

Using the Sapelo2 Cluster at the GACRC

Cluster New User Training Workshop

Georgia Advanced Computing Resource Center (GACRC)

EITS/University of Georgia

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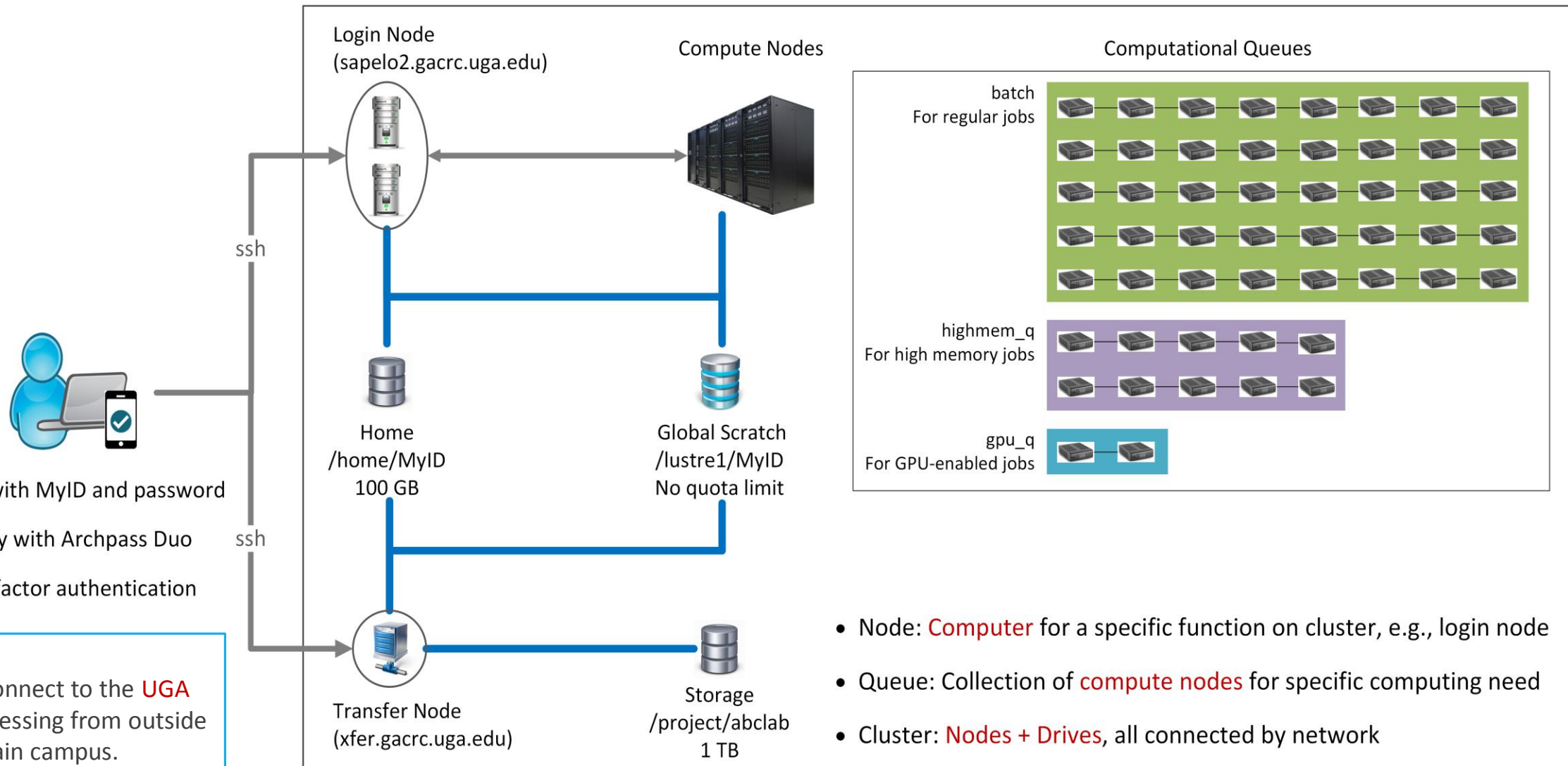
Outline

- GACRC
- Sapelo2 Cluster
 - Diagram
 - Overview
 - Four Directories
 - Four Computational Queues
 - Software Environment
- Job Submission Workflow
- GACRC Wiki and Support

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)

Sapelo2 Cluster



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

Sapelo2: A Linux HPC cluster (64-bit Centos 7)

➤ Two Nodes:

1. Login node for batch job workflow: MyID@sapelo2.gacrc.uga.edu
2. Transfer node for data transferring: MyID@xfer.gacrc.uga.edu

➤ Four Directories:

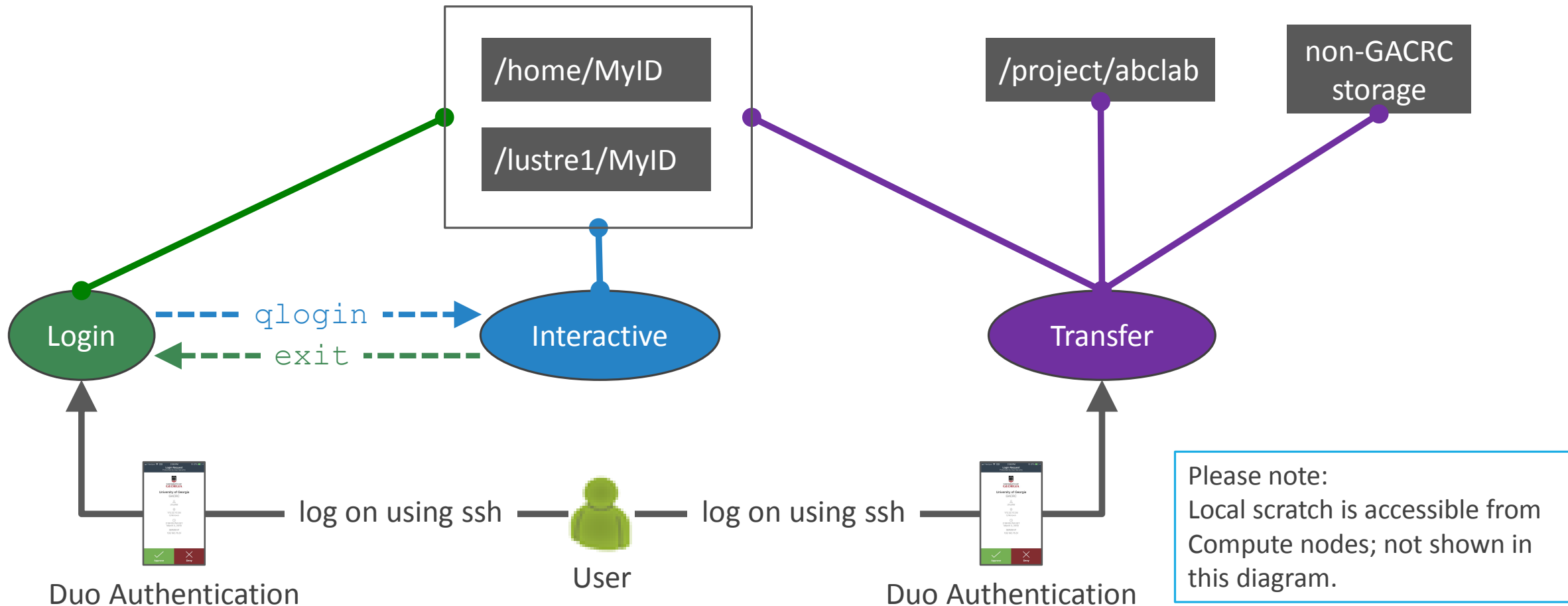
1. Home: Landing spot; 100GB quota; Backed-up
2. Global Scratch: High-performance job working space; NO quota; NOT backed-up
3. Local Scratch: Local storage on compute node; 200GB; NOT backed-up
4. Storage: Temporary data parking; 1TB quota; Backed-up (**ONLY accessible from Transfer node!**)

