GACRC Sapelo2 Cluster New User Training

Georgia Advanced Computing Resource Center (GACRC)

Enterprise Information Technology Services(EITS)

The University of Georgia

Outline

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- Sapelo2 Cluster
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  - Five Computational Partitions
  - Software Environment
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GACRC

- A high-performance-computing (HPC) center at the UGA
- 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

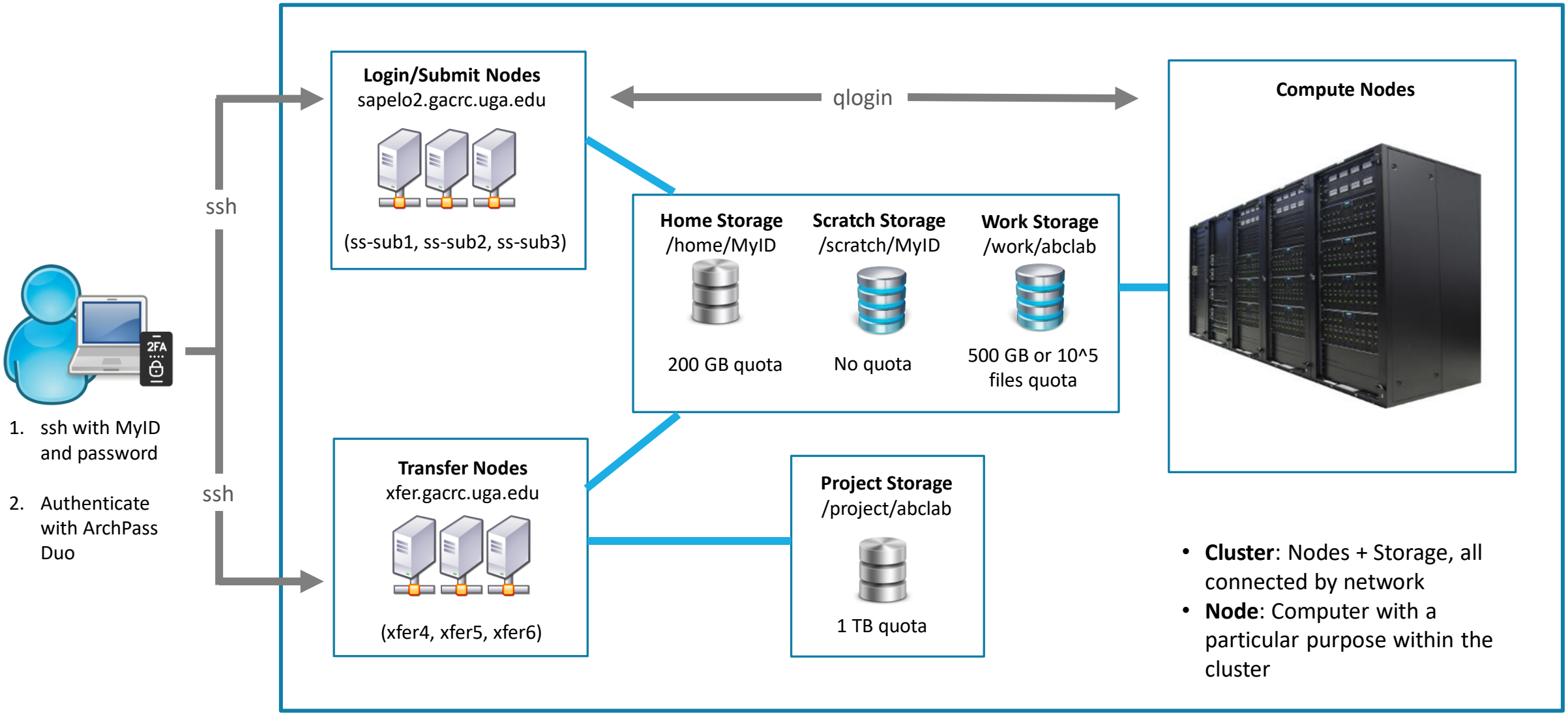
Wiki: http://wiki.gacrc.uga.edu

Help and Support: https://wiki.gacrc.uga.edu/wiki/Getting_Help

Web Site: http://gacrc.uga.edu

Kaltura Channel: https://kaltura.uga.edu/channel/GACRC/176125031

Sapelo2 Cluster



1. ssh with MyID and password
2. Authenticate with ArchPass Duo

- **Cluster**: Nodes + Storage, all connected by network
- **Node**: Computer with a particular purpose within the cluster

Note: You need to connect to the UGA network using VPN when accessing from outside of the **UGA main campus**.
UGA VPN: https://eits.uga.edu/access_and_security/infosec/tools/vpn/

Five Directories https://wiki.gacrc.uga.edu/wiki/Disk_Storage

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Directory	Name	Quota	Accessible from	Intended Use	Backed-up	Important Notes
/home/MyID	Home	200GB	**Login** **Transfer** **Compute**	Static data, e.g. 1. Scripts, source codes 2. Local software	Yes	Not for storing data of your jobs!
/scratch/MyID	Scratch	No Limit	**Login** **Transfer** **Compute**	Temporary files needed for currently running jobs	No	Clean up when your job finishes! Subject to "30-day purge" policy
/work/abclab	Work	500GB 10^5 files	**Login** **Transfer** **Compute**	Input files needed for repeated jobs	No	Clean up when your job finishes! Group sharing is possible
/project/abclab	Project	1TB (initial)	**Transfer**	Temporary data parking	Yes	Group sharing is possible
/lscratch	Local Scratch	200GB - 800GB	**Compute**	Jobs with heavy disk I/O operations	No	Clean up when job exits from node!

Scratch File System 30-Day Purge Policy

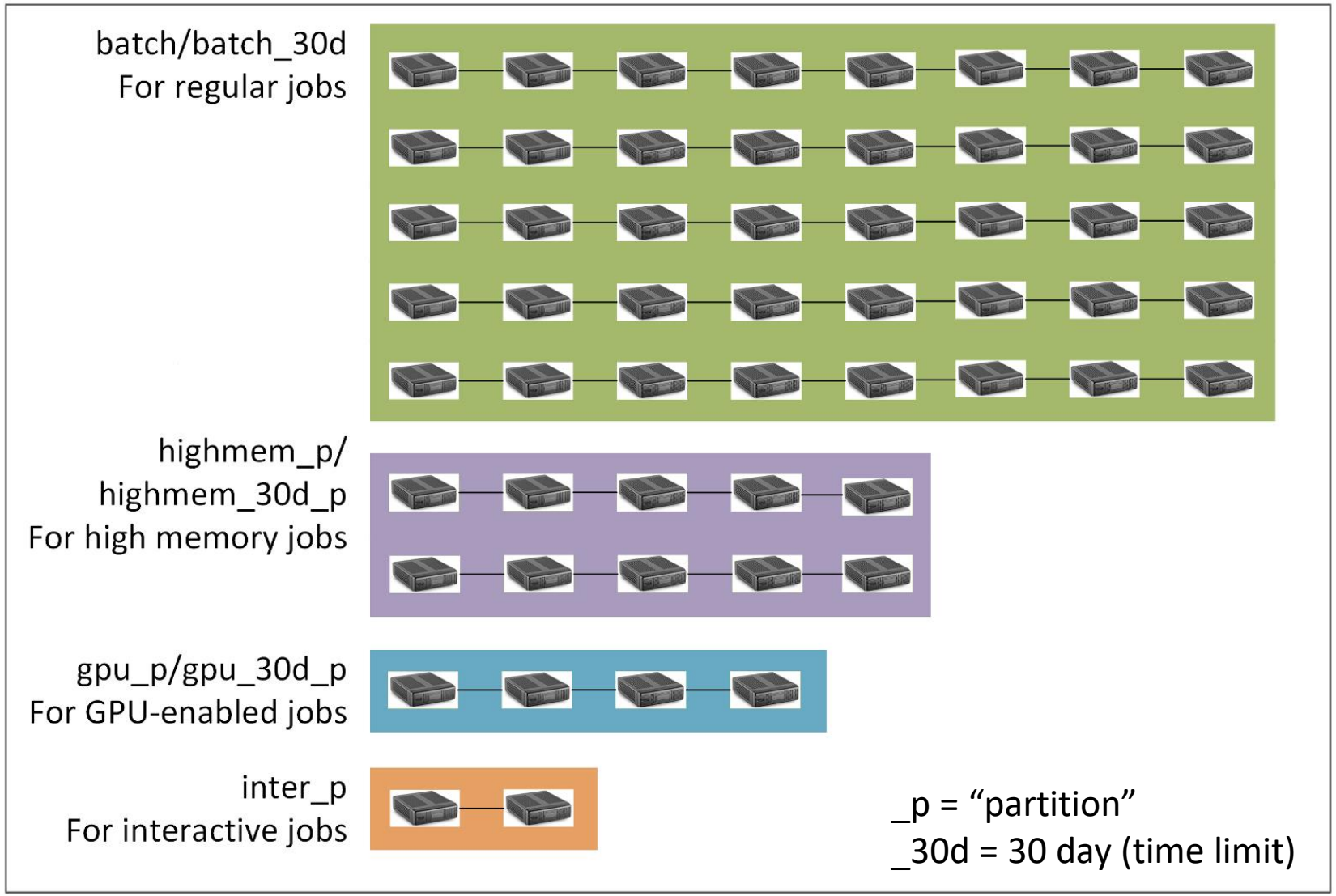
https://wiki.gacrc.uga.edu/wiki/Disk_Storage#Scratch_file_system

