Introduction to GACRC Teaching Cluster

Georgia Advanced Computing Resource Center (GACRC)

Enterprise Information Technology Services(EITS)

The University of Georgia

Outline

- GACRC
- Overview
- Working Environment
  - Three Folders
  - Three Computational Partitions
  - Software on Cluster
- Submit a Computational Batch Job
- Run Interactive Jobs
- GACRC Wiki and Support

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

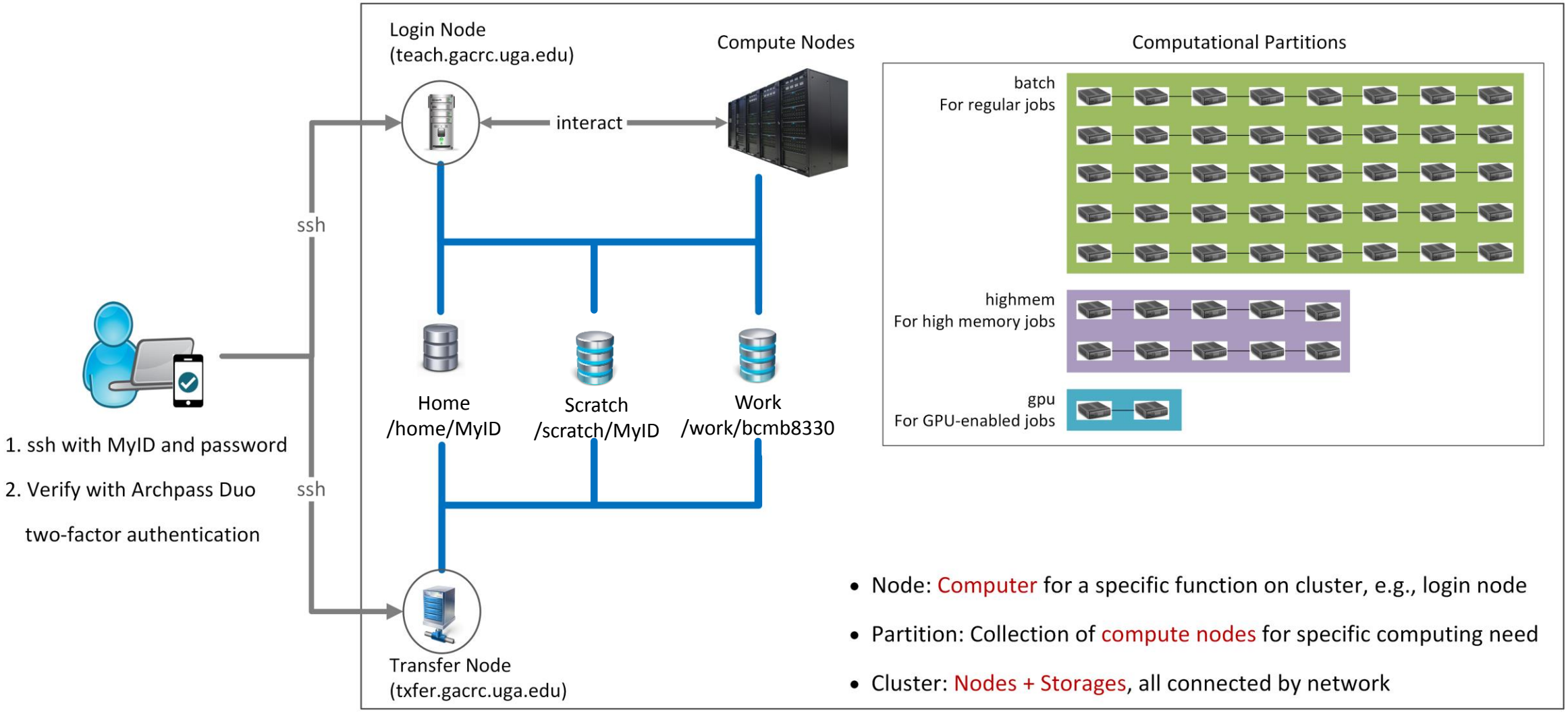
Wiki: http://wiki.gacrc.uga.edu

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

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

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

Teaching Cluster



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

Note: You need to connect to the UGA VPN at first when accessing from outside of the UGA main campus.