➤ Four Computational Queues: batch, highmem_q, gpu_q, groupBuyin_q

Four Directories

4 Directories	Role	Quota	Accessible from	Intended Use	Backed-up	Notes
/home/MyID	Home	100GB	Login Transfer	Static data: 1. Scripts, source codes 2. Local software	Yes	
/lustre1/MyID	Global Scratch	No Limit		Current job data: data being read/written by running jobs	No	User to clean up! *Subject to deletion in 30 days
/project/abclab	Storage	1TB (initial)	Transfer	Temporary data parking: non-current active data	Yes	Group sharing possible
/lscratch	Local Scratch	~200GB	Compute	Jobs with heavy disk I/O	No	1. User to clean up when job exits from the node! 2. Persistent data

Accessing Directories from Nodes



4 Computational Queues

Queue	Node Feature	Total Nodes	RAM(GB) /Node	Max RAM(GB) /Single-node Job	Cores /Node	Processor Type	GPU Cards /Node	InfiniBand
batch	Intel	30	64	62	28	Intel Xeon	N/A	Yes
		42	192	188	32	Intel Xeon (Skylake)		
	AMD	90	128	125	48	AMD Opteron		
highmem_q	Intel/AMD	4/1	1024	997	28	Intel Xeon		
	AMD/Intel	4/1	512	503	48	AMD Opteron		
gpu_q	GPU	2	128	125	16	Intel Xeon	8 NVIDIA K40	
		2	96/80	92/76	12		7 NVIDIA K20	
		4	192	188	32	Intel Xeon (Skylake)	1 NVIDIA P100	
groupBuyin_q	variable							

Software Environment

1. Software names are long and have a EasyBuild toolchain name associated to it
2. Complete module name: `Name/Version-toolchain`, e.g., `Python/2.7.14-foss-2016b`
3. Software names are case-sensitive!
 - `module avail` : List all available software modules installed on cluster
 - `module load moduleName` : Load a module into your working environment
 - `module list` : List modules currently loaded
 - `module unload moduleName` : Remove a module from working environment
 - `ml spider pattern` : Search module names matching a pattern (case-insensitive)

Job Submission Workflow

https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_Sapelo2

1. Log on to Login node using MyID and password, and two-factor authentication with Archpass Duo:
`ssh MyID@sapelo2.gacrc.uga.edu`
2. On Login node, change directory to global scratch : `cd /lustre1/MyID`
3. Create a working subdirectory for a job : `mkdir ./workDir`
4. Change directory to workDir : `cd ./workDir`
5. 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`
6. Make a job submission script in workDir : `nano ./sub.sh`
7. Submit a job from workDir : `qsub ./sub.sh`
8. Check job status : `qstat_me` or Cancel a job : `qdel JobID`

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

https://wiki.gacrc.uga.edu/wiki/Connecting#Connecting_to_Sapelo2

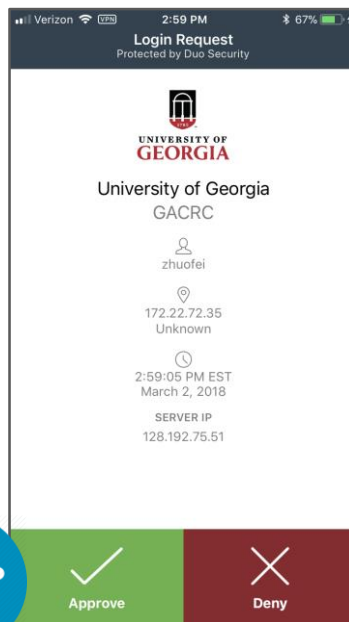
1. Open **Terminal** utility
2. Type command line: `ssh MyID@sapelo2.gacrc.uga.edu`
3. You will be prompted for your **MyID password**
4. Sapelo2 access requires ID verification using two-factor authentication with Archpass

Duo. If you are not enrolled in Archpass Duo, please refer to

https://eits.uga.edu/access_and_security/infosec/tools/archpass_duo/ on how to enroll