Any file that is not accessed or modified by a compute job in a time period no longer than 30 days will be automatically deleted off the /scratch file system.

Measures circumventing this policy will be monitored and actively discouraged.

- You have a list of those purgeable files located at /usr/local/var/lustre_stats/$USER.over30d.files.lst
- You are suggested to copy files from your /scratch directory to /project or outside of GACRC
- To get rid of files in your /scratch directory that you no longer need, move them to /scratch/trash/$USER
- The fastest way to save old files is to copy them to /project area, using the fpsync utility on xfer.gacrc.uga.edu
- When you archive data using tar on /scratch, please do not use z option (compression option). After you archived data by tar, you can use gzip to compress it.

Computational Partitions



Compute nodes are divided into groups called **partitions**. A **partition** is a collection of compute nodes for a particular computing need.

Computational Partitions

https://wiki.gacrc.uga.edu/wiki/Job_Submission_partitions_on_Sapelo2
https://wiki.gacrc.uga.edu/wiki/Systems#Sapelo2

Type	Partition	Time limit	Max jobs Running	Max jobs Submit	Notes
Regular	batch	7 days	250	10,000	Regular nodes
	highmem_p		15	100	For running high memory jobs
	gpu_p		18	20	For running GPU-enabled jobs
Long-term	batch_30d	30 days	1	2	30-day partition counterparts
	highmem_30d_p				
	gpu_30d_p		2		
Interactive	inter_p	2 days	3	20	Regular nodes, for interactive jobs.
Buy-in	name_p	variable			Partitions that target different groups' buy-in nodes. The name string is specific to each group.

Partition	Total Nodes	Max Mem(GB) /Single-node job	Cores /Node	Processor Type	GPU Cards /Node
batch batch_30d	~275	120	**64**	AMD EPYC	N/A
			32		
			48	AMD Opteron	
		180	32	Intel Xeon Skylake	
		58	28	Intel Xeon Broadwell	
highmem_p highmem_30d_p	~30	500	32	AMD EPYC	N/A
			48	AMD Opteron	
		990	**64**	AMD EPYC	
			28	Intel Xeon Broadwell	
			48	AMD Opteron	
gpu_p gpu_30d_p	~10	**180**	**32**	Intel Xeon Skylake	1 NVDIA P100
		120	16	Intel Xeon	8 NVIDIA K40m
		90	12		7 NVIDIA K20Xm
name_p	variable				

Software Environment

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

- Approximately 900 software modules are installed (as of March 2021)
- Most modules are compiled EasyBuild (EB) toolchains GCC-8.3.0 or foss-2019b.
- Name format: Name/Version-Toolchain, e.g., Python/3.8.2-GCCcore-8.3.0 (case-sensitive)
- Module commands:
  - ml spider *pattern* : Search module names matching a *pattern*
  - ml *moduleName* : Load a module into your working environment
    - **DO NOT LOAD/USE MODULES ON THE LOGIN/SUBMIT NODES! (ss-sub1, ss-sub2, ss-sub3, etc…)**
  - ml av : List all available software modules installed on cluster
  - ml : List modules currently loaded
  - ml *-moduleName* : Remove a module from working environment
  - ml purge : Remove all modules from working environment

Important Tip using Software

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

- When you load more than one software modules, toolchain compatibility is the most important thing you need to pay attention to
- If you load more than one module and some toolchains are incompatible, your job will end up with failing dependencies or Lmod errors, such as:

Lmod has detected the following error:
These module(s) exist but cannot be loaded as requested

✗
ml Python/3.7.4-GCCcore-8.3.0
ml Perl/5.28.0-GCCcore-7.3.0

✓
ml Python/3.7.4-GCCcore-8.3.0
ml Perl/5.30.0-GCCcore-8.3.0

✗
ml Beast/2.6.3-foss-2019b
ml Perl/5.28.0-GCCcore-7.3.0

✓
ml Beast/2.6.3-foss-2019b
ml Perl/5.30.0-GCCcore-8.3.0

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 your scratch space: `cd /scratch/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 WinSCP 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 : `sbatch ./sub.sh`
8. Check job status : `squeue --me` or Cancel a job : `scancel jobID`

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

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

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@localhost ~]$
[zhuofei@localhost ~]$ ssh zhuofei@sapelo2.gacrc.uga.edu      ← Log on
Password:                                                     ← Input MyID password!
……
Enter a passcode or select one of the following options:
 1. Duo Push to XXX-XXX-5758
 2. Phone call to XXX-XXX-5758
 3. Phone call to XXX-XXX-1925
 4. SMS passcodes to XXX-XXX-5758

Passcode or option (1-5): 1                                   ← Select Duo authentication option!
Success. Logging you in...
Last login: Tue Sep 15 11:22:42 2020 from 128.192.75.65

