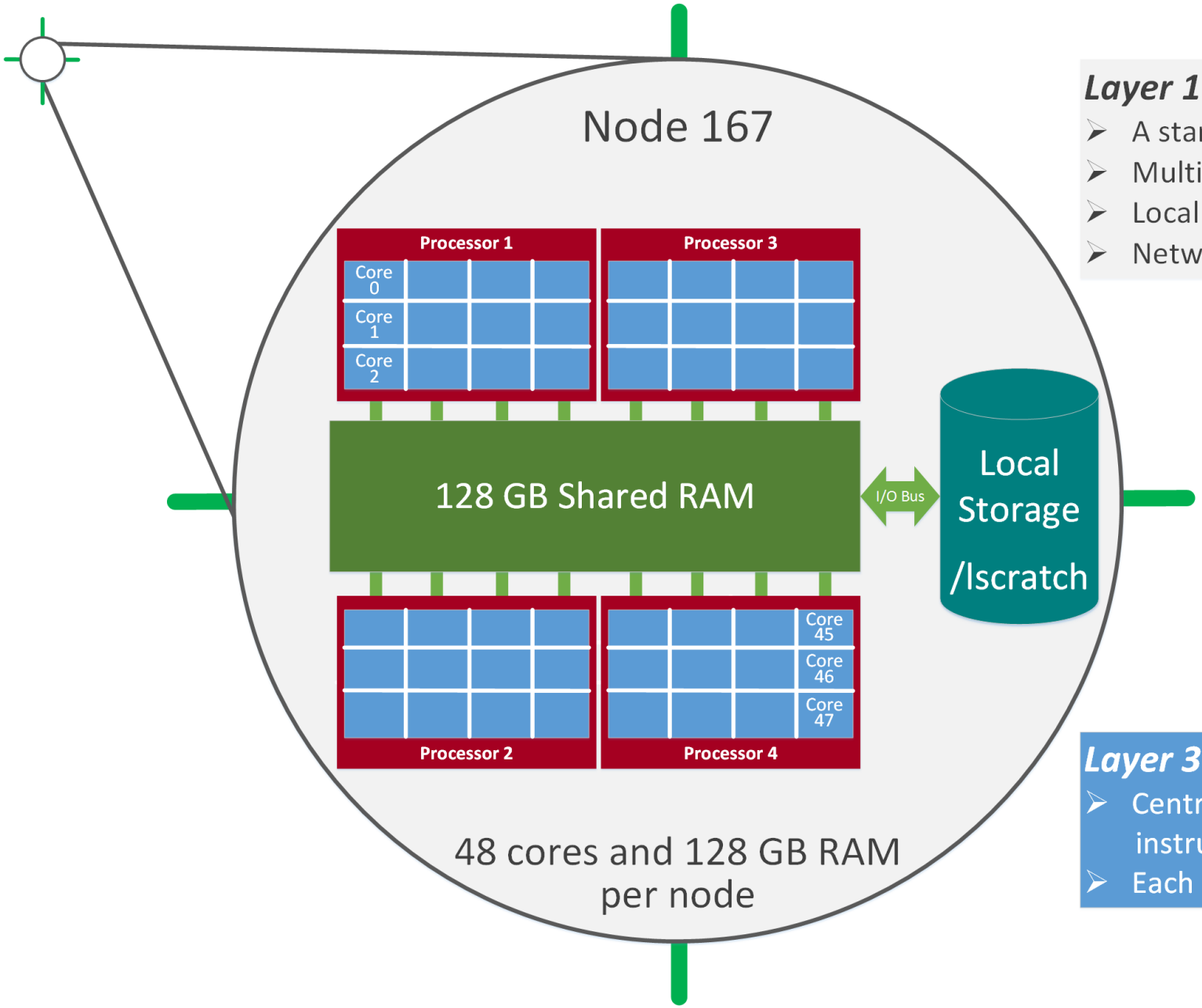


Computing Resources

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

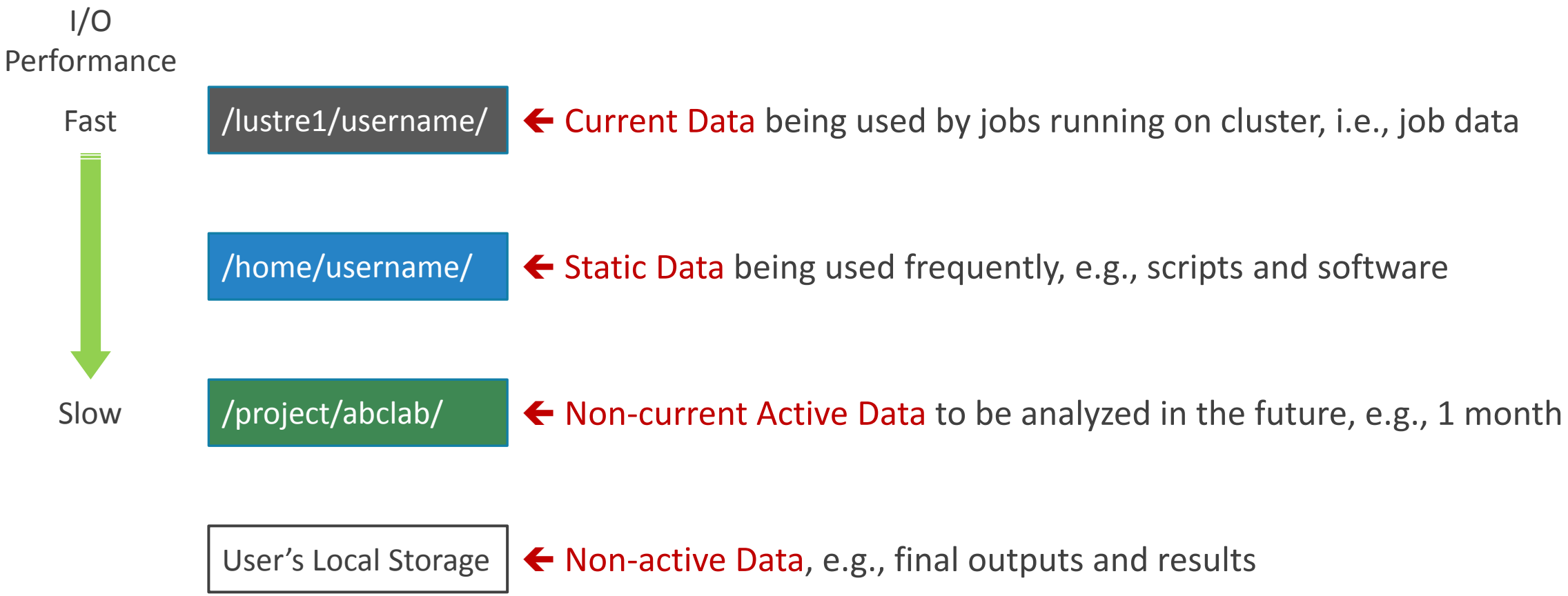
- Central processing unit (CPU) reading and executing instructions independently
- Each core is assigned to a software thread

