Georgia Advanced Computing Resource Center
UNIVERSITY OF GEORGIA

Introduction to HPC Using Sapelo Cluster at GACRC

Level 1/2

Georgia Advanced Computing Resource Center (GACRC)

EITS/University of Georgia

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Outline

- GACRC
- What is Sapelo cluster?
- Job Submission Workflow
- Work on Sapelo
- Guideline and Practical Tips

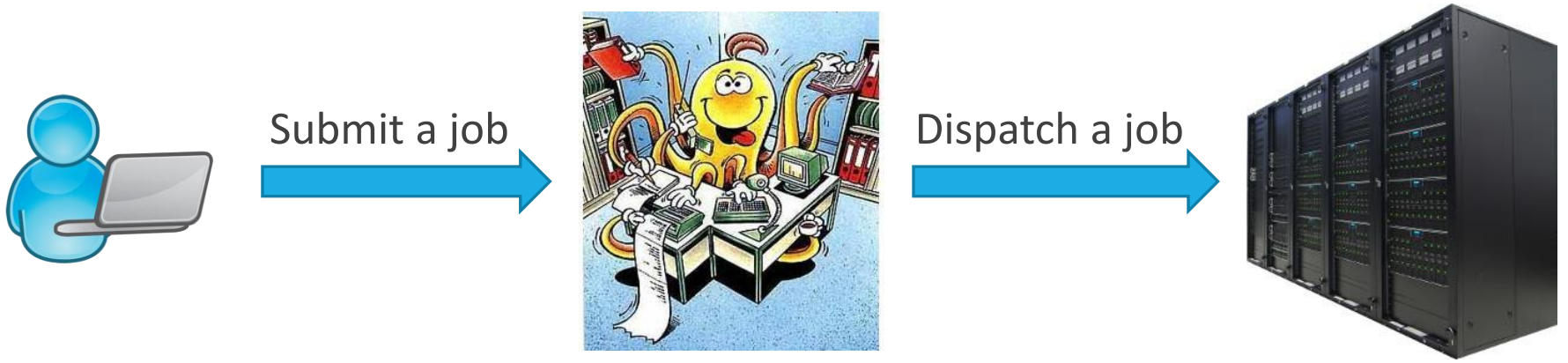
GACRC

- We are a high-performance-computing (HPC) center at UGA
- We provide to the UGA research and education community an advanced computing environment:
  - HPC computing and networking infrastructure located at the Boyd Data Center
  - Comprehensive collection of scientific, engineering and business applications
  - Consulting and training services
- http://wiki.gacrc.uga.edu (GACRC Wiki)
- https://wiki.gacrc.uga.edu/wiki/Getting_Help (GACRC Support)
- http://gacrc.uga.edu (GACRC Web)

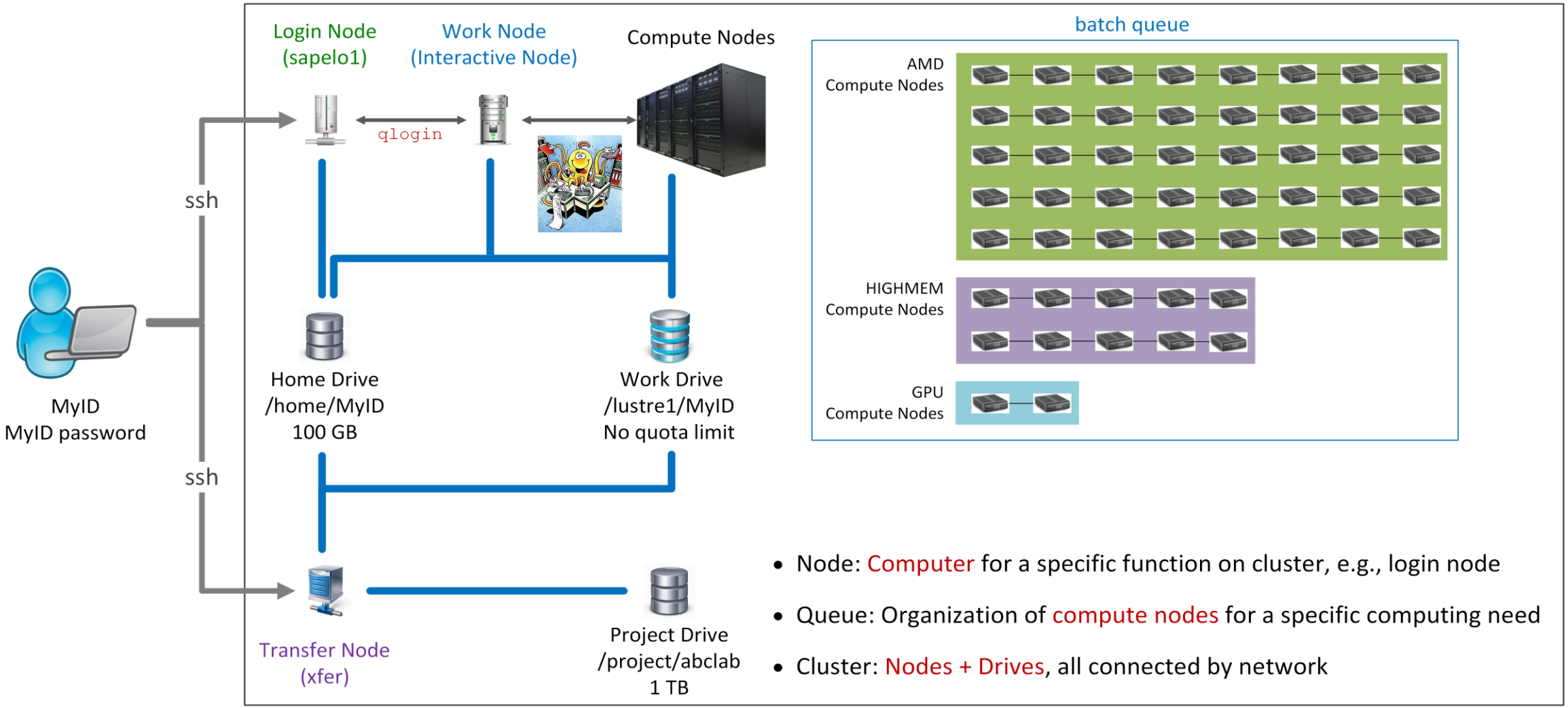
What is a Cluster?