zhuofei@ss-sub1 ~$                                            ← I am on login node ss-sub1!
```

Step1 (Cont.) - Windows using PuTTY

1. Download and install PuTTY: https://www.putty.org/

2. Detailed downloading and installation instructions:

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

3. Detailed configuring and usage instructions:

   https://wiki.gacrc.uga.edu/wiki/How_to_Install_and_Configure_PuTTY#Configuring_PuTTY

Step1 (Cont.) - Windows using PuTTY

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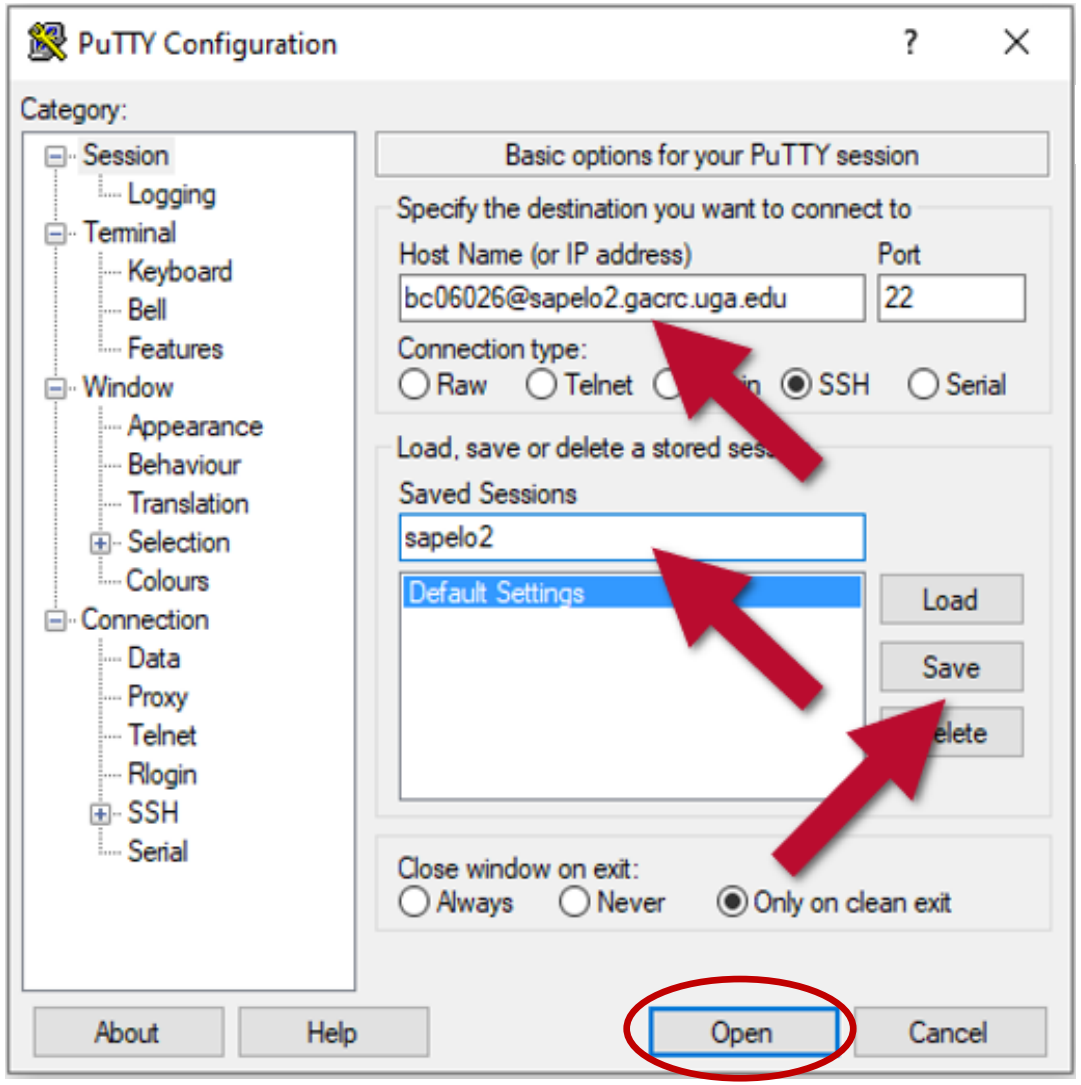
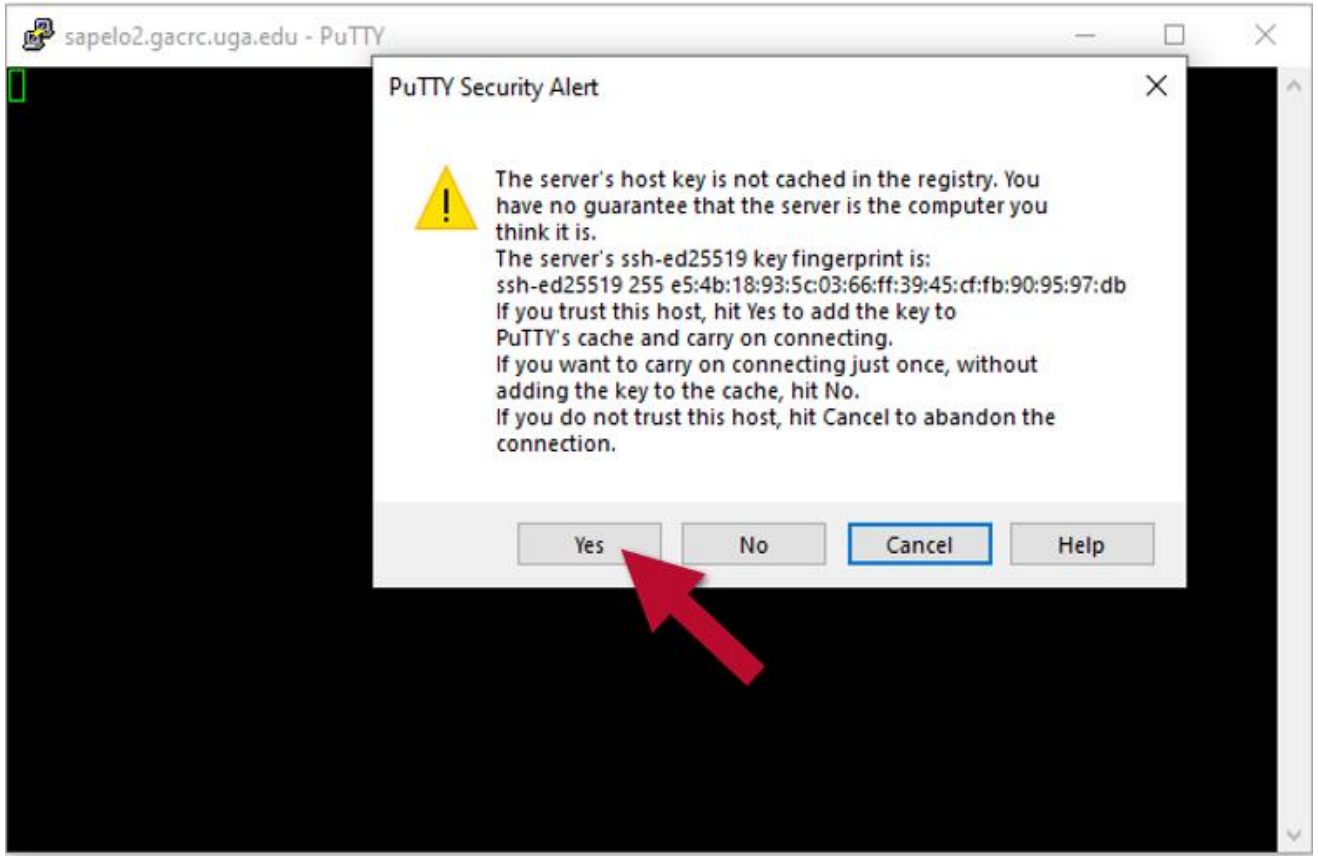


The first time you connect to login node, PuTTY will give you this security alert window. Please click "Yes"



Step1 (Cont.) - Windows using PuTTY

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Next you will enter your UGA MyID password and initiate DUO authentication procedure:

sapelo2.gacrc.uga.edu - PuTTY

```
Using username "bc06026".
Keyboard-interactive authentication prompts from server:
|
| UGA DUO authentication is required for SSH/SCP access to
| GACRC systems.
|
| UGA DUO is a two-factor authentication service which
| requires a password (one factor) and a code, phone,
| or device (second factor) to successfully authenticate.
|
| If you are not enrolled in the UGA DUO service please
| visit the UGA DUO service self-service portal to enroll
| and configure or manage your DUO enabled devices.
|
| https://eits.uga.edu/access_and_security/infosec/tools/duo/portal/
|
| For additional help with UGA DUO authentication or to
| report an issue please visit:
|
| https://eits.uga.edu/access_and_security/infosec/tools/archpass/
|
| Password:
```

← UGA MyID password

sapelo2.gacrc.uga.edu - PuTTY

```
| requires a password (one factor) and a code, phone,
| or device (second factor) to successfully authenticate.
|
| If you are not enrolled in the UGA DUO service please
| visit the UGA DUO service self-service portal to enroll
| and configure or manage your DUO enabled devices.
|
| https://eits.uga.edu/access_and_security/infosec/tools/duo/portal/
|
| For additional help with UGA DUO authentication or to
| report an issue please visit:
|
| https://eits.uga.edu/access_and_security/infosec/tools/archpass/
| 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-5758
|  3. Phone call to XXX-XXX-1925
|  4. Phone call to XXX-XXX-3535
|  5. SMS passcodes to XXX-XXX-5758
|
| Passcode or option (1-5): 1
```

← DUO option

Step2: On Login node change directory to global scratch

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

```
zhuofei@ss-sub1 ~$ pwd
/home/zhuofei
```

← this is my home directory!

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

```
zhuofei@ss-sub1 ~$ cd /scratch/zhuofei/
zhuofei@ss-sub1 zhuofei$ pwd
/scratch/zhuofei
```

← this is my scratch space!

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

```
zhuofei@ss-sub1 zhuofei$ ls
user_test
```

Step3 - 4: Create and cd to a working subdirectory

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

```
zhuofei@ss-sub1 zhuofei$ mkdir workDir
zhuofei@ss-sub1 zhuofei$ ls
user_test  workDir
```

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

```
zhuofei@ss-sub1 zhuofei$ cd workDir
zhuofei@ss-sub1 workDir$ pwd
/scratch/zhuofei/workDir
zhuofei@ss-sub1 workDir$ ls
```

← it is empty!

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

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

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:/scratch/zhuofei/workDir/
```