Working Environment

https://wiki.gacrc.uga.edu/wiki/Systems#Teaching_cluster

- Two nodes, your "username" is your MyID for both of them:
  1. For batch job workflow, the host to log into is teach.gacrc.uga.edu
  2. For file transfers, the host to log into is txfer.gacrc.uga.edu

- Three Directories:
  1. /home/MyID: directory for static data (e.g., scripts, software, etc…)
  2. /scratch/MyID: working space for running computational jobs
  3. /work/bcmb8330: directory for storing data
     a. /work/bcmb8330/MyID : data storage space for individual user in class
     b. /work/bcmb8330/instructor_data : data shared with class by the instructor

- Three Partitions:
  1. batch: for running regular computational jobs
  2. highmem: for running high-memory jobs
  3. gpu: for running GPU jobs

Working Environment (cont.)

- Software
  1. Software names are long and have a Easybuild toolchain name associated to it
  2. Complete module name: Name/Version-toolchain, e.g., Python/3.8.2-GCCcore-8.3.0
  3. Software names are case-sensitive!
     - `module spider pattern` : Search modules using a name pattern (case-insensitive)
     - `module load/unload moduleName` : Load/remove a module
     - `module avail` : List all available modules on the cluster
     - `module list` : List modules currently loaded
     - `module purge` : Remove all modules from working environment

Submit a Batch Job

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

1. Log on to Login node using MyID and password, and two-factor authentication with Archpass Duo:

   `ssh MyID@teach.gacrc.uga.edu`
2. Change directory to /scratch directory: `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

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

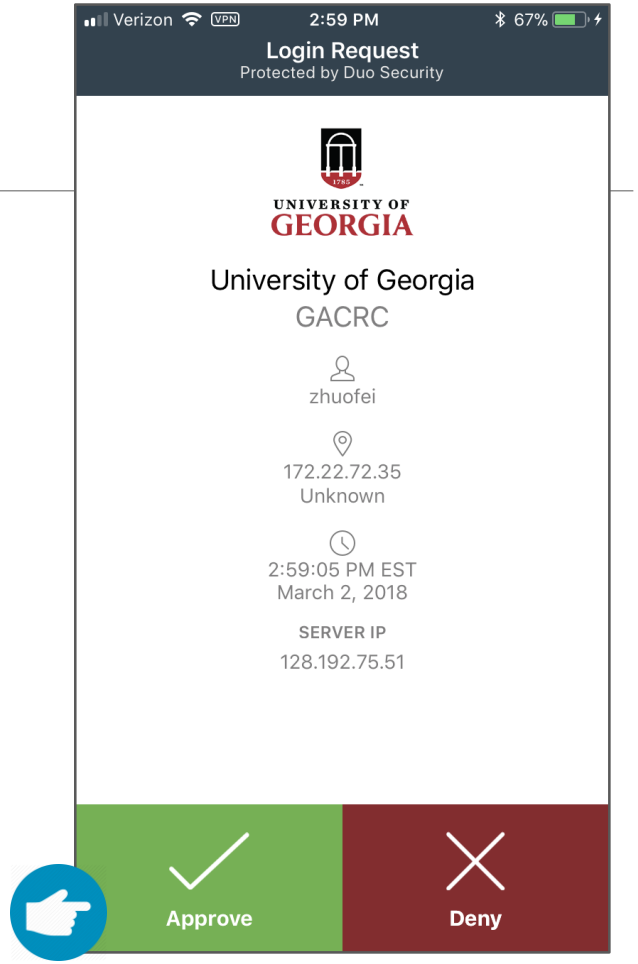
1. Teaching cluster access requires verification using two-factor authentication with Archpass Duo. If you are not enrolled in Archpass Duo, please refer to https://eits.uga.edu/access_and_security/infosec/tools/archpass_duo/ on how to enroll

2. If you are connecting from off-campus, please first connect to the UGA VPN and then connect to teach.gacrc.uga.edu. Information on how to use the VPN is available at https://eits.uga.edu/access_and_security/infosec/tools/vpn/