When you work on cluster, 3 roles are working:

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



Sapelo Cluster Diagram



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

Sapelo Cluster Overview

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

- Operating System: 64-bit CentOS Linux 6.5
- You can log on (open connection) to:

  Login (username@sapelo1.gacrc.uga.edu) : edit script, submit batch job (not suggested!)

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

- Login → (qlogin) → Work Node : edit script, submit batch job, run interactive job

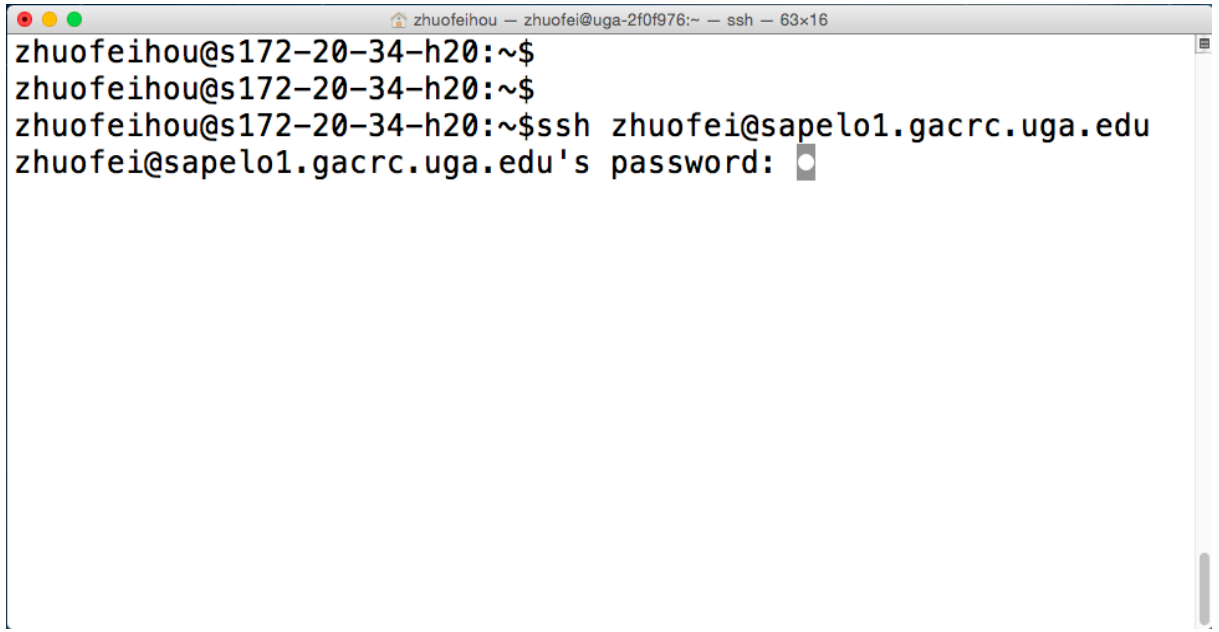
Job Submission Workflow

1. Log on to Login node: `ssh MyID@sapelo1.gacrc.uga.edu`
2. From Login node, transfer to Work node: `qlogin`
3. On Work node, change directory to global scratch: `cd /lustre1/username`
4. Create a working subdirectory for a job: `mkdir ./workDir`
5. Change directory to workDir: `cd ./workDir`
6. Transfer data from local computer to workDir: use `scp` or SSH File Transfer to connect Transfer node

   Transfer data on cluster to workDir: log on to Transfer node and then use `cp` or `mv`
7. Make a job submission script in workDir: `nano ./sub.sh`
8. Submit a job from workDir: `qsub ./sub.sh`
9. Check job status: `qstat_me` or Cancel a job: `qdel JobID`

Step1: Log on to Login node - Mac/Linux using ssh

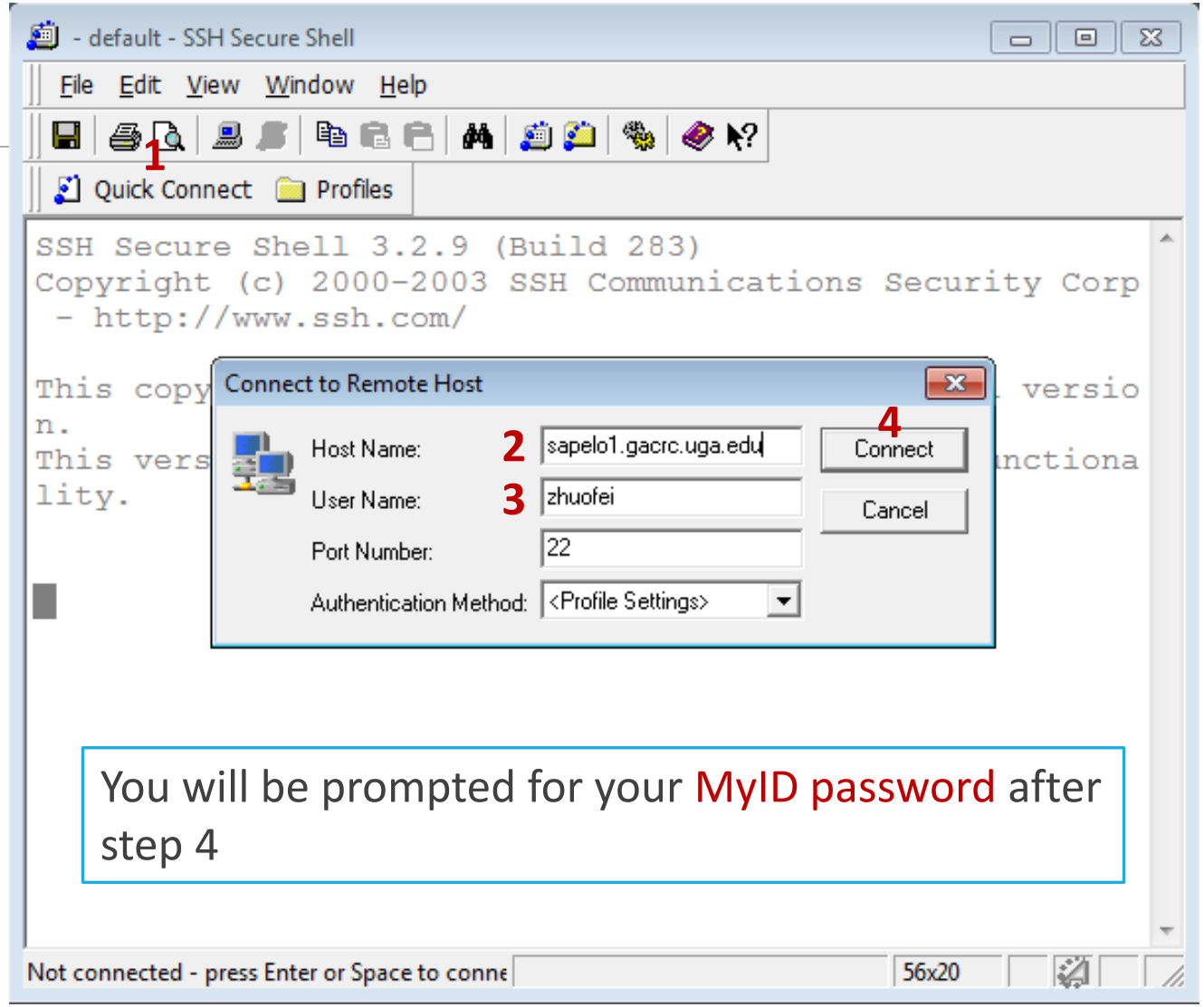
1. Open Terminal utility
2. Type command line: `ssh MyID@sapelo1.gacrc.uga.edu`
3. You will be prompted for your MyID password (when you type in the password, the prompt blinks and does not move)