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

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

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

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

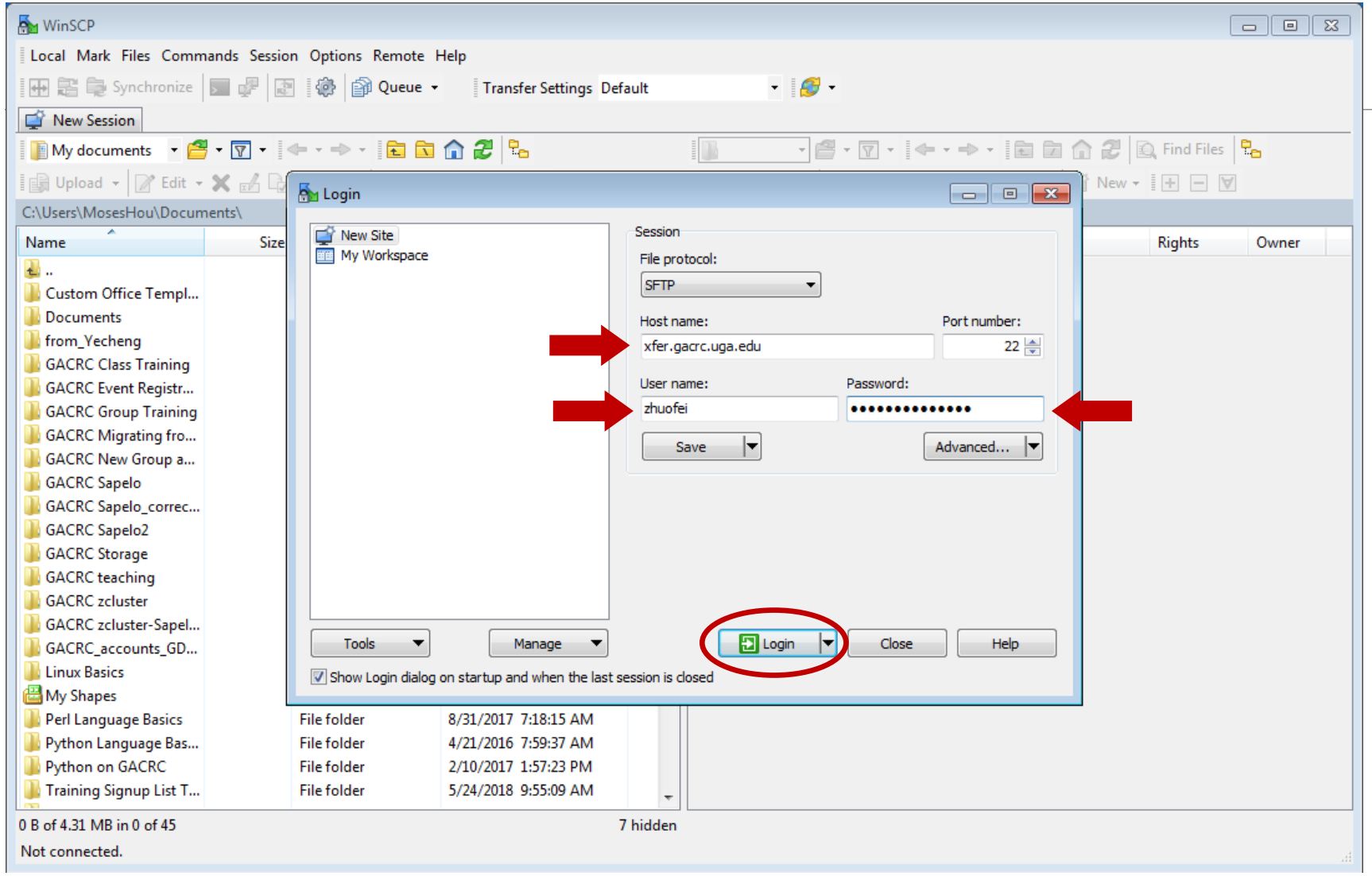
Step5 (Cont.) - Windows using WinSCP

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

1. You need to connect to cluster's Transfer node (xfer.gacrc.uga.edu)
2. Use WinSCP on local computer
   - WinSCP can be downloaded from https://winscp.net/eng/index.php
   - Default installation procedure is simple
3. Alternative FileZilla https://wiki.gacrc.uga.edu/wiki/Transferring_Files#Using_FileZilla