Step1 (Cont.) - Mac/Linux using ssh

Use Terminal utility on
Mac or Linux!



```
zhuofei@s172-20-19-h149:~$
zhuofei@s172-20-19-h149:~$
zhuofei@s172-20-19-h149:~$ssh zhuofei@sapelo2.gacrc.uga.edu ← Log on
Password: ← Input MyID password!
Duo two-factor login for zhuofei

Enter a passcode or select one of the following options:

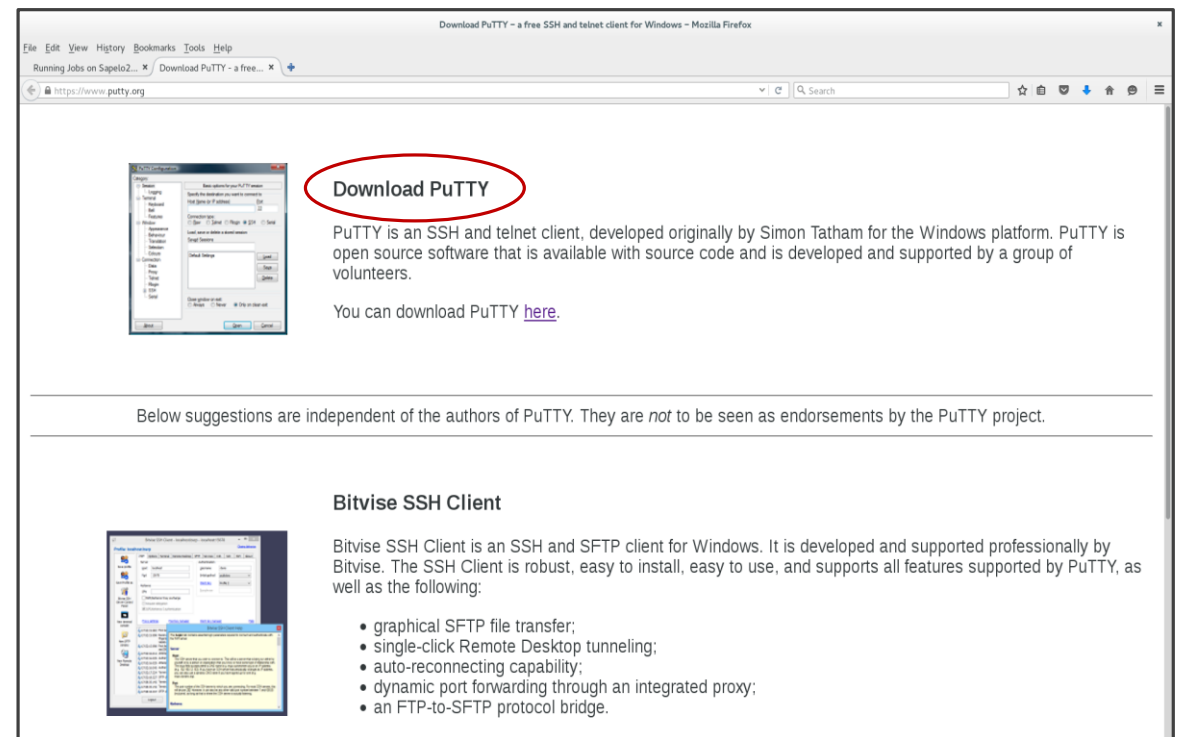
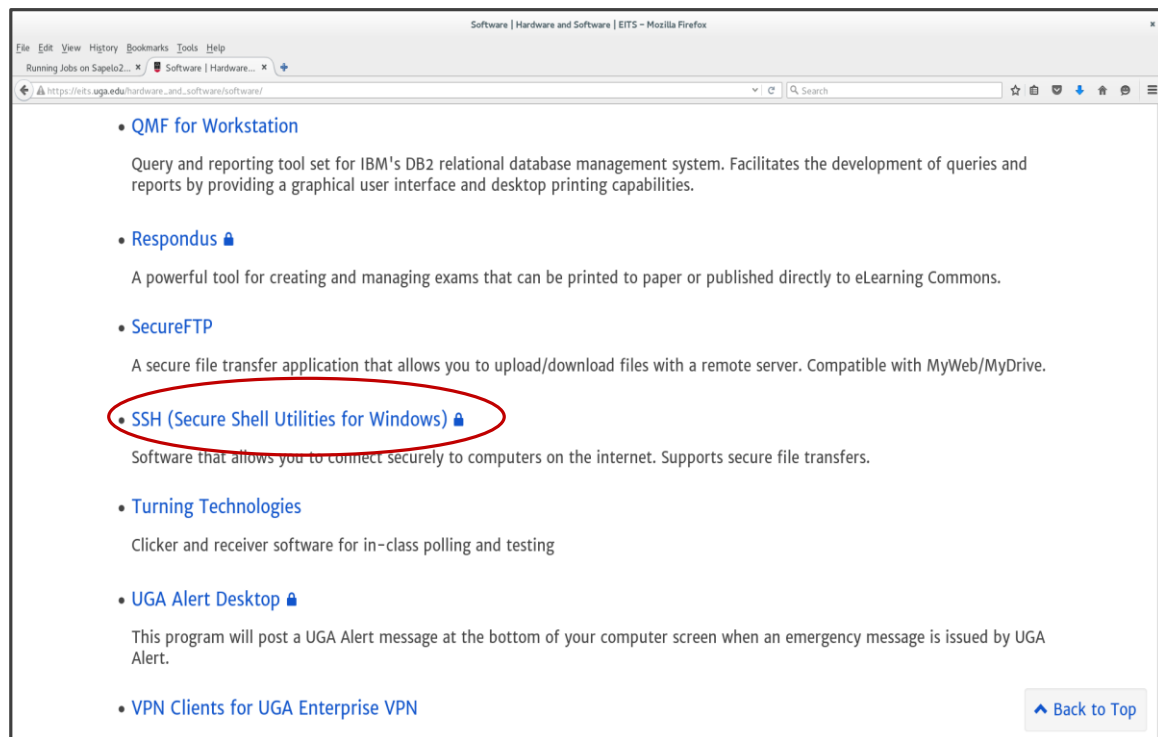