Step1 (Cont.) - Windows

Download to install:

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



Step2: From Login node go to Work node using qlogin

- Once you logged on Login node, your current directory will be your home directory:

```
zhuofei@uga-2f0f976:~ $ pwd
/home/zhuofei                    ← that's my home dir on cluster!
```

- Type `qlogin` command on your command line:

```
zhuofei@uga-2f0f976:~ $ qlogin
qsub: waiting for job 2983350.pbs.scm to start
qsub: job 2983350.pbs.scm ready

zhuofei@n148:~ $                 ← now I am on a Work node with index of n148
```

Step2 (Cont.)

- Once you are on Work node, your current directory will be your home directory:

```
zhuofei@n148:~ $ pwd
/home/zhuofei                    ← that's my home dir on cluster!
```

- Type `exit` command on your command line to go back to Login node:

```
zhuofei@n148:~ $ exit
logout

qsub: job 2983575.pbs.scm completed
zhuofei@uga-2f0f976:~ $          ← now I am back on Login node
```

Step3: On Work node, change directory to global scratch

- Use `cd` command to change your current directory to /lustre1/MyID

```
zhuofei@n148:~ $ cd /lustre1/zhuofei
zhuofei@n148:/lustre1/zhuofei $ pwd
/lustre1/zhuofei                    ← that's my working space on cluster!
```

- Use `ls` command to take a look in /lustre1/MyID

```
zhuofei@n148:/lustre1/zhuofei $ ls
user_test  workDir_Alex
```

Step4: Create a working subdirectory for a job

- Use `mkdir` command to make a subdirectory in /lustre1/MyID

```
zhuofei@n148:/lustre1/zhuofei $ mkdir workDir
zhuofei@n148:/lustre1/zhuofei $
```

- Use `ls` command to take a look in /lustre1/MyID

```
zhuofei@n148:/lustre1/zhuofei $ ls
user_test   workDir   workDir_Alex
```

← a new folder workDir was created!

Step5: Change directory to workDir

- Use `cd` command to change your current directory to /lustre1/MyID/workDir

```
zhuofei@n148:/lustre1/zhuofei $ cd workDir
zhuofei@n148:/lustre1/zhuofei/workDir $
```

- Use `ls` command to take a look in /lustre1/MyID/workDir

```
zhuofei@n148:/lustre1/zhuofei/workDir $ ls
zhuofei@n148:/lustre1/zhuofei/workDir $
```

← It is empty!

Step6: Transfer data from local computer to workDir - Mac/Linux

1. You need to connect to cluster's Transfer node (xfer.gacrc.uga.edu)
2. Open Terminal utility on local computer to use scp (-r) [Source] [Target]

E.g. 1: working on local computer, from Local ➔ workDir on cluster

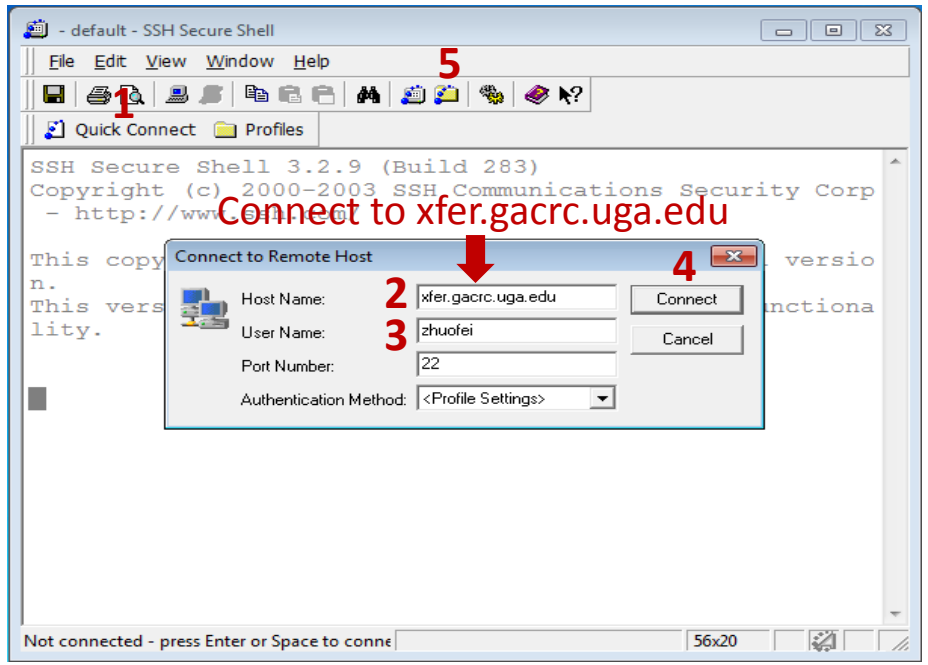
```
scp ./file zhuofei@xfer.gacrc.uga.edu:/lustre1/zhuofei/workDir/
scp -r ./folder/ zhuofei@xfer.gacrc.uga.edu:/lustre1/zhuofei/workDir/
```