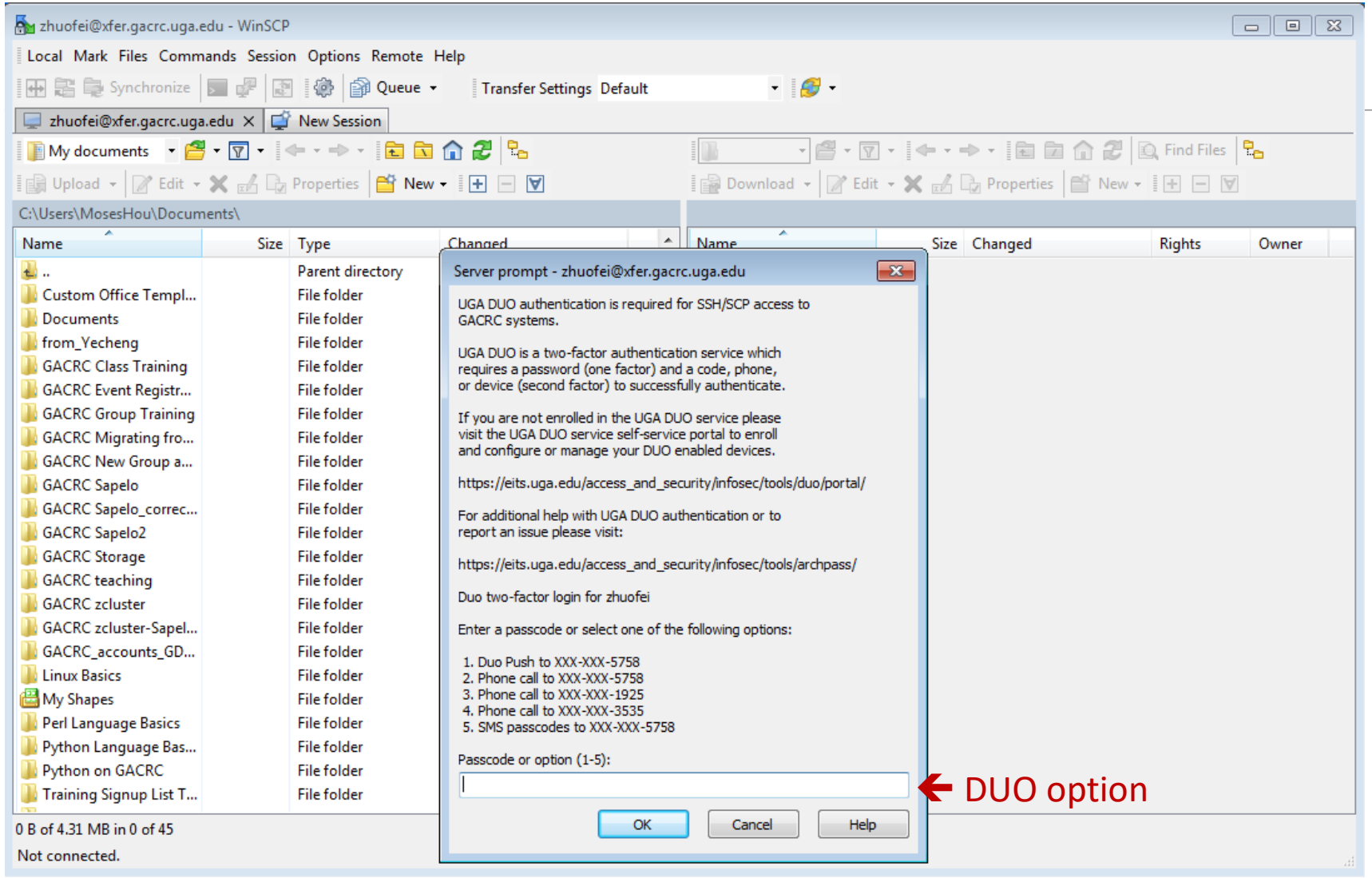
Step5 (Cont.) - Windows using WinSCP

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



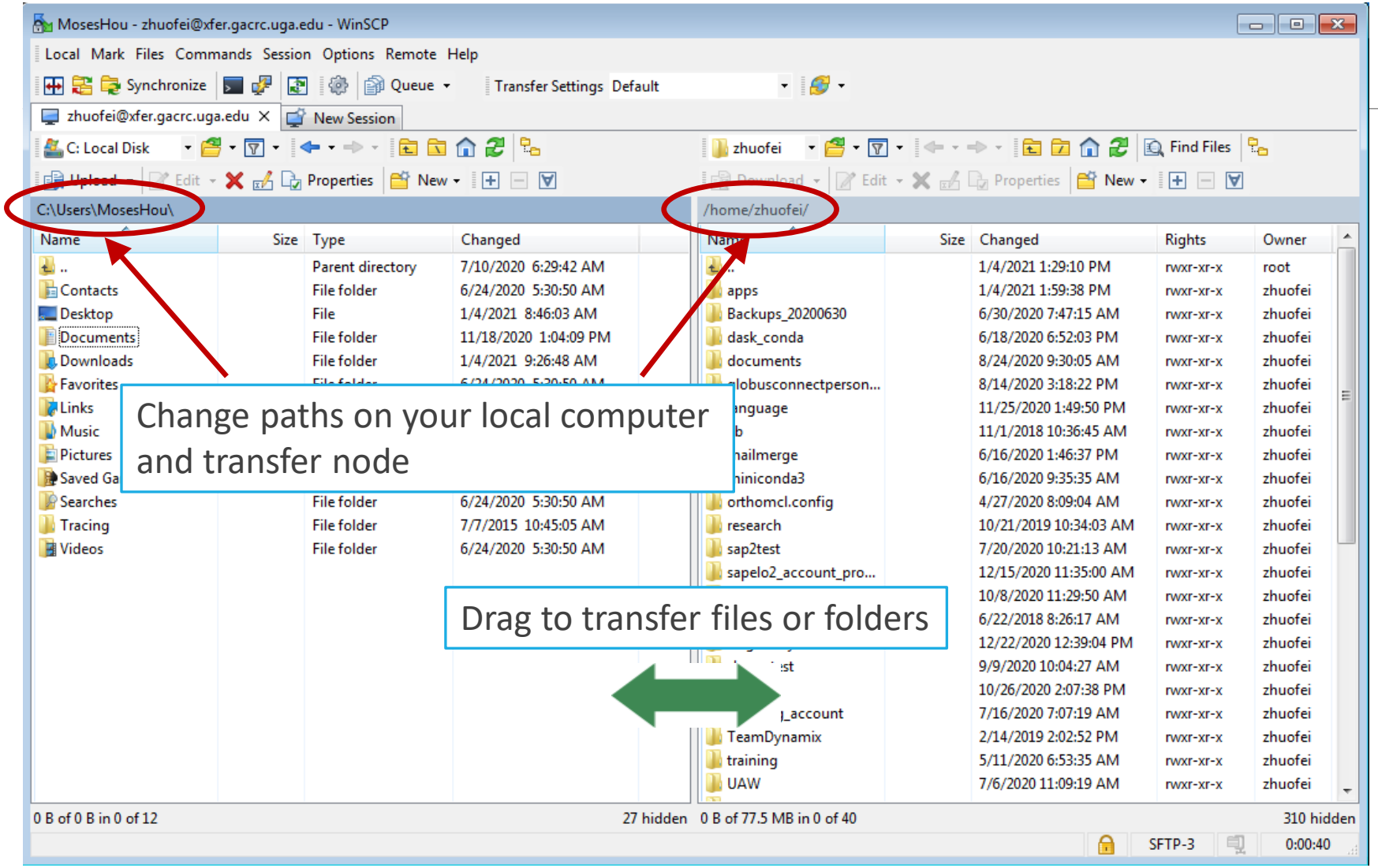
Step5 (Cont.) - Windows using WinSCP

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



Step5 (Cont.) - Windows using WinSCP

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



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 15-16)
  - ✓ Windows: use PuTTY to log in MyID@xfer.gacrc.uga.edu (page 17-19)
- Landing folder: /home/MyID (Home)
- You can transfer data between following directories on cluster using cp or mv:
  1. /home/MyID (Home)
  2. /scratch/MyID (Scratch)
  3. /work/abclab (Work)
  4. /project/abclab (Project)
- Most file systems on Transfer are *auto-mounted* upon *the first time full-path access*, e.g., cd /project/abclab/

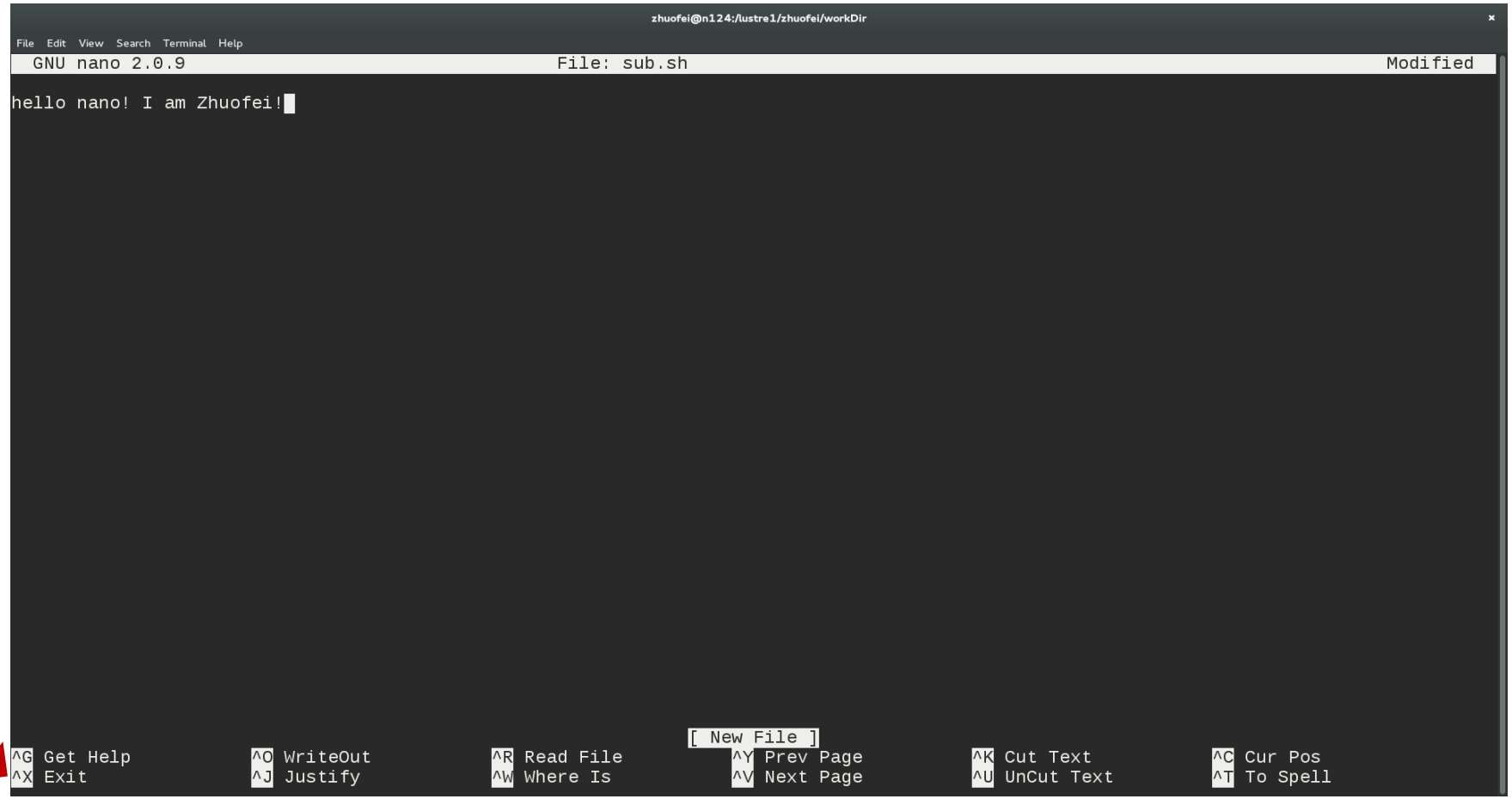
Step6: Make a job submission script in workDir

https://wiki.gacrc.uga.edu/wiki/Sample_batch_job_submission_scripts_on_Sapelo2

```
$ nano sub.sh
```

nano is a simple text editor on Linux. You are welcome to use other editors like vim or emacs.