1. Duo Push to XXX-XXX-5758
2. Phone call to XXX-XXX-1925
3. Phone call to XXX-XXX-5758
4. SMS passcodes to XXX-XXX-5758

Passcode or option (1-4): 1 ← Select Duo login option!

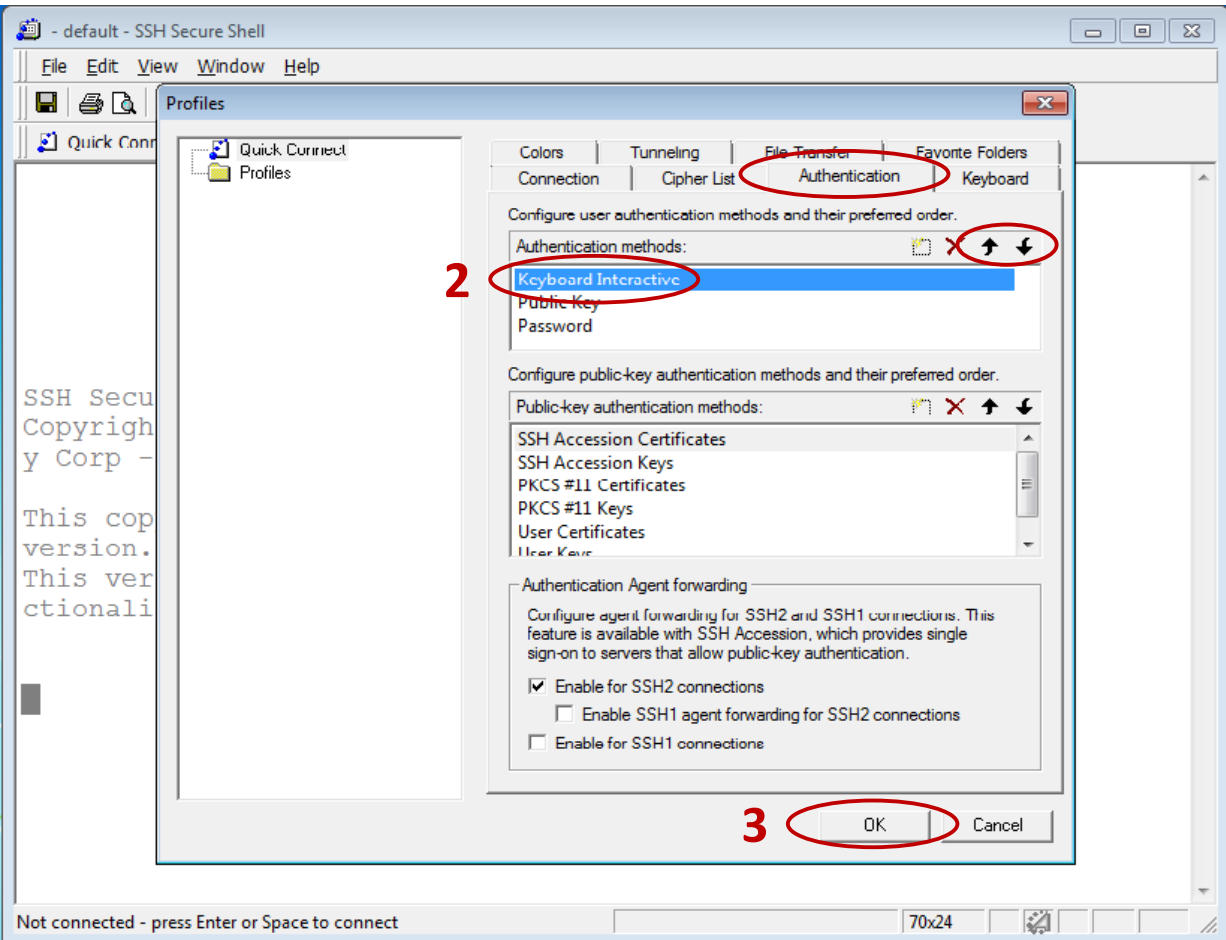
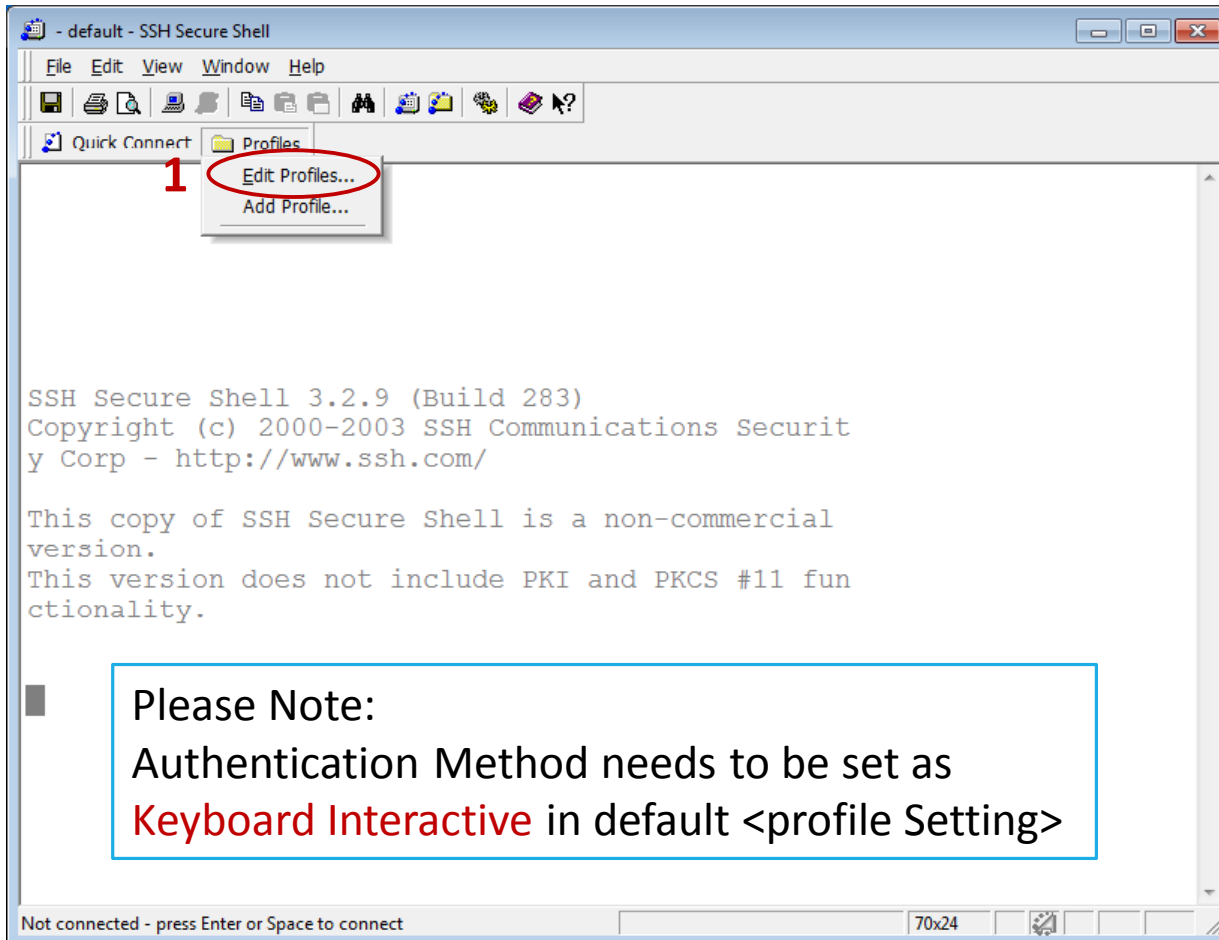
Pushed a login request to your device...
Success. Logging you in...
zhuofei@sapelo2-sub2 ~$
zhuofei@sapelo2-sub2 ~$ ← I am on sapelo2-sub2!
```