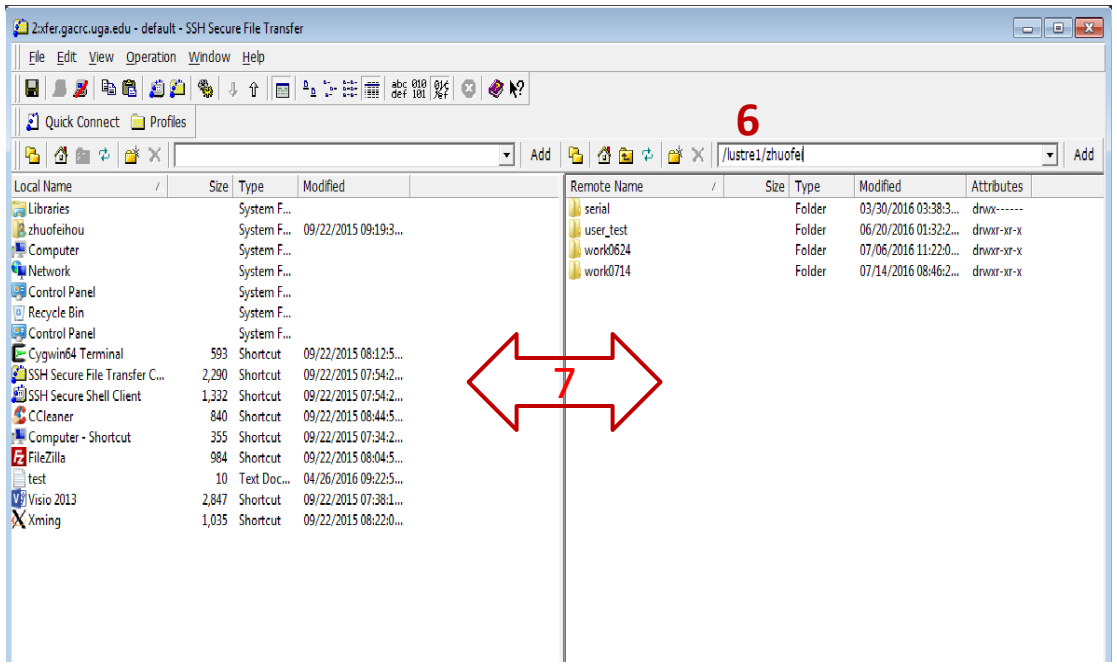
E.g. 2: working on local computer, from workDir on cluster ➔ Local

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

Step6 (Cont.) - Windows

1. You need to connect to cluster's Transfer node (xfer.gacrc.uga.edu)
2. Use SSH File Transfer or FileZilla or WinSCP on local computer





Step6 (Cont.): Transfer data on cluster to workDir

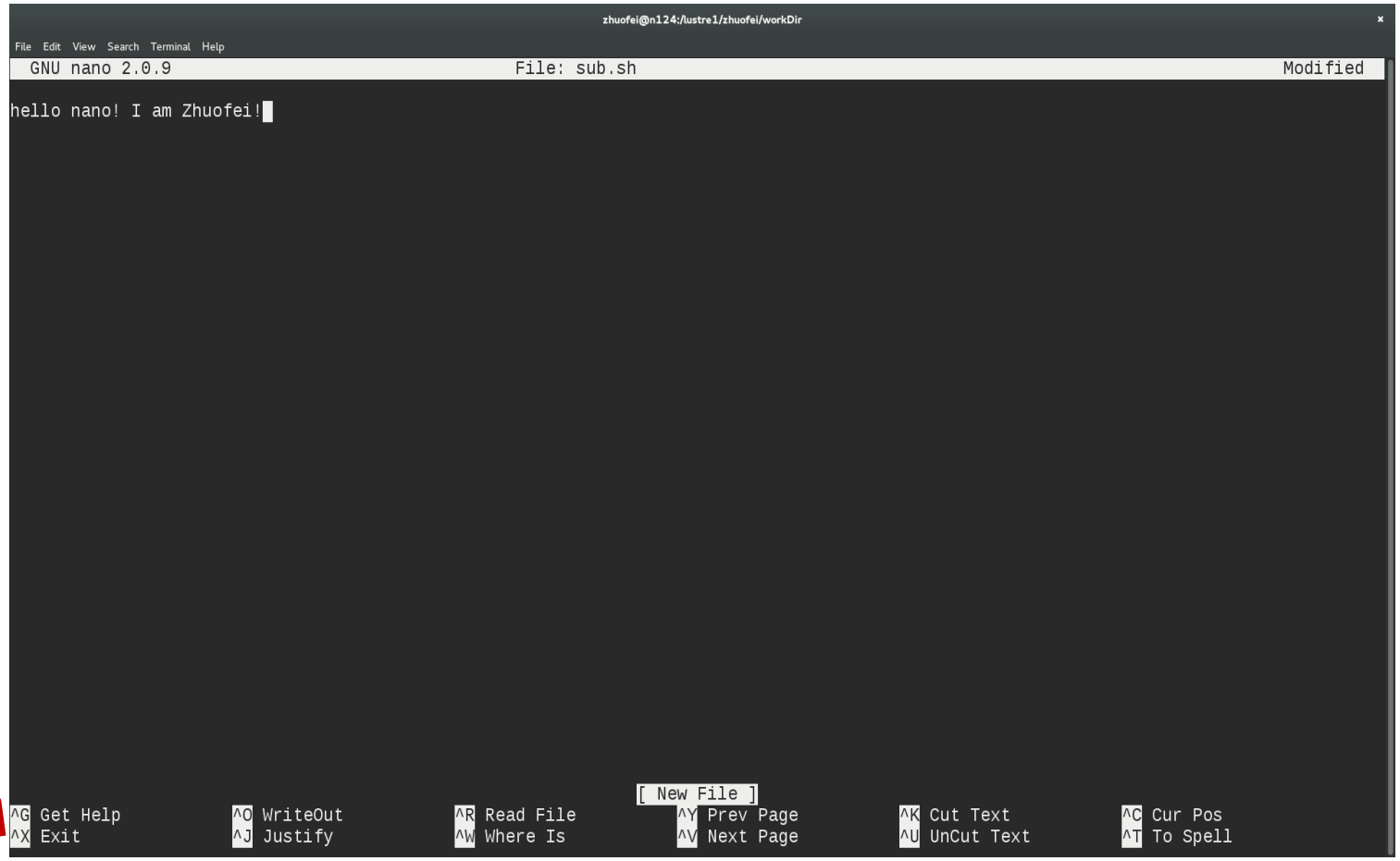
- Log on to Transfer node (xfer.gacrc.uga.edu)
  - ✓ Mac/Linux: ssh MyID@xfer.gacrc.uga.edu (page 8)
  - ✓ Windows: use SSH Secure Client app (page 9)
- Landing directory: /home/MyID (Sapelo home)
- Transfer data between folders on cluster using cp, mv
- Filesystems you can access using full path:
  1. /home/MyID/ : Sapelo home directory (landing directory)
  2. /lustre1/MyID/ : Sapelo global scratch directory
  3. /project/abclab/ : Non-current active data temporary parking
- Most file systems on Transfer are *auto-mounted* upon *the first time full-path access*, e.g., cd /project/abclab/