Ctrl-x to save file and quit from nano



```
  GNU nano 2.3.1                File: sub.sh                          Modified

#!/bin/bash
#SBATCH --job-name=testBowtie2          # Job name (testBowtie2)
#SBATCH --partition=batch               # Queue name (batch)
#SBATCH --ntasks=1                      # Run single task using one CPU core on a single node
#SBATCH --mem=4G                        # Job memory limit (4 GB)
#SBATCH --time=1:00:00                  # Time limit hrs:min:sec or days-hours:minutes:seconds
#SBATCH --export=NONE                   # Do not load any users' explicit environment variables
#SBATCH --output=%x_%j.out              # Standard output, testBowtie2_1234.out
#SBATCH --error=%x_%j.err               # Standard error log, testBowtie2_1234.err
#SBATCH --mail-type=END,FAIL            # Mail events (BEGIN, END, FAIL, ALL)
#SBATCH --mail-user=username@uga.edu    # Where to send mail

cd $SLURM_SUBMIT_DIR                    # Change directory to job submission directory
ml Bowtie2/2.4.1-GCC-8.3.0              # Load software module and run bowtie2 below

bowtie2  -x  ./index/lambda_virus  -U  ./myreads.fq  -S  output.sam

^G Get Help    ^O WriteOut    ^R Read File   ^Y Prev Page   ^K Cut Text
^X Exit        ^J Justify     ^W Where Is    ^V Next Page   ^U UnCut Te
```

To run the demo example, please copy these files into your working dir:

```
cp  -r /usr/local/training/Sapelo2/*  .
```

Step7: Submit a job from workDir using sbatch

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

```
zhuofei@ss-sub1 workDir$ pwd
/scratch/zhuofei/workDir
zhuofei@ss-sub1 workDir$ ls
index  myreads.fq  sub.sh
zhuofei@ss-sub1 workDir$ sbatch sub.sh
Submitted batch job 32860
```

sub.sh is a 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

Step8: Check job status using squeue --me

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

```
zhuofei@ss-sub1 workDir$ squeue --me
JOBID PARTITION     NAME     USER  ST      TIME  NODES    NODELIST(REASON)
32862     batch testBowt  zhuofei  PD      0:00      1    (None)
32861     batch testBowt  zhuofei   R      0:05      1    c5-19
32860     batch testBowt  zhuofei   R      4:37      1    c5-19
32859     batch testBowt  zhuofei  CD      9:29      1    b1-2
```

R : job is Running
PD : job is PenDing, waiting for resources to become available
CD : job is CompleteD and is not longer running
CA : job is CAnceled and is not longer running
F : job is Failed (crashed) on the node and is not longer running

Note: “TIME” is the elapsed wall-clock time of your job running on cluster, instead of the CPU time.

Step8: Check job status using squeue --me -l

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

```
zhuofei@ss-sub1 workDir$ squeue --me -l
Tue Sep 15 15:00:51 2020
JOBID PARTITION     NAME     USER    STATE       TIME TIME_LIMI  NODES NODELIST(REASON)
32866     batch testBowt  zhuofei  RUNNING       0:14   1:00:00      1 rc6-10
32865     batch testBowt  zhuofei  RUNNING       0:30   1:00:00      1 rc6-10
32864     batch testBowt  zhuofei  RUNNING       0:33   1:00:00      1 rc6-10
```

Step8 (Cont.): Cancel job using scancel

https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_Sapelo2#How_to_cancel_.28delete.29_a_running_or_pending_job

```
zhuofei@ss-sub1 workDir$ squeue --me -l
Tue Sep 15 15:08:27 2020
JOBID PARTITION     NAME     USER    STATE       TIME TIME_LIMI  NODES NODELIST(REASON)
32869     batch testBowt  zhuofei  RUNNING       0:01   1:00:00      1 c5-19
32868     batch testBowt  zhuofei  RUNNING       0:05   1:00:00      1 c5-19
32867     batch testBowt  zhuofei  RUNNING       0:10   1:00:00      1 c5-19
zhuofei@ss-sub1 workDir$
zhuofei@ss-sub1 workDir$ scancel 32867
zhuofei@ss-sub1 workDir$ squeue --me -l
Tue Sep 15 15:08:45 2020
JOBID PARTITION     NAME     USER    STATE       TIME TIME_LIMI  NODES NODELIST(REASON)
32867     batch testBowt  zhuofei COMPLETI       0:26   1:00:00      1 c5-19
32869     batch testBowt  zhuofei  RUNNING       0:19   1:00:00      1 c5-19
32868     batch testBowt  zhuofei  RUNNING       0:23   1:00:00      1 c5-19
zhuofei@ss-sub1 workDir$ squeue --me -l
Tue Sep 15 15:08:50 2020
JOBID PARTITION     NAME     USER    STATE       TIME TIME_LIMI  NODES NODELIST(REASON)
32869     batch testBowt  zhuofei  RUNNING       0:19   1:00:00      1 c5-19
32868     batch testBowt  zhuofei  RUNNING       0:23   1:00:00      1 c5-19
```

```
bc06026@b1-24 workdir$ sacct
       JobID    JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
3326893      testBowti+      batch gacrc-ins+          1    RUNNING      0:0
3326893.bat+      batch           gacrc-ins+          1    RUNNING      0:0
3326893.ext+     extern           gacrc-ins+          1    RUNNING      0:0


bc06026@b1-24 workdir$ sacct -X
       JobID    JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
3326893      testBowti+      batch gacrc-ins+          1    RUNNING      0:0


bc06026@b1-24 workdir$ sacct -X --format jobid,state
       JobID      State
------------ ----------
3326893         RUNNING
bc06026@b1-24 workdir$
```

```
zhuofei@ss-sub1 workDir$ sacct-gacrc
JobID JobName  User  Partition  NodeList  AllocNodes  NTasks  NCPUS ReqMem MaxVMSize  State  CPUTime  Elapsed  Timelimit ExitCode WorkDir
------------ ---------- ---------- ---------- --------------- ---------- -------- ---------- ---------- ---------- ---------- ---------- ---------- -------- ------------------------------
275          bowti+   zhuofei  batch    rc6-10       1          1    4Gn                COMPLETED  00:09:13  00:09:13  01:00:00  0:0 /scratch/zhu..
275.batch    batch                      rc6-10       1      1   1    4Gn     396868K  COMPLETED  00:09:13  00:09:13            0:0
275.extern   extern                     rc6-10       1      1   1    4Gn     142616K  COMPLETED  00:09:13  00:09:13            0:0
276          amberjob shtsai  gpu_p    c4-23        1          1    10Gn               CANCELLED+ 00:03:19  00:03:19  02:00:00  0:0 /scratch/sht..
276.batch    batch                      c4-23        1      1   1    10Gn    221140K  CANCELLED  00:03:20  00:03:20            0:15
276.extern   extern                     c4-23        1      1   1    10Gn    169800K  COMPLETED  00:03:19  00:03:19            0:0
277          mpitest  shtsai  batch    c2-[11-12]   2          24   600Mc              COMPLETED  04:01:12  00:10:03  02:00:00  0:0 /scratch/sht..
277.batch    batch                      c2-11        1      1   12   600Mc   221268K  COMPLETED  02:00:36  00:10:03            0:0
277.extern   extern                     c2-[11-12]   2      2   24   600Mc   169800K  COMPLETED  04:01:12  00:10:03            0:0
277.0        orted                      c2-12        1      1   1    600Mc   265640K  COMPLETED  00:00:01  00:00:01            0:0
278          bash     shtsai  inter_p  c2-4         1          1    2Gn                RUNNING    00:13:37  00:13:37  12:00:00  0:0 /scratch/sht..
278.extern   extern                     c2-4         1      1   1    2Gn                RUNNING    00:13:37  00:13:37            0:0
278.0        bash                       c2-4         1      1   1    2Gn                RUNNING    00:13:37  00:13:37            0:0
```

```
zhuofei@ss-sub1 workDir$ sacct-gacrc-v 47939

JobID          47939
JobName        testBowti+
User           zhuofei
Partition      batch
NodeList       c1-3
AllocNodes     1
State          RUNNING
CPUTime        00:00:28
Elapsed        00:00:28
Timelimit      01:00:00
ExitCode       0:0
WorkDir        /scratch/zhuofei/workDir_sapelo2
NTasks         1
NCPUS          1
ReqMem         4Gn
```

```
zhuofei@ss-sub1 workDir$ seff 37259
Job ID: 37259
Cluster: tc2
User/Group: zhuofei/gacrc-instruction
State: COMPLETED (exit code 0)
Cores: 1
CPU Utilized: 00:09:45
CPU Efficiency: 99.66% of 00:09:47 core-walltime
Job Wall-clock time: 00:09:47
Memory Utilized: 197.34 MB
Memory Efficiency: 4.82% of 4.00 GB
```