Storage Environment

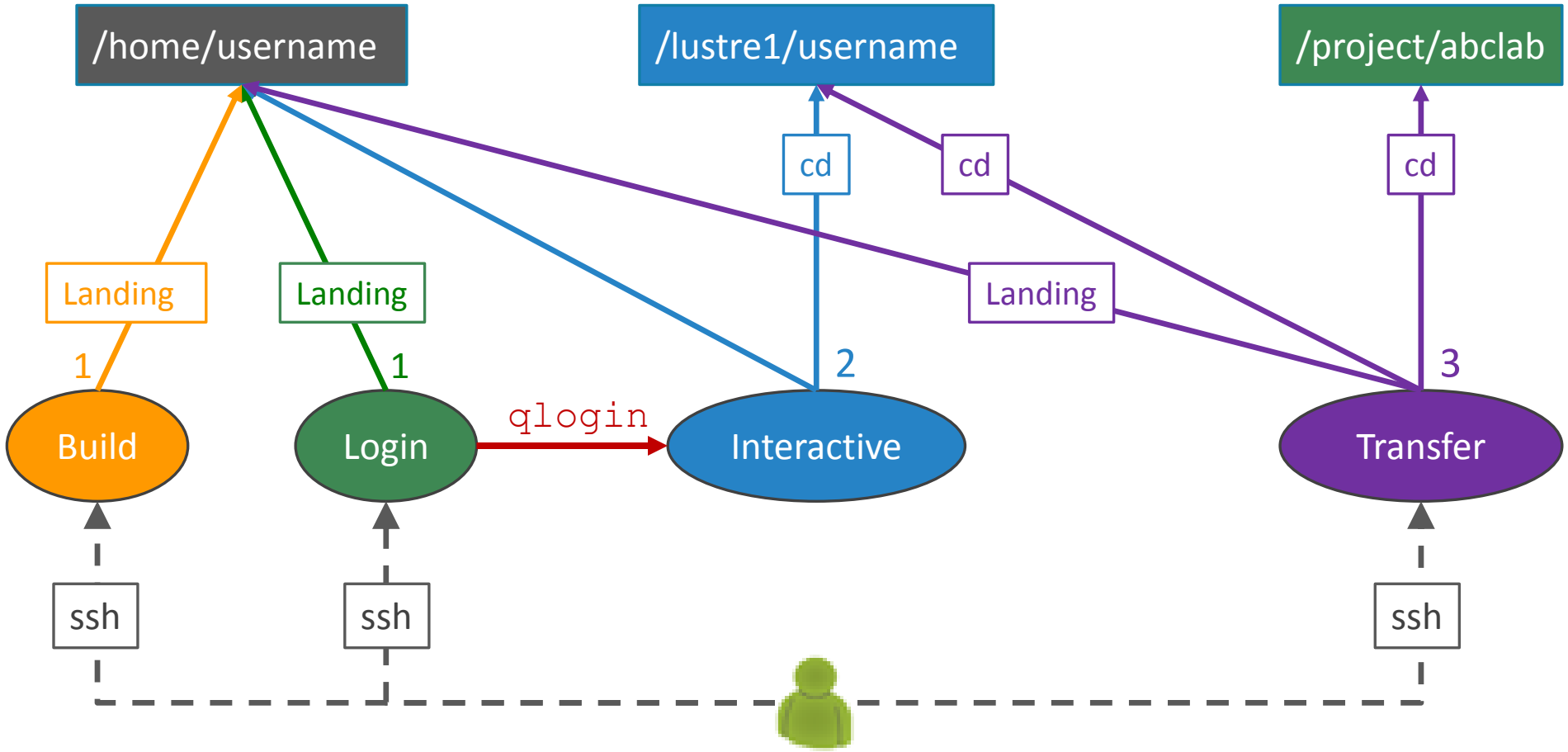
4 Filesystems	Role	Quota	Accessible from	Intended Use	Notes
/home/username/	Home	100GB	sapelo1.gacrc.uga.edu (Login) Interactive nodes (Interactive) xfer.gacrc.uga.edu (Transfer) build1.gacrc.uga.edu (Build) compute nodes (Compute)	Highly static data being used frequently, e.g., scripts, local software	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	Auto-moved to /project if 30 days no modification*
/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