Step7: Make a job submission script in workDir using nano

```
$ nano sub.sh
```

nano is a small and friendly text editor on Linux.

Ctrl-x to save file and quit from nano



Step7 (Cont.)

1. Copy a template from GACRC Wiki Software:

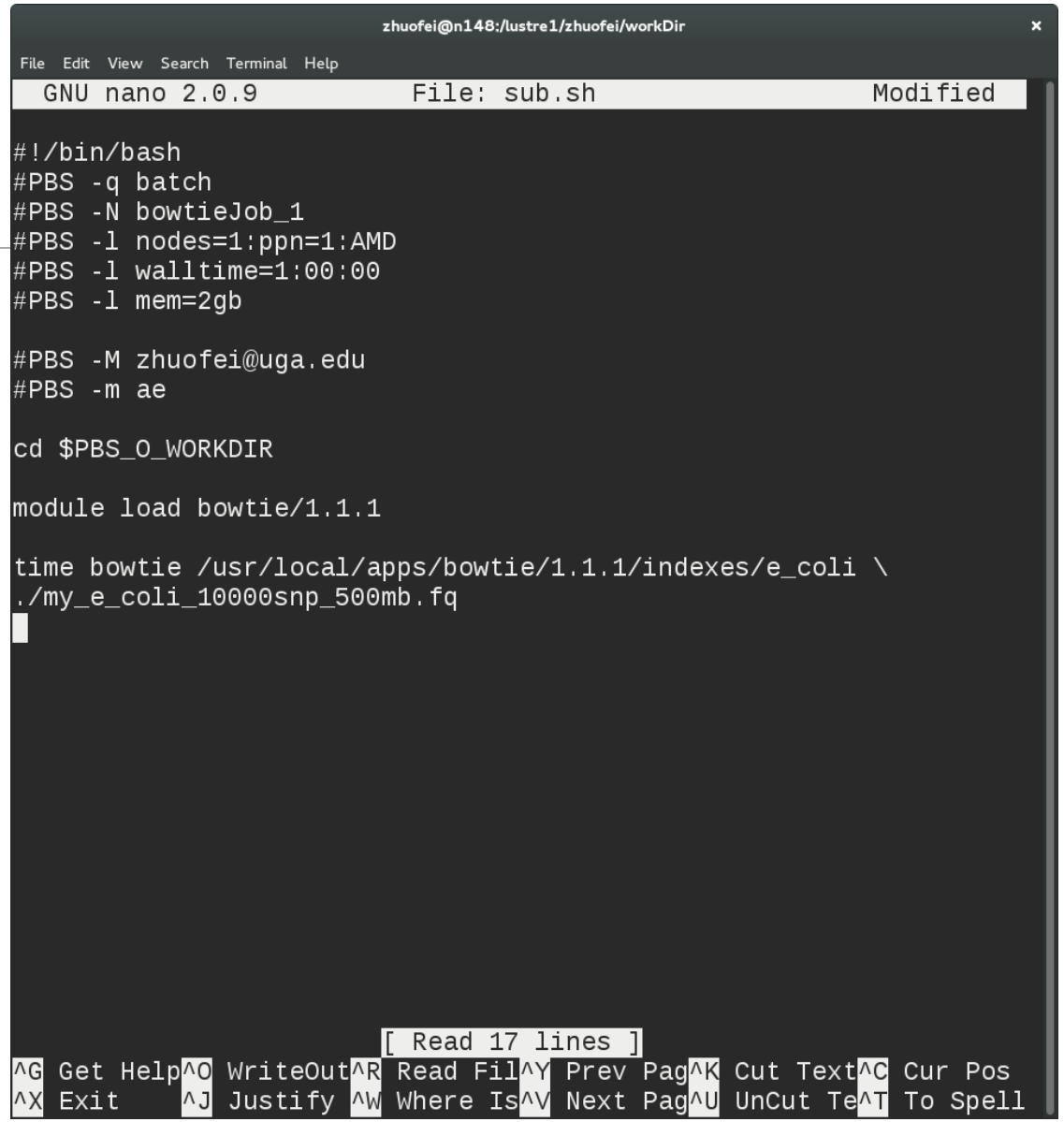
https://wiki.gacrc.uga.edu/wiki/Bowtie-Sapelo

2. Modify it as needed for your computing

Note: To run this example, you need to copy input data to your current working folder:

cp /usr/local/training/my_e_coli_10000snp_500mb.fq .

http://bowtie-bio.sourceforge.net/tutorial.shtml



Step8: Submit a job from workDir using qsub

```
zhuofei@n148:/lustre1/zhuofei/workDir $ pwd
/lustre1/zhuofei/workDir
zhuofei@n148:/lustre1/zhuofei/workDir $ ls
my_e_coli_10000snp_500mb.fq  sub.sh
zhuofei@n148:/lustre1/zhuofei/workDir $ qsub sub.sh
2987391.pbs.scm
```

sub.sh is job submission script to

1. specify computing resources:
2. load software using module load
3. run any Linux commands you want to run
4. run the software

Step9: Check job status using qstat_me

```
zhuofei@n148:/lustre1/zhuofei/workDir $ qstat_me
Job ID                  Name             User            Time Use S Queue
----------------------- ---------------- --------------- -------- - -----
2987177.pbs             STDIN            zhuofei         00:05:01 R s_interq
2987391.pbs             bowtieJob_1      zhuofei         00:00:35 C batch
2987401.pbs             bowtieJob_1      zhuofei                0 R batch
2987402.pbs             bowtieJob_1      zhuofei                0 Q batch
```

R : job is running
C : job completed (or canceled or crashed) and is not longer running. Jobs stay in this state for 1 hour
Q : job is pending, waiting for resources to become available

Note: “Time Use” is the CPU time, instead of the wall-clock time of your job staying on cluster!