Step1 (Cont.) - Windows using SSH Secure Utilities

1. Download and install SSH Secure Utilities: http://eits.uga.edu/hardware_and_software/software/
2. You can use PuTTY as an alternative: <https://www.putty.org/>



Step1 (Cont.) - Windows using SSH Secure Utilities



Please Note:
Authentication Method needs to be set as
Keyboard Interactive in default <profile Setting>

Step1 (Cont.) - Windows using SSH Secure Utilities

4

SSH Secure Shell 3.2.9 (Build 283)
Copyright (c) 2000-2003 SSH Communications Security Corp
- http://www.ssh.com/

This copy of SSH Secure Shell is a non-commercial version. This version does not include PKI and PKCS #11 functionality.

Connect to Remote Host

Host Name: 5 sapelo2.gacrc.uga.edu
User Name: 6 zhuofei
Port Number: 22
Authentication Method: <Profile Settings>

7

8. You will be prompted for UGA MyID password after Step 7

Not connected - press Enter or Space to connect

Copyright (c) 2000-2003 SSH Communications Security Corp
- http://www.ssh.com/

This copy of SSH Secure Shell is a non-commercial version. This version does not include PKI and PKCS #11 functionality.

Duo two-factor login for zhuofei

Enter a passcode or select one of the following options:

1. Duo Push to XXX-XXX-5758
2. Phone call to XXX-XXX-1925
3. Phone call to XXX-XXX-5758
4. SMS passcodes to XXX-XXX-5758

Passcode or option (1-4): 1

9. Select Duo login option!

Pushed a login request to your device...
Success. Logging you in...
zhuofei@sapelo2-sub1 ~\$
zhuofei@sapelo2-sub1 ~\$

10

Approve Deny

Connected to sapelo2.gacrc.uga.edu

Step2: On Login node change directory to global scratch

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

```
zhuofei@sapelo2-sub2 ~$ pwd  
/home/zhuofei
```

← this is my home directory!

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

```
zhuofei@sapelo2-sub2 /$ cd /lustre1/zhuofei  
zhuofei@sapelo2-sub2 zhuofei$ pwd  
/lustre1/zhuofei
```

← this is my global scratch folder!

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

```
zhuofei@sapelo2-sub2 zhuofei$ ls  
user_test  workDir_Alex  workDir_bk
```


Step3 - 4: Create and cd to a working subdirectory

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

```
zhuofei@sapelo2-sub2 zhuofei$ mkdir workDir
zhuofei@sapelo2-sub2 zhuofei$ ls
user_test  workDir  workDir_Alex  workDir_bk
```

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

```
zhuofei@sapelo2-sub2 zhuofei$ cd workDir
zhuofei@sapelo2-sub2 workDir$ ls
zhuofei@sapelo2-sub2 workDir$
```

← it is empty!