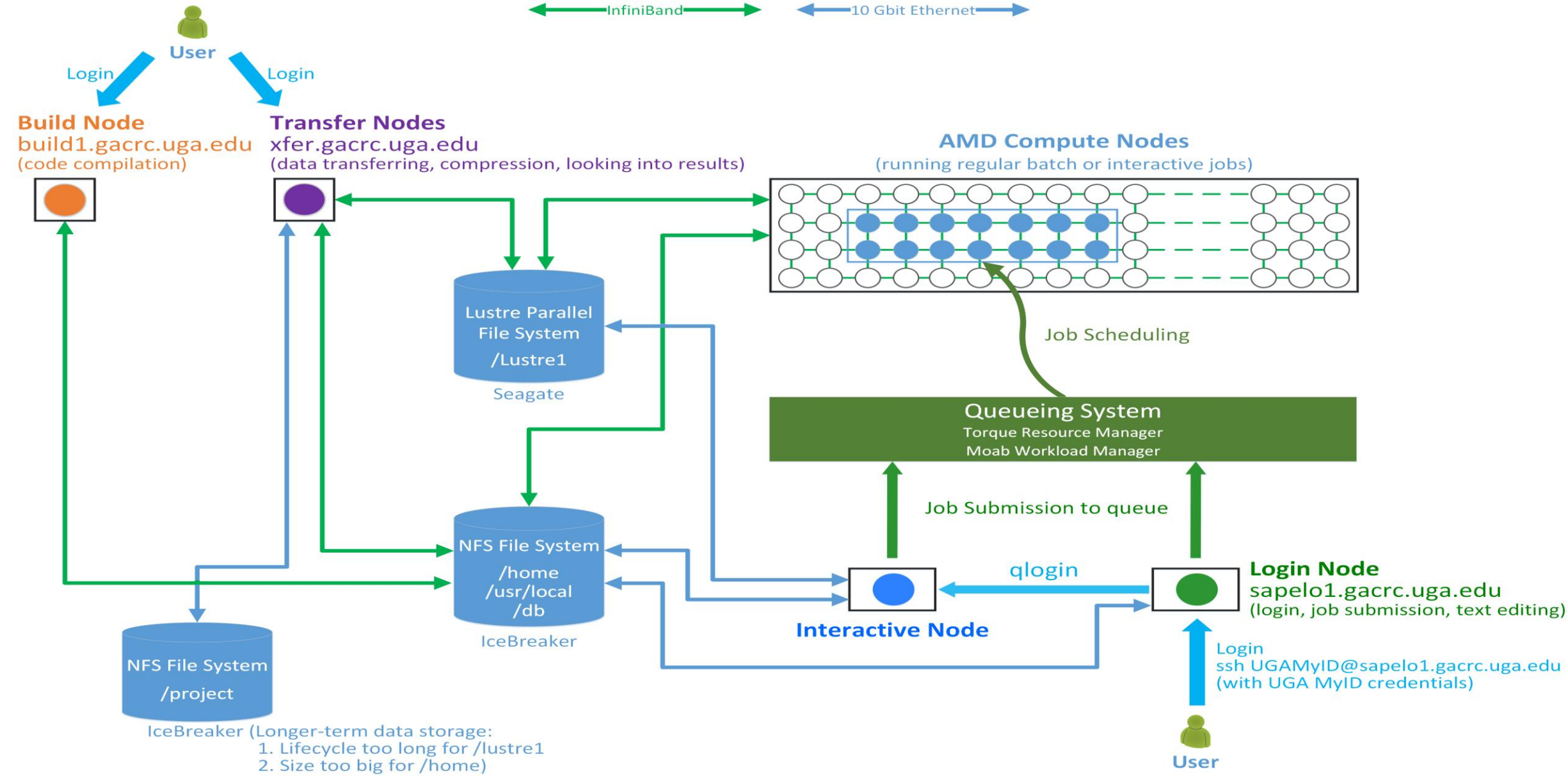
7 Main Functions	On/From-Node	Related Filesystem
Login Landing	Login or Transfer or Build	/home/username (Home) (Always!)
Batch Job Submitting	Login	/home/username (Home)
	Interactive	/lustre1/username (Scratch) (Suggested!) /home/username (Home)
Interactive Job Running		/lustre1/username (Scratch) /home/username (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

Next Page

The New GACRC Linux HPC Cluster Operational Diagram



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
```

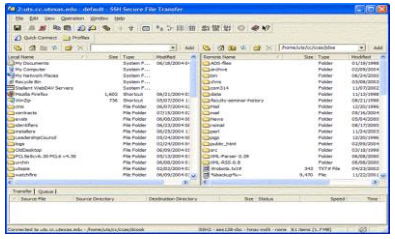
8.

```
$ 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:

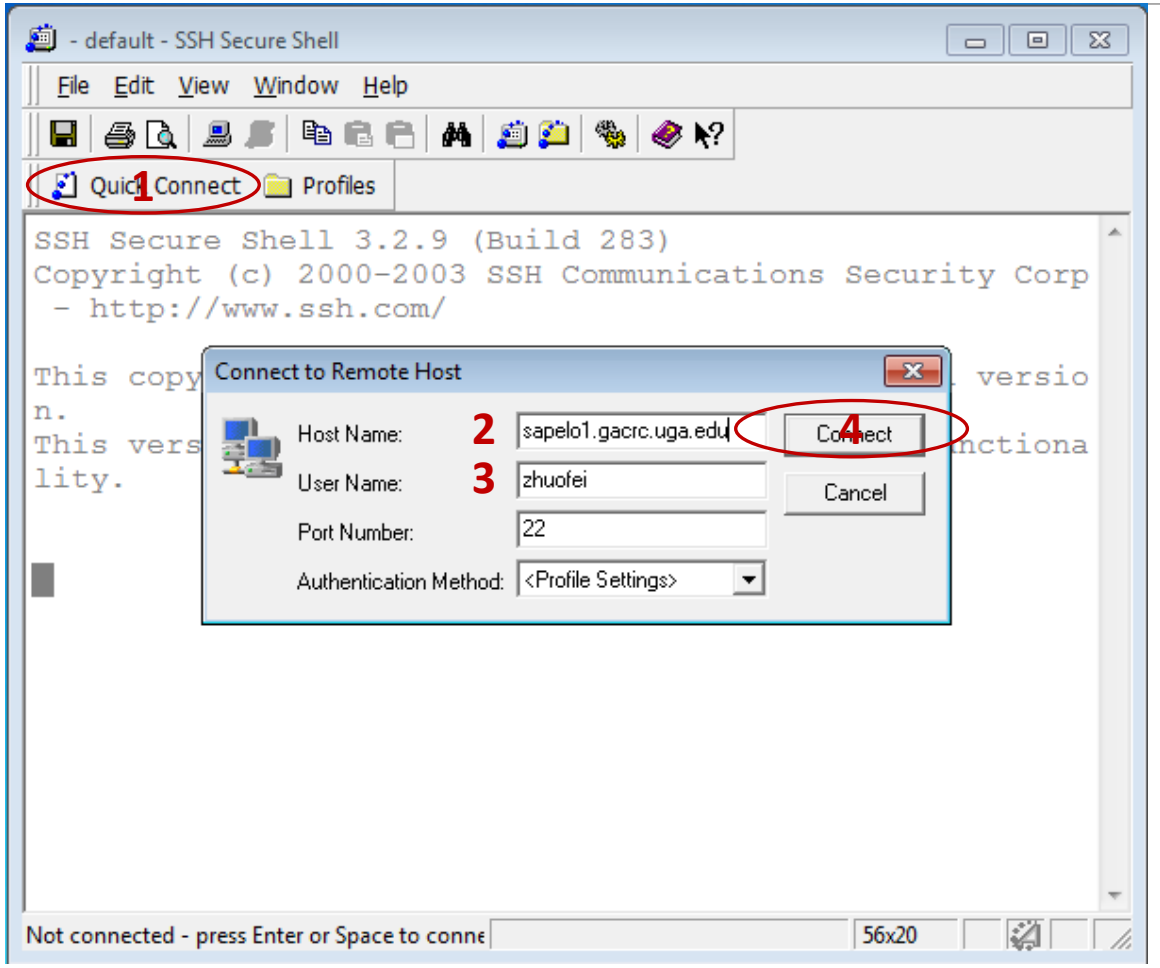
```
zhuofei@sapelo1.gacrc.uga.edu's password:
```