Step9 (Cont.): Cancel job using qdel

```
zhuofei@n148:/lustre1/zhuofei/workDir $ qdel 2987402
zhuofei@n148:/lustre1/zhuofei/workDir $ qstat_me
Job ID                    Name             User            Time Use S Queue
------------------------- ---------------- --------------- -------- - ------
2987177.pbs               STDIN            zhuofei         00:05:01 R s_interq
2987391.pbs               bowtieJob_1      zhuofei         00:00:35 C batch
2987401.pbs               bowtieJob_1      zhuofei                0 R batch
2987402.pbs               bowtieJob_1      zhuofei                0 C batch
```

Step9 (Cont.): Check Job using qstat –n –u MyID

```
zhuofei@n14:/lustre1/zhuofei/workDir $ qstat -n -u zhuofei

pbs.scm:

                                                                  Req'd  Req'd       Elap
Job ID          Username Queue    Jobname      SessID NDS   TSK  Memory Time      S Time
--------------- -------- -------- ---------- ------ ---- ----- ------ --------- - --------
2991949.pbs.scm  zhuofei  s_interq STDIN       819642    1     1  --     12:00:00 R 00:00:34
   n14/31
2991951.pbs.scm  zhuofei  batch    bowtieJob_1 842001    1     1  2gb    01:00:00 R 00:00:06
   n101/28
2991952.pbs.scm  zhuofei  batch    bowtieJob_1 844269    1     1  2gb    01:00:00 R 00:00:04
   n101/30
2991953.pbs.scm  zhuofei  batch    bowtieJob_1 844885    1     1  2gb    01:00:00 R 00:00:04
   n101/31
```

Note: “Elap Time” is the wall-clock time, instead of the CPU time, which qstat_me can give you!

Step9 (Cont.): Check all Jobs on cluster using qstat

```
$ qstat
Job ID                    Name             User            Time Use S Queue
------------------------------------------------------------------------
2392787.pbs               G_s-Butyl_0_opt  gtp72866        101:34:5 R batch
2392792.pbs               G_s-Butyl_20_opt gtp72866        56:14:32 R batch
2393599.pbs               ...80-oz0.6-K220 rbchan          89:99:59 R batch
2395891.pbs               NoRiver_jul_2008 hluo76                 0 Q batch
2395893.pbs               NoRiver_jul_2012 hluo76                 0 Q batch
2396261.pbs               ...opyl_freq_005 gtp72866        31:55:56 R batch
2396297.pbs               ...opyl_freq_041 gtp72866        202:53:1 R batch
2400998.pbs               ...rrect_lab4.sh xwwang          844:06:3 R batch
2406268.pbs               abundTrinity3    mpodio                 0 Q batch
2423833.pbs               L80-307          jx57780         393:37:1 C batch
2423838.pbs               L80-312          jx57780         373:57:4 C batch
2513741.pbs               ...3012_ah100_00 byang           00:00:00 R batch
2513743.pbs               ...4012_ah070_01 byang           138:22:3 R batch
.
.
.
```

Note: qstat command will give you a long list of all jobs from all users on cluster!

Workflow Diagram

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`

7. `nano ./sub.sh`

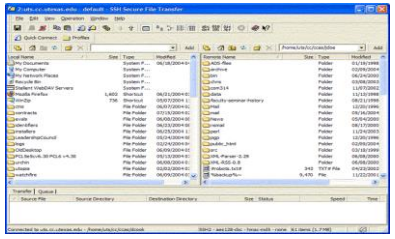
```
#!/bin/bash
#PBS -q batch
#PBS -N bowtieJob_1
#PBS -l nodes=1:ppn=1:AMD
#PBS -l walltime=1:00:00
#PBS -l mem=2gb

#PBS -M zhuofei@uga.edu
#PBS -m ae

cd $PBS_O_WORKDIR

module load bowtie/1.1.1
……
```

lustre1

6. Linux/Mac user:

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

Windows user:



8. `$ qsub sub.sh`

9. `$ qstat_me or qdel JobID`

Computing Resources

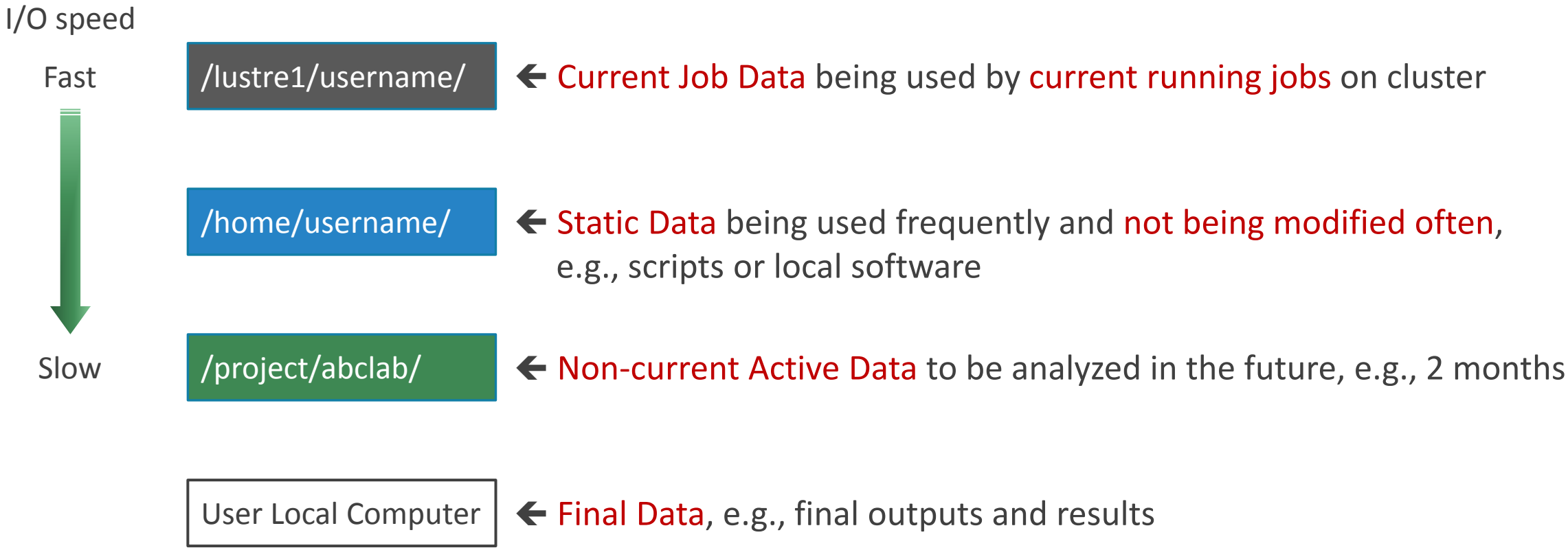
Queue	Node Feature	Total Nodes	RAM(GB) /Node	Max RAM(GB) /Single-node Job	Cores /Node	Processor	GPU	GPU Cards /Node	InfiniBand
batch	AMD	112	128	**126**	**48**	AMD Opteron	N/A		Yes
		4	256	252					
	HIGHMEM	6	512	504					
		4	1024 (1)	997					
			1024 (3)		28	Intel Xeon			
	GPU	2	128	126	16		NVIDIA K40m	8	
	abcnode (buy-in)	85	variable	variable	variable	variable	variable	variable	