Step5: Transfer data from local computer to workDir - Mac/Linux

https://wiki.gacrc.uga.edu/wiki/Transferring_Files

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/ .
```

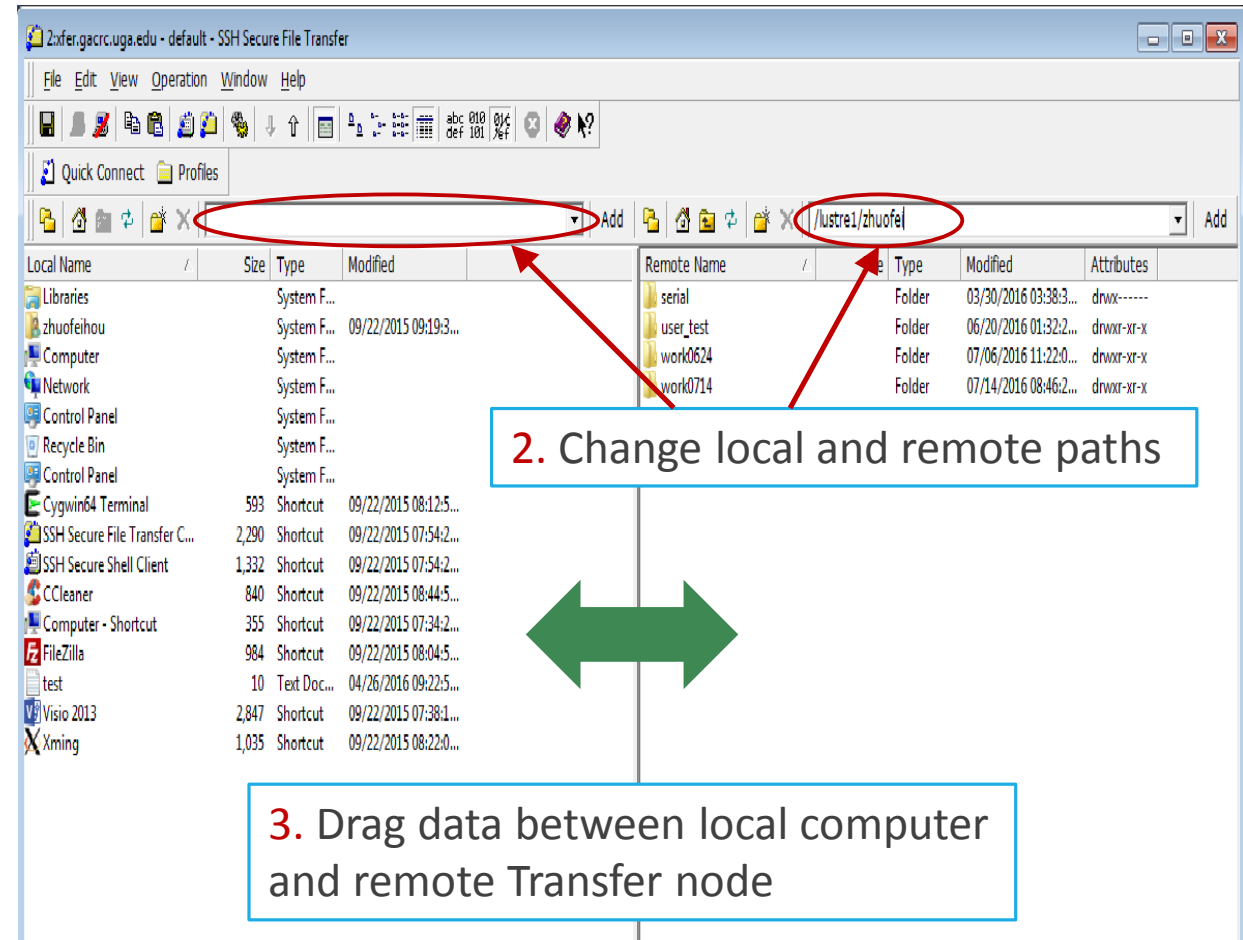
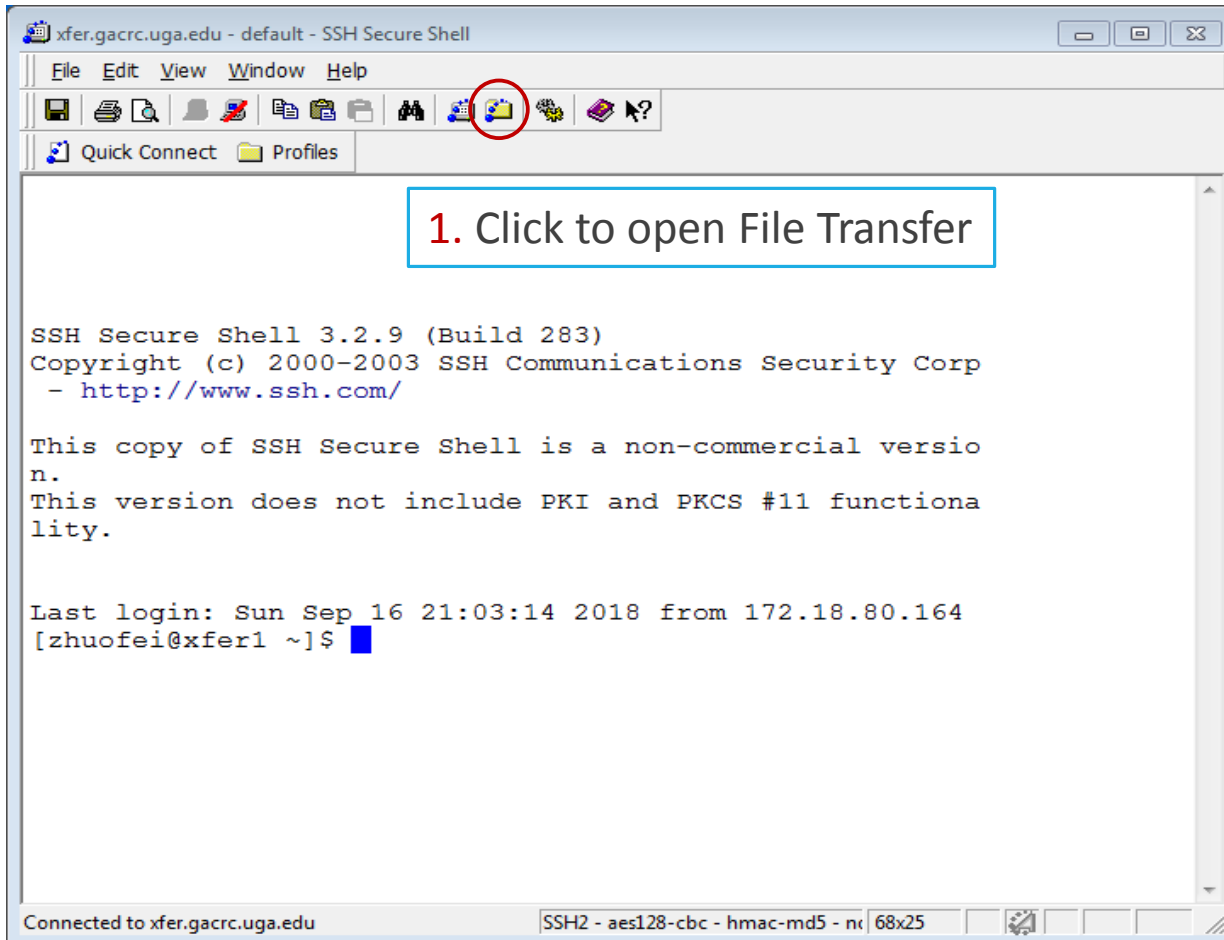
Step5 (Cont.) - Windows using SSH Secure Utilities

1. You need to connect to cluster's Transfer node (xfer.gacrc.uga.edu)
2. Use **SSH File Transfer** on local computer (alternative FileZilla or WinSCP)
3. Steps 1-8 are the same as steps on page 14-15, except for Host Name in step 5:

Host Name: xfer.gacrc.uga.edu

4. Step 9-10 are not required for logging on Transfer node, as of 2018-09-18
5. Once you log on, use File Transfer of SSH Secure Utilities, as shown on next page

Step5 (Cont.) - Windows using SSH Secure Utilities



Step5 (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 12)
 - ✓ Windows: use SSH Secure Utilities (page 19)
- Landing folder: `/home/MyID` (Home)
- Transfer data between folders on cluster using `cp`, `mv`
- Directories you can access using full path:
 1. `/home/MyID`
 2. `/lustre1/MyID`
 3. `/project/abclab`
- Most file systems on Transfer are *auto-mounted* upon the first time *full-path* access, e.g.,
`cd /project/abclab/`

Step6: Make a job submission script in workDir

https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_Sapelo2#Job_submission_Scripts

```
$ nano sub.sh
```

nano is a small and friendly text editor on Linux.

Ctrl-x to save file and quit from nano



```
zhuofei@n124:/lustre1/zhuofei/workDir
GNU nano 2.0.9 File: sub.sh Modified
hello nano! I am Zhuofei!
[ New File ]
^G Get Help      ^O WriteOut      ^R Read File     ^Y Prev Page     ^K Cut Text      ^C Cur Pos
^X Exit          ^J Justify       ^W Where Is     ^V Next Page     ^U UnCut Text    ^T To Spell
```

Step6 (Cont.)

1. Sample script on GACRC Wiki Software page:
<https://wiki.gacrc.uga.edu/wiki/Bowtie2-Sapelo2>
2. Modify it as needed for your computing

To run this example, you need to copy 3 files into your current working dir:

```
cp /usr/local/training/sub.sh .  
cp /usr/local/training/myreads.fq .  
cp -r /usr/local/training/index .
```

```
zhuofei@sapelo2-sub2:/lustre1/zhuofei/workDir  
File Edit View Search Terminal Help  
GNU nano 2.3.1 File: sub.sh Modified  
#PBS -S /bin/bash ← default Linux bash shell  
#PBS -q batch ← use batch queue  
#PBS -N bowtie2_test ← job name  
#PBS -l nodes=1:ppn=1: ← 1 compute node and 1 core from the node  
#PBS -l mem=2gb ← total RAM memory (enforced!)  
#PBS -l walltime=1:00:00 ← job running time on cluster (wall-clock time)  
  
#PBS -M zhuofei@uga.edu  
#PBS -m ae  
  
cd $PBS_0_WORKDIR  
  
module load Bowtie2/2.3.3-foss-2016b  
  
time bowtie2 -p 1 -x ./index/lambda_virus -U ./myreads.fq -S output.sam  
^G Get Help ^O WriteOut ^R Read File ^Y Prev Page ^K Cut Text ^C Cur Pos  
^X Exit ^J Justify ^W Where Is ^V Next Page ^U UnCut Tex ^T To Spell
```

Step7: Submit a job from workDir using qsub

https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_Sapelo2#How_to_submit_a_job_to_the_batch_queue

```
zhuofei@sapelo2-sub2 workDir$ pwd
/lustre1/zhuofei/workDir
zhuofei@sapelo2-sub2 workDir$ ls
index myreads.fq sub.sh
zhuofei@sapelo2-sub2 workDir$ qsub sub.sh
11943.sapelo2
```

sub.sh is job submission script to

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

Step8: Check job status using qstat_me

https://wiki.gacrc.uga.edu/wiki/Monitoring_Jobs_on_Sapelo2

```
zhuofei@sapelo2-sub2 workDir$ qstat_me
Job ID           Name           User           Time Use  S Queue
-----
11943.sapelo2   bowtie2_test   zhuofei       00:06:40  C batch
11944.sapelo2   bowtie2_test   zhuofei       00:05:17  R batch
11946.sapelo2   bowtie2_test   zhuofei       00:12:51  R batch
11947.sapelo2   bowtie2_test   zhuofei              0  R batch
11948.sapelo2   bowtie2_test   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 24 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!

Step8 (Cont.): Cancel job using qdel

https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_Sapelo2#How_to_delete_a_running_or_pending_job

```
zhuofei@sapelo2-sub2 workDir$ qdel 11947
zhuofei@sapelo2-sub2 workDir$ qstat_me
```

Job ID	Name	User	Time Use	S	Queue
11943.sapelo2	bowtie2_test	zhuofei	00:06:40	C	batch
11944.sapelo2	bowtie2_test	zhuofei	00:05:17	R	batch
11946.sapelo2	bowtie2_test	zhuofei	00:12:51	R	batch
11947.sapelo2	bowtie2_test	zhuofei	00:00:09	C	batch
11948.sapelo2	bowtie2_test	zhuofei	00:00:00	Q	batch



job 11947 status is changed from R to C
C status will stay in list for ~24 hour

Step8 (Cont.): Check Job using qstat -n -u MyID

https://wiki.gacrc.uga.edu/wiki/Monitoring_Jobs_on_Sapelo2

```
zhuofei@sapelo2-sub2 workDir$ qstat -n -u zhuofei
```

```
dispatch.ecompute:
```

Job ID	Username	Queue	Jobname	SessID	NDS	TSK	Req'd Memory	Req'd Time	S	Elap Time
12175.sapelo2	zhuofei	batch	bowtie2_test	132442	1	1	2gb	01:00:00	R	00:23:44
n238/0	← job is running on node238/CPU0									
12176.sapelo2	zhuofei	batch	bowtie2_test	67226	1	1	2gb	01:00:00	R	00:20:44
n237/0										
12177.sapelo2	zhuofei	batch	bowtie2_test	119643	1	1	2gb	01:00:00	R	00:05:44

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

Step8 (Cont.): Check all Jobs on cluster using qstat

https://wiki.gacrc.uga.edu/wiki/Monitoring_Jobs_on_Sapelo2

```

zhuofei@sapelo2-sub2 workDir$ qstat
Job ID          Name          User          Time Use S Queue
-----
11267.sapelo2   L80-500       jx57780       164:32:5   R batch
11269.sapelo2   L80-502       jx57780       164:55:5   C batch
11270.sapelo2   L80-503       jx57780       165:38:5   C batch
11607.sapelo2   canu          gd98309       3414:46:   R bergman_q
11726.sapelo2   ..._3_constoptTS sm39091       3157:30:   R wheeler_q
11729.sapelo2   ..._2_constoptTS sm39091       2731:29:   R wheeler_q
11790.sapelo2   sp2_run19b_dye castelao      4412:52:   C batch
11804.sapelo2   ...e-4_Nnoise=64 cotter        98:26:20   R batch
11806.sapelo2   ...e-4_Nnoise=64 cotter        98:14:22   R batch
11987.sapelo2   ..._th_W18-T5-L4 qbcg          08:02:40   C batch
11989.sapelo2   matlabjob     zhyw86        0 C batch
11990.sapelo2   ..._1_constoptTS sm39091       445:42:1   R wheeler_q
11991.sapelo2   ..._1_constoptTS sm39091       444:51:4   R wheeler_q
11992.sapelo2   ..._cl_W18-T3-D1 qbcg          03:04:21   C batch
.
.