([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
  - /panfs/pstor.storage/home/abclab/username/ : zcluster home
  - /escratch4/username/ : zcluster scratch
  - /project/abclab/ : long-term active data storage
- ✓ 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 ./
```

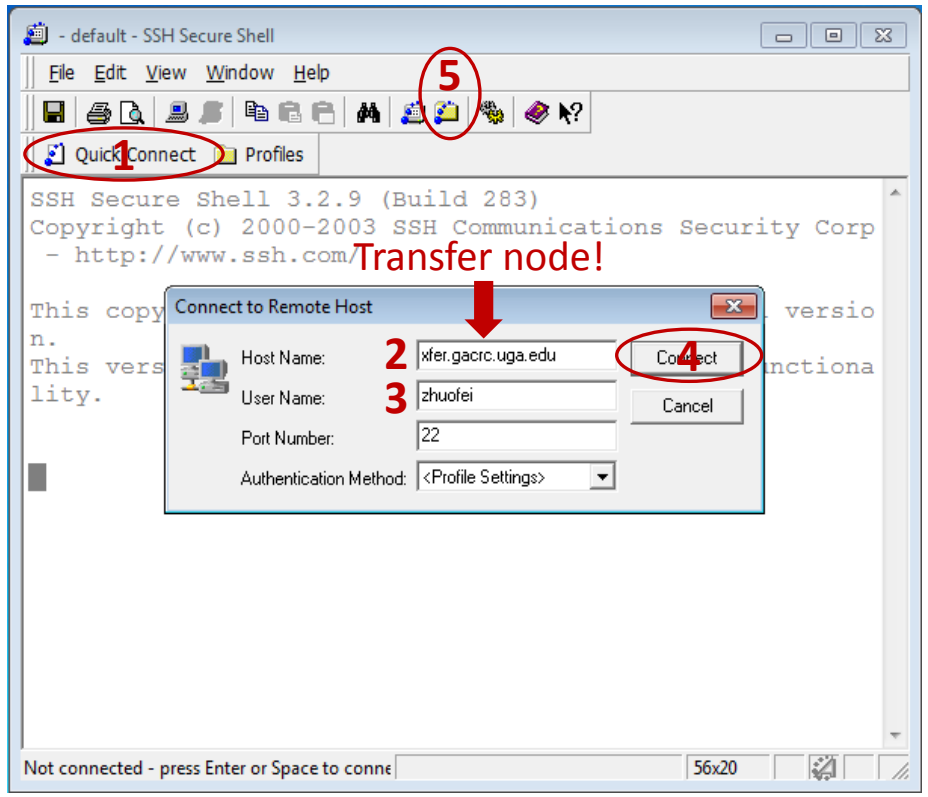
```
scp -r zhuofei@xfer.gacrc.uga.edu:/lustre1/zhuofei/workDir/folder/ ./
```

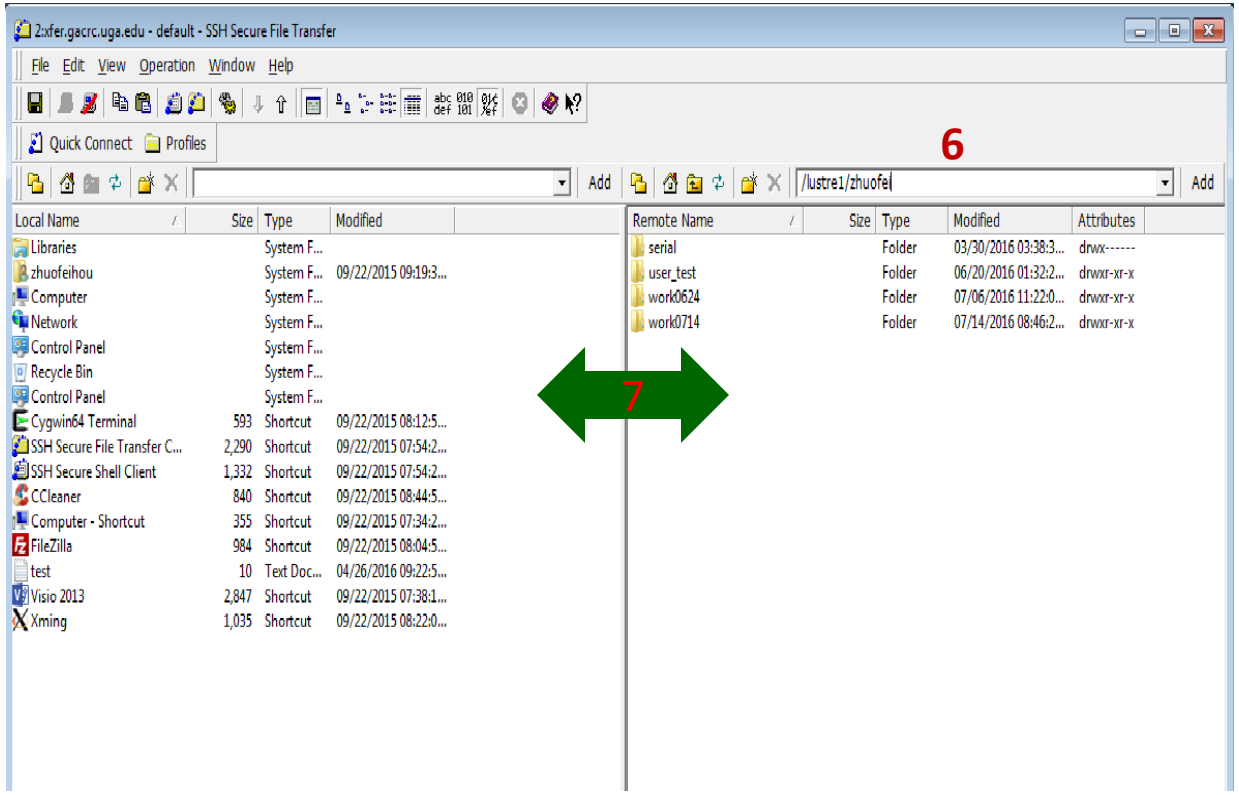
- On Window: SSH Secure Shell File Transfer, FileZilla, WinSCP (next page)

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

User's local  

 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	➔ 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 2>&1	➔ 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!