Storage Environment

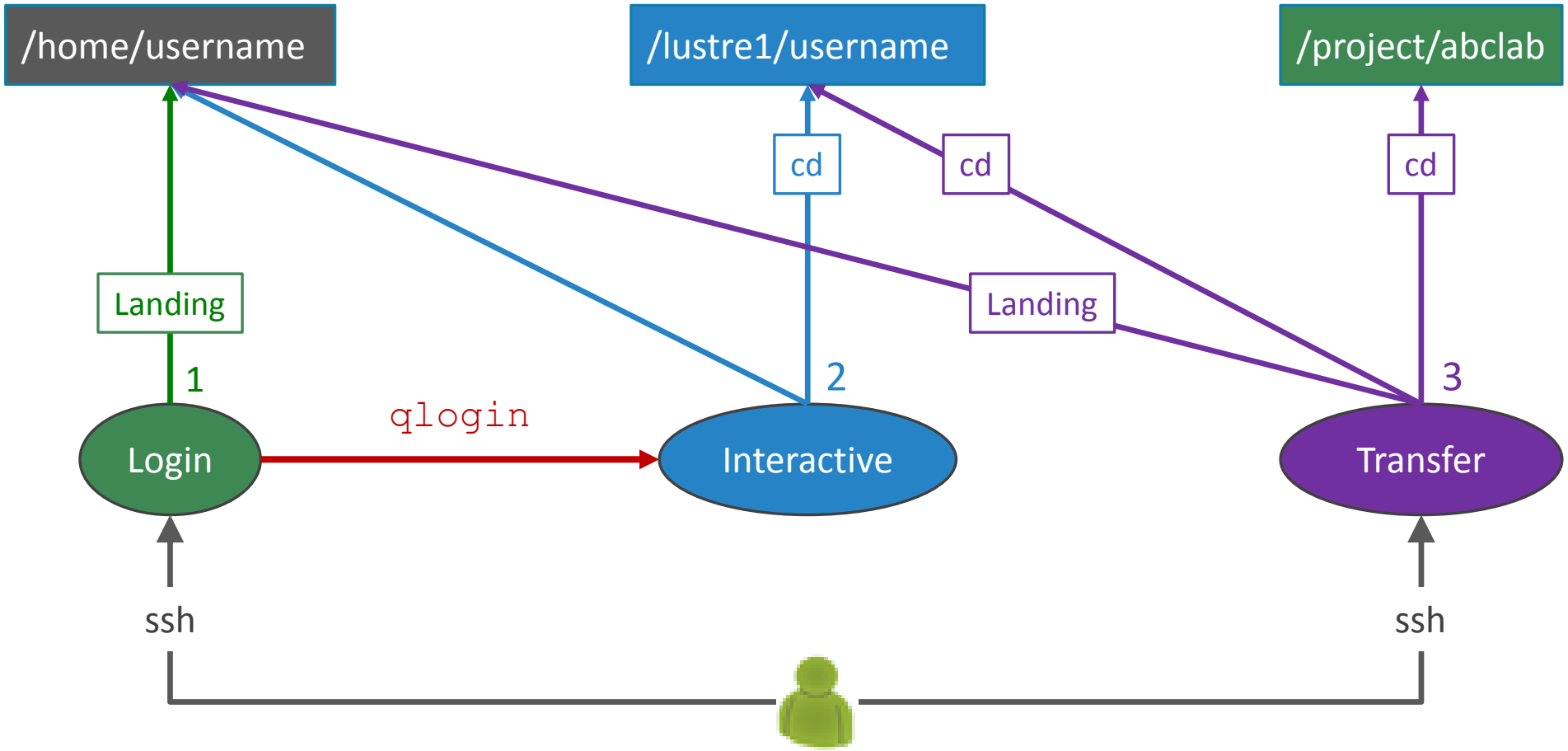
4 Filesystems	Role	Quota	Accessible from	Intended Use	Notes
/home/username/	Home	100GB	sapelo1.gacrc.uga.edu (Login) Interactive nodes (Interactive) xfer.gacrc.uga.edu (Transfer) compute nodes	**Static data** being used frequently, e.g., scripts, source codes, local software	Snapshots
/lustre1/username/	Global Scratch	No Limit	Interactive nodes (Interactive) xfer.gacrc.uga.edu (Transfer) compute nodes	**Current job data** being read from/written into by jobs running on cluster	**User to clean up!** Subject to deletion in 30 days*
/tmp/lscratch/	Local Scratch	N/A	individual compute node	Jobs with heavy disk I/O	**User to clean up!** When job exists from the node!
/project/abclab/	Storage	1TB (Initial)	xfer.gacrc.uga.edu (Transfer)	**Temporary data parking** for non-current active data	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 (Cont.) - Intended Use of Directories



Storage Environment (Cont.) – Accessing Directories from Nodes



Storage Environment (Cont.)