Obtain Job Details

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

Option 1: `squeue --me` for details of a pending or running jobs

Option 2: `sacct` or `sacct-gacrc(-v)` for details of computing resource usage of a running or finished job

Option 3: `seff` for details of computing resource usage of a finished job

Option 4: Email notification from finished jobs (completed, canceled, or crashed), if using:

```
#SBATCH --mail-user=username@uga.edu

#SBATCH --mail-type=ALL
```

Interactive jobs

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

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

Description	Command
Start an interactive session	qlogin
Start an interactive session with X forwarding	xqlogin

qlogin	srun --pty -p inter_p --mem=2G --nodes=1 --ntasks-per-node=1 --time=12:00:00 --job-name=qlogin bash -l
xqlogin	srun --pty --x11 -p inter_p --mem=2G --nodes=1 --ntasks-per-node=1 --time=12:00:00 --job-name=xqlogin bash -l

GACRC Wiki http://wiki.gacrc.uga.edu
Kaltura channel https://kaltura.uga.edu/channel/GACRC/176125031

System: https://wiki.gacrc.uga.edu/wiki/Systems#Sapelo2

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

Software: https://wiki.gacrc.uga.edu/wiki/Software_on_Sapelo2

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

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

Sample scripts : https://wiki.gacrc.uga.edu/wiki/Sample_batch_job_submission_scripts_on_Sapelo2

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

GACRC Help and 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

When you ask GACRC to test or troubleshoot your jobs, Please make sure of the correctness of your datasets being used!

GACRC Service Catalog

Georgia Advanced Computing Resource Center (GACRC) service catalog

Services (11)

Account Creation
For a research group's PI to request user accounts for group members on the GACRC computing systems.

Class Account Creation
For an instructor to request user accounts for students attending a course that will need to use GACRC computing systems.

Class Account Modification
For instructors to request changes to be made in previously requested class account.

Computing Lab Modification/Deletion

General Internal

General Support
Report issues and request help with GACRC systems, except for software installation requests and account/lab creation requests.

Lab Creation
For a research group's PI to register a computing lab on the GACRC computing systems

Modify/Delete Account
For PIs to request changes in or deletion of user accounts on GACRC computing systems.

Software Installation/Update
Request software and common application database (e.g. NCBI blast databases) installation and upgrade.

My Recent Requests

- home directory is not fully provisioned: ss57215
- GACRC Sapelo2 New Lab/Use Account Request 2018-11-14_preTraining
- GACRC Sapelo2 Cluster New Lab/Use Account Request 2018-11-05_preTraining
- provision 5 user accounts for ugahelpdesk group
- GACRC Sapelo2 New Lab/Use Account Request 2018-10-22_preTraining

View All Recent Requests >

Popular Services

- EITS Help Desk Support Request
- MyID Account Request
- Change Request
- 02 Restricted VPN Access
- Terry Classroom & Meeting Room Support

View All Popular Services >

My Recently Visited Services

- Modify/Delete Account
- Class Account Creation

Service - General Support - Mozilla Firefox

File Edit View History Bookmarks Tools Help

Mail - zhuofei@uga.edu | Service - General Support

https://uga.teamdynamix.com/TDClient/Requests/ServiceDet?ID=25844

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General Support

If you do not have a myid, please mail gacrc-help@uga.edu, and we will respond promptly.

The purpose of this form is to provide a method to report issues and to request help with GACRC systems.

Please use this form for all questions and support needs (e.g. to report issues, to troubleshoot jobs, to request resources or grant writing help, etc). Please do not use this form for software installation requests or lab/user account management, which all have separate forms.

Please refer to the GACRC documentation for information on GACRC resources, how to connect and transfer files, how to run jobs, installed software list, training schedule, and a FAQ.

The link to this documentation is https://wiki.gacrc.uga.edu

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General Support

+ Show Help − Hide Help

Report issues and request help with GACRC systems, except for software installation requests and account/lab creation requests.

Short Description *

Email *

MyID *

Phone Number *

Support Needed For

- [ ] Galaxy
- [ ] Sapelo2
- [ ] Teaching Cluster
- [ ] Work Filesystem
- [ ] Home Filesystem
- [ ] Scratch Filesystem
- [ ] Project Filesystem
- [ ] Xfer Nodes
- [ ] Other

Lab *

Slurm job states

Code	State	Meaning
R	Running	Job is running on compute node(s)
PD	Pending	Job is waiting for compute node(s)
CD	Completed	Job completed
CG	Completing	Job is completing
CA	Canceled	Job was canceled
F	Failed	Job terminated with non-zero exit code
NF	Node Fail	Job terminated due to failure of node(s)

Commands for submitting and canceling jobs

Description	Slurm Command
Submit a batch job to queue	sbatch sub.sh
Delete a job from queue	scancel <jobID>
Cancel all your job(s)	scancel -u <username>
Cancel all your pending job(s)	scancel -t PENDING -u <username>
Cancel your job(s) by job name	scancel --name <jobname>
Cancel an element (index) of an array job (jobID)	scancel <jobID>_<index>

Commands for monitoring jobs

Description	Slurm Command
Command	squeue or squeue -l
Job status of all your jobs	squeue --me or squeue --me -l
Job status of a job	squeue -j <jobID>
Job status of job(s) from a user	squeue -u <username>
Job status with details	scontrol show job <job ID> scontrol show job -dd <job ID>
Job's resource usage	sacct-gacrc
View job batch script	scontrol write batch_script <job ID> [filename]

Slurm headers for running a Serial (single-core) job

https://wiki.gacrc.uga.edu/wiki/Sample_batch_job_submission_scripts_on_Sapelo2

```
#!/bin/bash
#SBATCH --job-name=testBowtie2          # Job name (testBowtie2)
#SBATCH --partition=batch               # Queue name (batch)
#SBATCH --ntasks=1                      # Run in a single task using one CPU core on a single node
#SBATCH --mem=4G                        # Job memory limit (4 GB)
#SBATCH --time=1:00:00                  # Time limit hrs:min:sec or days-hours:minutes:seconds
#SBATCH --export=NONE                   # Do not load any users' explicit environment variables
#SBATCH --output=%x_%j.out              # Standard output log, e.g., testBowtie2_1234.out
#SBATCH --error=%x_%j.err               # Standard error log, e.g., testBowtie2_1234.err
#SBATCH --mail-type=END,FAIL            # Mail events (BEGIN, END, FAIL, ALL)
#SBATCH --mail-user=username@uga.edu    # Where to send mail

cd $SLURM_SUBMIT_DIR                    # Change directory to job submission directory
ml Bowtie2/2.4.1-GCC-8.3.0              # Load software module and run bowtie2 below
bowtie2  -x  ./index/lambda_virus  -U  ./myreads.fq  -S  output.sam
```

Slurm headers for running a Threaded job

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```
#!/bin/bash
#SBATCH --job-name=testBowtie2          # Job name (testBowtie2)
#SBATCH --partition=batch               # Queue name (batch)
#SBATCH --nodes=1                       # Run all processes on a single node
#SBATCH --ntasks=1                      # Run in a single task on a single node
#SBATCH --cpus-per-task=8               # Number of CPU cores per task (8)
#SBATCH --mem=10G                       # Job memory limit (10 GB)
#SBATCH --time=1:00:00                  # Time limit hrs:min:sec or days-hours:minutes:seconds
#SBATCH --export=NONE                   # Do not load any users' explicit environment variables
#SBATCH --output=%x_%j.out              # Standard output log, e.g., testBowtie2_1234.out
#SBATCH --error=%x_%j.err               # Standard error log, e.g., testBowtie2_1234.err
#SBATCH --mail-type=END,FAIL            # Mail events (BEGIN, END, FAIL, ALL)
#SBATCH --mail-user=username@uga.edu    # Where to send mail

cd $SLURM_SUBMIT_DIR
ml Bowtie2/2.4.1-GCC-8.3.0
bowtie2  -p  8  -x  ./index/lambda_virus  -U  ./myreads.fq  -S  output.sam
```

Slurm headers for running an Array job

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```
#!/bin/bash
#SBATCH --job-name=testBowtie2Array        # Job name (testBowtie2Array)
#SBATCH --partition=batch                  # Queue name (batch)
#SBATCH --ntasks=1                         # Run in a single task using one CPU core on a single node
#SBATCH --mem=4G                           # Job memory limit (4 GB)
#SBATCH --time=1:00:00                     # Time limit hrs:min:sec or days-hours:minutes:seconds
#SBATCH --export=NONE                      # Do not load any users' explicit environment variables
#SBATCH --output=%x_%j.out                 # Standard output log, e.g., testBowtie2Array_1234.out
#SBATCH --error=%x_%j.err                  # Standard error log, e.g., testBowtie2Array_1234.err
#SBATCH --array=0-9                        # Array element range from 0 to 9, i.e. 10 element jobs

cd $SLURM_SUBMIT_DIR
ml Bowtie2/2.4.1-GCC-8.3.0                 # Original data is split into 10 pieces and run in each element job
bowtie2  -x  ./index/lambda_virus  -U  ./myreads_$SLURM_ARRAY_TASK_ID.fq \
-S  output_$SLURM_ARRAY_TASK_ID.sam
```