```

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

Step8 (Cont.): Check all Jobs on cluster using qstat

https://wiki.gacrc.uga.edu/wiki/Monitoring_Jobs_on_Sapelo2

```
zhuofei@sapelo2-sub2 workDir$ qstat
Job ID          Name                User                Time Use S Queue
-----
11267.sapelo2   L80-500             jx57780             164:32:5 R batch
11269.sapelo2   L80-502             jx57780             164:55:5 C batch
11270.sapelo2   L80-503             jx57780             165:38:5 C batch
11607.sapelo2   canu                gd98309             3414:46: R bergman_q
11726.sapelo2   ..._3_constoptTS   sm39091             3157:30: R wheeler_q
11729.sapelo2   ..._2_constoptTS   sm39091             2731:29: R wheeler_q
11790.sapelo2   sp2_run19b_dye     castelao            4412:52: C batch
11804.sapelo2   ...e-4_Nnoise=64   cotter              98:26:20 R batch
11806.sapelo2   ...e-4_Nnoise=64   cotter              98:14:22 R batch
11987.sapelo2   ..._th_W18-T5-L4   qbcg                08:02:40 C batch
11989.sapelo2   matlabjob          zhyw86              0 C batch
11990.sapelo2   ..._1_constoptTS   sm39091             445:42:1 R wheeler_q
11991.sapelo2   ..._1_constoptTS   sm39091             444:51:4 R wheeler_q
11992.sapelo2   ..._cl_W18-T3-D1   qbcg                03:04:21 C 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 MyID@sapel01.gacrc.uga.edu`



Windows user:



Login



2. `cd /lustre1/MyID`

3. `mkdir ./workDir`

4. `cd ./workDir`



lustre1

6. `nano ./sub.sh`

```
#PBS -S /bin/bash
#PBS -q batch
#PBS -N bowtie2_test
#PBS -l nodes=1:ppn=1
#PBS -l mem=2gb
#PBS -l walltime=1:00:00

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

cd $PBS_O_WORKDIR

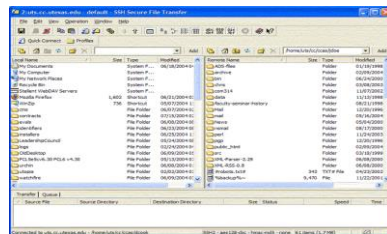
module load Bowtie2/2.3.3-foss-2016b.....
```

5. Linux/Mac user:

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



Windows user:



8. `$ qstat_me or qdel JobID`

7. `$ qsub sub.sh`

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

Running Jobs: https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_Sapelo2

Monitoring Jobs: https://wiki.gacrc.uga.edu/wiki/Monitoring_Jobs_on_Sapelo2

Job Submission Queue: https://wiki.gacrc.uga.edu/wiki/Job_Submission_Queues

Software: <https://wiki.gacrc.uga.edu/wiki/Software>

Transfer File: https://wiki.gacrc.uga.edu/wiki/Transferring_Files

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

Training: <https://wiki.gacrc.uga.edu/wiki/Training>

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

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

➤ **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

Please note to make sure the correctness of datasets being used by your jobs!

Request Support

* indicates Required fields.

Your Name *

MyID *

E-mail *

Phone Number

Brief Description

Request Details *

(less than 2,000 characters)

Cluster

sapelo2 sapelo teach other

* For questions on cluster or software, please include the command/script used, working path and working nodes (interactive / queue name) if applicable.

* For software installation, please specify software name, version and include link to the software if applicable.

* Please review your message on the next page and then click the Submit button.

Appendix: Examples of Batch Serial/Threaded/MPI Job Scripts

https://wiki.gacrc.uga.edu/wiki/Sample_Scripts

- 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
 - ✓ maximum wallclock time
 2. load software using **ml load** (for cluster software)
 3. run any Linux commands you want to run, e.g., pwd, mkdir, cd, echo, etc.
 4. run the software
 - **Input data** for analysis, if have
- Common queueing commands you need:
 - **qsub, qstat_me, qstat, qdel**
 - **qstat -f, showq**

Example 1: **Serial job script** running NCBI Blast+ using **1 CPU**

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

cd $PBS_O_WORKDIR

ml load BLAST+/2.6.0-foss-2016b-Python-2.7.14
time blastn [options] ...
```

- Linux default shell (bash)
- **Queue name** (batch)
- Job name (testBlast)
- **Number of nodes** (1), **number of cores** (1), **node feature is NOT needed!**
- Maximum amount of **RAM memory** (20 GB) is **enforced** by the cluster!
- **Maximum wall-clock time** (48 hours) for the job, default **6** minutes
- Compute node will use the directory from which the job is submitted as the working directory, i.e., /lustre1/MyID/workDir
- Load the module of ncbiblast+, version 2.6.0
- Run blastn with 'time' command to measure the amount of time it takes to run the application

<https://wiki.gacrc.uga.edu/wiki/BLAST%2B-Sapelo2>

*Example 2: Threaded job script running NCBI Blast+ using 4 CPUs

```
#PBS -S /bin/bash
#PBS -q batch
#PBS -N testBlast
#PBS -l nodes=1:ppn=4
#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

ml load BLAST+/2.6.0-foss-2016b-Python-2.7.14

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

→ Number of nodes (1), number of cores (4)
Number of cores requested (4) = Number of threads (4)

→ Email address to receive a notification for computing resources
→ Send email notification when job aborts (a) or terminates (e)
→ Standard error file (testBlast.e12345) will be merged into standard out file (testBlast.o12345)

→ Run blastn with 4 threads (-num_threads 4)

*Example 3: MPI job script running RAxML using 2 full nodes

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

```
#PBS -q batch
```

```
#PBS -N testRAxML
```

```
#PBS -l nodes=2:ppn=28
```

```
#PBS -l walltime=120:00:00
```

```
#PBS -l mem=100gb
```

→ Number of nodes (2), number of cores (28)

Total cores requested = $2 \times 28 = 56$

We suggest, Number of MPI Processes (50) \leq Number of cores requested (56)

```
cd $PBS_O_WORKDIR
```

```
ml load RAxML/8.2.11-foss-2016b-mpi-avx
```

→ To run raxmlHPC-MPI-AVX, MPI version using OpenMPI

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

→ Run raxmlHPC-MPI-AVX with 50 MPI processes (-np 50),
default 56

Guideline Tips

- Do NOT use Login node to run CPU/memory intensive jobs directly → submit jobs to queue!
- Do NOT use Login Node to upload/download large data to/from cluster → use Transfer node!
- Do NOT use home dir for storing large job data → use global scratch /lustre1/MyID
- Do NOT park data on global or local scratch → clean up when job finished or exits from node
- NO large memory job running on batch or jlm_q → use highmem_q
- NO small memory job running on highmem_q → use batch or jlm_q
- 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! ✅

Thank You!

Telephone Support

EITS Help Desk: 706-542-3106

Monday – Thursday: 7:30 a.m. – 7:30 p.m.

Friday: 7:30 a.m. – 6 p.m.

Saturday – Sunday: 1 p.m. – 7 p.m.

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