7 Main Functions	Related Filesystem	Related Node
Login Landing	/home/username (Home) (Always!)	Login or Transfer
Batch Job Submitting	/home/username (Home)	Login
	/lustre1/username (Global Scratch) (Suggested!) /home/username (Home)	Interactive
Interactive Job Running	/lustre1/username (Global Scratch) /home/username (Home)	
Data Transferring, Archiving , Compressing	/lustre1/username (Global Scratch) /home/username (Home)	Transfer
Non-current Active Data Temporary Parking	/project/abclab (Project Storage)	
Job Data Temporarily Storing	/lustre1/username (Global Scratch) /tmp/lscratch (Local Scratch)	Compute

Software Environment

- The cluster uses environment modules to define the various paths for software packages (more than 600 and expanding daily!)
- `module avail`: List all available modules (centralized installation):

```
$ module avail

------------------------------------------------------------ /usr/local/modulefiles ------------------------------------------------------------
Core/StdEnv                      fftw/3.3.4/pgi149-mvapich200      mafft/7.273-e                 python/2.7.8
Data/cache/moduleT.new           fftw/3.3.4/pgi149-omp183   (D)    mageck/0.5                    python/2.7.13
Data/cache/moduleT        (D)    find_cns/07212016                 mageck-vispr/02242017         python/3.4.3
Data/system.txt                  fineradstructure/12092016         magickwand/0.2                python/3.5.1          (D)
R/3.0.3                          finestructure/2.0.7               magma/2.22-9                  pytorch/0.1.9
R/3.1.2                          flash/1.2.11                      mahotas/1.4.3                 pytorch/02272017      (D)
R/3.2.1                          flex/2.6.0/gcc/4.7.4              masurca/3.1.3                 qiime/1.9.1
R/3.2.3                          flex/2.6.0/pgi/14.10              matlab/R2015aSP1              qt/4.8
R/3.3.1                   (D)    freebayes/1.0.1                   matlab/R2015b                 quast/4.1
StdEnv                    (D)    freesurfer/6.0.0                  matlab/R2016b             (D) quast/4.2             (D)
……
```

Software Environment (Cont.)

- `module list`: List modules currently loaded:

```
$ module list

Currently Loaded Modules:
  1) moab/8.1.1   2) StdEnv
```

- `module load`: Load the needed module:
- `module unload`: Remove a module

```
$ module load python/2.7.8
$module load R/3.2.3
$ module list

Currently Loaded Modules:
  1) moab/8.1.1   2) StdEnv   3) python/2.7.8   4) R/3.2.3
```

- `module spider`: Search a module:

```
$ module spider R/3.2.3
----------------------------------------------------------------------------
R: R/3.2.3
----------------------------------------------------------------------------
Description:
     statistics package ……
```

Work on Sapelo - Useful Links

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

GACRC Wiki Running Jobs: https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_Sapelo

GACRC Wiki Software: https://wiki.gacrc.uga.edu/wiki/Software

GACRC Wiki Linux Command: https://wiki.gacrc.uga.edu/wiki/Command_List

GACRC Wiki Training: https://wiki.gacrc.uga.edu/wiki/Training

GACRC User Account Request: https://wiki.gacrc.uga.edu/wiki/User_Accounts

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

Work on Sapelo - Get Help

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 – Get 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

Work on Sapelo - Run Batch Jobs

- Components you need to run a job:
  - Software already installed (cluster software or the one installed by yourself)
  - Job submission script to
    1. specify computing resources:
       - ✓ number of nodes and cores
       - ✓ amount of memory
       - ✓ node's feature
       - ✓ maximum wallclock time
    2. load software using module load (for cluster software)
    3. run any Linux commands you want to run, e.g., pwd, mkdir, cd, echo, etc.
    4. run the software
- Common queueing commands you need:
  - qsub, qstat_me, qstat, qdel
  - showjobs, checkjob, showq

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 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=20gb
#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), default 96

```
#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

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), default 54

Work on Sapelo - 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
```

Option 1: qstat -f JobID (running jobs or finished jobs in 1 hour)

```
$ qstat -f 1426778
Job Id: 1426778.pbs.scm
    Job_Name = BS2_GFF_range_methylator5-10.py
    Job_Owner = gent@uga-2f0f976.scm
    resources_used.cput = 76:54:46
    resources_used.energy_used = 0
    resources_used.mem = 44136kb
    resources_used.vmem = 90200kb
    resources_used.walltime = 76:50:04
    job_state = C
    queue = batch
     .
    Error_Path = uga-2f0f976.scm:/home/gent/scripts/BS2_GFF_range_methylator5-10.py.e1426778
    exec_host = n2/7
    Output_Path = uga-2f0f976.scm:/home/gent/scripts/BS2_GFF_range_methylator5-10.py.o1426778
     .
    Resource_List.mem = 2gb
    Resource_List.nodect = 1
    Resource_List.nodes = 1:ppn=1:AMD
    Resource_List.walltime = 480:00:00
    .
    Variable_List = PBS_O_QUEUE=batch,PBS_O_HOME=/home/gent, …… ,
                    PBS_O_WORKDIR=/home/gent/scripts,
```

Option 2: showjobs JobID (finished jobs over 1 hour, but ≤ 7 days)

```
$ showjobs 1426778
Job Id             : 1426778.pbs.scm
Job Name           : BS2_GFF_range_methylator5-10.py
Output File        : uga-2f0f976.scm:/home/gent/scripts/BS2_GFF_range_methylator5-10.py.o1426778
Error File         : uga-2f0f976.scm:/home/gent/scripts/BS2_GFF_range_methylator5-10.py.e1426778
Working Directory  : /home/gent/scripts
Home Directory     : /home/gent
Submit Arguments   : BS2_GFF_range_methylator5-10.py.sh
User Name          : gent
Group Name         : krdlab
Queue Name         : batch
Wallclock Limit    : 20:00:00:00
Wallclock Duration: 3:04:50:04
CPUTime            : 3:04:54:46
Memory Used        : 43.1Mb
Memory Limit       : 2gb
vmem Used          : 88.1Mb
Submit Time        : Mon Mar 27 20:51:01 2017
Start Time         : Tue Mar 28 03:06:41 2017
End Time           : Fri Mar 31 07:58:32 2017
Exit Code          : 0
Master Host        : n2
```

Option 3: 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:  n5/4-27
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
```

Work on Sapelo - Check Queue Status using 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`

- The stdout .o file and stderr .e file are to be written into files at the finishing time of a job.

  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

Thank You!