Slurm headers for running a Threaded (OpenMP) job

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```
#!/bin/bash
#SBATCH --job-name=testOpenMP                # Job name (testOpenMP)
#SBATCH --partition=batch                    # Queue name (batch)
#SBATCH --nodes=1                            # Run all processes on a single node
#SBATCH --ntasks=1                           # Run in a single task on a single node
#SBATCH --cpus-per-task=12                   # Number of CPU cores per task (12)
#SBATCH --mem=10G                            # Job memory limit (10 GB)
#SBATCH --export=NONE                        # Do not load any users' explicit environment variables
#SBATCH --time=24:00:00                      # Time limit hrs:min:sec or days-hours:minutes:seconds
#SBATCH --output=%x_%j.log                   # Standard output and error log, e.g., testOpenMP_1234.log
#SBATCH --mail-type=END,FAIL                 # Mail events (BEGIN, END, FAIL, ALL)
#SBATCH --mail-user=username@uga.edu         # Where to send mail

cd $SLURM_SUBMIT_DIR
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK  # Sets the number of threads to use for OpenMP parallel regions
ml foss/2019b                                # Load toolchain module
./myProgram.x                                # Run your program binary compiled with OpenMP
```

Slurm headers for running an MPI job

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```
#!/bin/bash
#SBATCH --job-name=testMPI                # Job name (tesMPI)
#SBATCH --partition=batch                 # Queue name (batch)
#SBATCH --nodes=2                         # Run on two nodes
#SBATCH --ntasks-per-node=16              # How many tasks on each node; Number of tasks=32=MPI ranks
#SBATCH --cpus-per-task=1                 # Number of CPU cores per task; 16 CPU cores per node
#SBATCH --mem-per-cpu=500M                # Memory per allocated CPU; 8GB (500MB*16) memory per node
#SBATCH --time=24:00:00                   # Time limit hrs:min:sec or days-hours:minutes:seconds
#SBATCH --export=NONE                     # Do not load any users' explicit environment variables
#SBATCH --output=%x_%j.log                # Standard output and error log, e.g., testMPI_1234.log
#SBATCH --mail-type=END,FAIL              # Mail events (BEGIN, END, FAIL, ALL)
#SBATCH --mail-user=username@uga.edu      # Where to send mail

cd $SLURM_SUBMIT_DIR
ml foss/2019b                             # Load toolchain module
mpirun -n 32 ./myProgram.x                # Run your program binary compiled with OpenMPI with 32 ranks
```

Slurm headers for running a Hybrid MPI/OpenMP job

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```
#!/bin/bash
#SBATCH --job-name=testHybrid              #  Job name (testHybrid)
#SBATCH --partition=batch                  #  Queue name (batch)
#SBATCH --nodes=2                          #  Run on two nodes
#SBATCH --ntasks-per-node=8                #  How many tasks on each node; Number of tasks=16=MPI ranks
#SBATCH --cpus-per-task=4                  #  Number of CPU cores per task; 32 CPU cores per node
#SBATCH --mem-per-cpu=500M                 # Memory per allocated CPU; 16GB (500MB*32) memory per node
#SBATCH --time=24:00:00                    # Time limit hrs:min:sec or days-hours:minutes:seconds
#SBATCH --export=NONE                      # Do not load any users' explicit environment variables
#SBATCH --output=%x_%j.log                 # Standard output and error log
#SBATCH --mail-type=END,FAIL               # Mail events (BEGIN, END, FAIL, ALL)
#SBATCH --mail-user=username@uga.edu       # Where to send mail

cd $SLURM_SUBMIT_DIR                       # Change directory to job submission directory
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK    # Sets the number of threads to use for OpenMP parallel regions
ml foss/2019b                              # Load toolchain module
mpirun -n 16 ./myProgram.x                 # Run your program binary compiled with OpenMPI with 16 ranks
```

Slurm headers for running a GPU job

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```
#!/bin/bash
#SBATCH --job-name=amber                    # Job name
#SBATCH --partition=gpu_p                   # Partition (queue) name, i.e., gpu_p
#SBATCH --gres=gpu:1                        # Requests one GPU device; --gres=gpu:P100:1, --gres=gpu:K40:1
#SBATCH --ntasks=1                          # Run a single task
#SBATCH --cpus-per-task=2                   # Number of CPU cores per task
#SBATCH --mem=40gb                          # Job memory request
#SBATCH --time=10:00:00                     # Time limit hrs:min:sec
#SBATCH --export=NONE                       # Do not load any users' explicit environment variables
#SBATCH --output=%x_%j.out                  # Standard output and error log, e.g., amber_1234.out
#SBATCH --mail-type=END,FAIL                # Mail events (BEGIN, END, FAIL, ALL)
#SBATCH --mail-user=username@uga.edu        # Where to send mail

cd $SLURM_SUBMIT_DIR
ml Amber/18-fosscuda-2018b-AmberTools-18-patchlevel-10-8
mpiexec $AMBERHOME/bin/pmemd.cuda -O -i ./prod.in -o prod_c4-23.out  -p ./dimerFBP_GOL.prmtop -c ./restart.rst \
-r prod.rst -x prod.mdcrd
```

Slurm headers for running a Singularity container

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```
#!/bin/bash
#SBATCH --job-name=test_sortmerna          # Job name
#SBATCH --partition=batch                  # Partition (queue) name
#SBATCH --ntasks=1                         # Run on a single CPU
#SBATCH --mem=8gb                          # Job memory request
#SBATCH --time=02:00:00                    # Time limit hrs:min:sec
#SBATCH --export=NONE                      # Do not load any users' explicit environment variables
#SBATCH --output=sortmerna.%j.out          # Standard output log, e.g., sortmerna.1234.out
#SBATCH --error=sortmerna.%j.err           # Standard error log, e.g., sortmerna.1234.err
#SBATCH --cpus-per-task=4                  # Number of CPU cores per task
#SBATCH --mail-type=END,FAIL               # Mail events (NONE, BEGIN, END, FAIL, ALL)
#SBATCH --mail-user=username@uga.edu       # Where to send mail

cd $SLURM_SUBMIT_DIR
singularity exec /apps/singularity-images/sortmerna-3.0.3.simg sortmerna --threads 4 --ref db.fasta,db.idx --reads file.fa \
--aligned base_name_output
```

Guideline Tips

- Do NOT use Login node to run CPU/memory intensive tasks directly ➔ submit jobs to compute nodes!
- Do NOT use Login Node to transfer data between your local computer and cluster ➔ use Transfer node!
- Do NOT use Home for storing job data ➔ use /scratch/MyID
- Do NOT park data in Scratch or Local Scratch ➔ clean up when job finishes or exits from node
- Do NOT park data permanently in Project ➔ download data to your local drive
- NO large memory job running on batch partition ➔ use highmem_p
- NO small memory job running on highmem_p partition ➔ use batch
- In general, <u>number of threads you want to run with a parallel job = number of cores requested</u>
- When you archive data using tar on /scratch, please do not use z option (compression option). After you achieved data by tar, you can use gzip to compress it.

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.

Georgia Advanced Computing Resource Center

101-108 Computing Services building

University of Georgia

Athens, GA 30602

https://gacrc.uga.edu/