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

1. Open Terminal utility
2. Type command line: `ssh MyID@teach.gacrc.uga.edu`
3. You will be prompted for your UGA MyID password
4. You will verify your login using Archpass Duo authentication

```
ssh zhuofei@teach.gacrc.uga.edu        ← 1. use ssh to open connection

UGA DUO authentication is required for SSH/SCP access to GACRC
systems. For additional help with UGA DUO authentication or to
report an issue please visit: https://eits.uga.edu/access_and_security...

Password:        ← 2. Enter your MyID password
                      When you enter password, no stars or dots will show
                      as you are typing. Please type password carefully!
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 5. SMS passcodes to XXX-XXX-5758 (next code starts with: 1)

Passcode or option (1-5): 1          ← 3. Select Duo option
Success. Logging you in...
Last login: Mon Aug  3 11:11:58 2020 from 172.18.114.119
zhuofei@teach-sub1 ~$                ← 4. Logged on!
```



5. Verify login using Duo

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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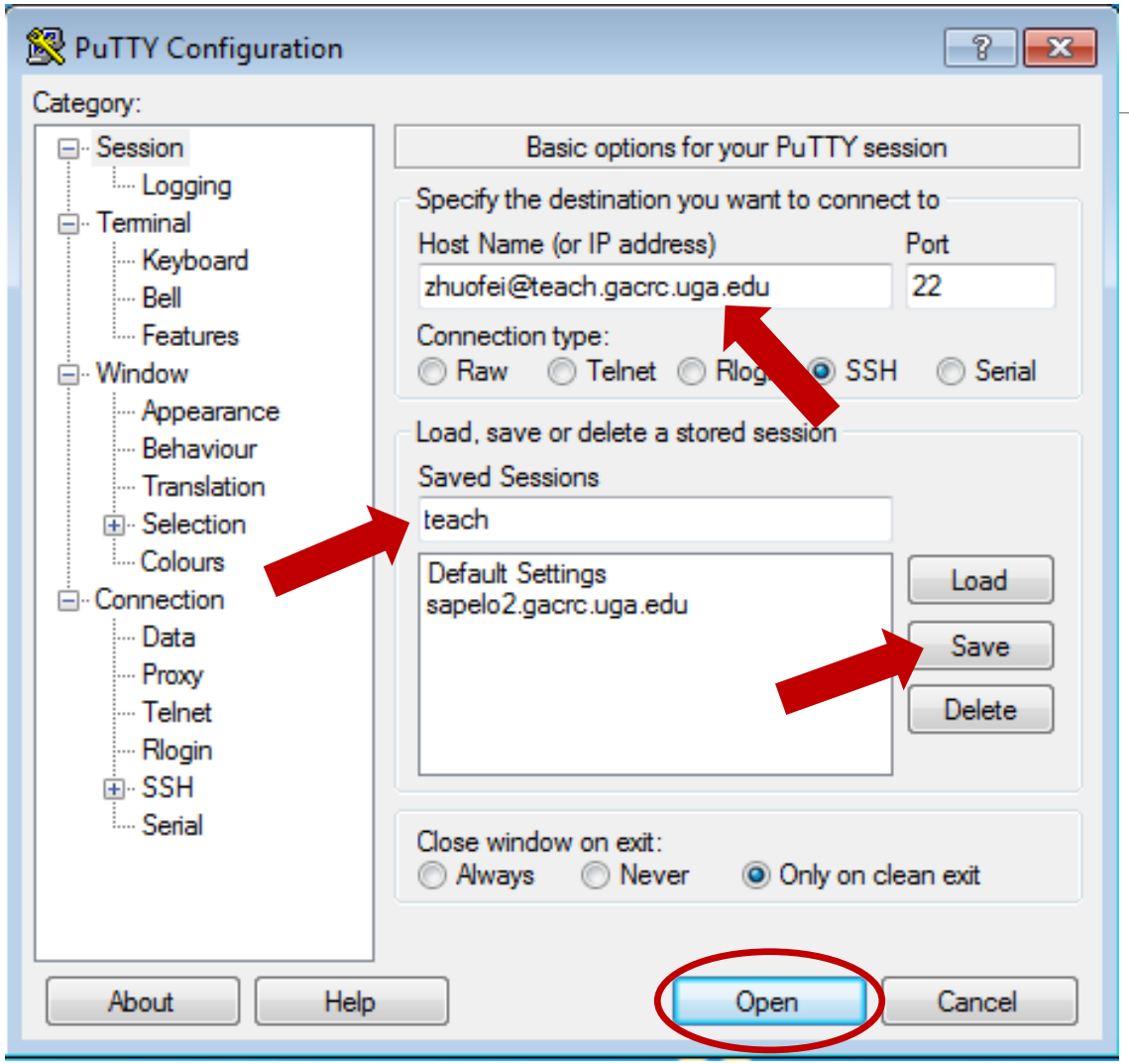
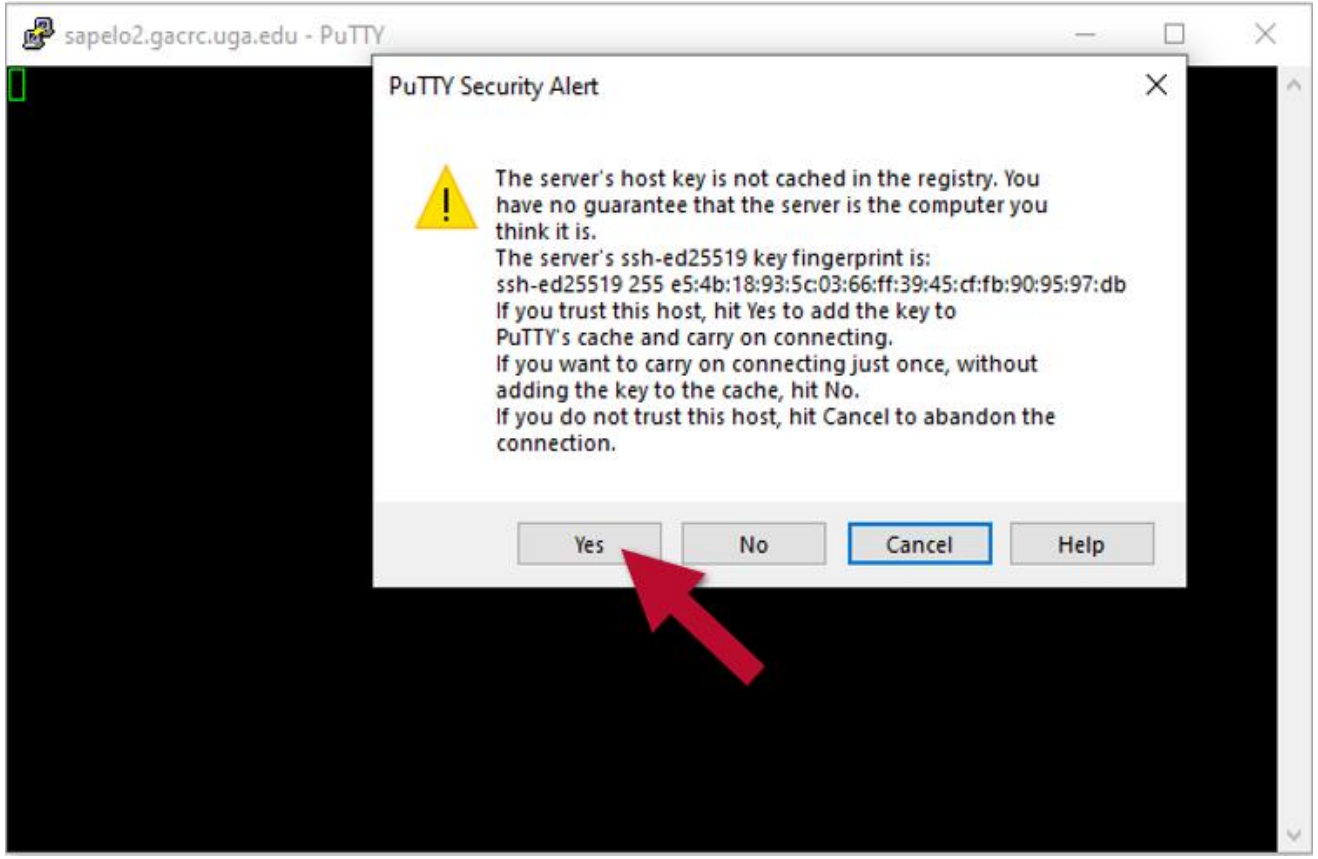


The first time you connect to login node, PuTTY will give you this security alert window. Please click "Yes"



Step1 (Cont.) - Windows using PuTTY

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

zhuofei@teach-sub1:~

```
Using username "zhuofei".
Keyboard-interactive authentication prompts from server:
| Password:                    ← UGA 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-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   ← Select DUO option
End of keyboard-interactive prompts from server
Success. Logging you in...
Last login: Thu Jan  7 10:20:01 2021 from 128.192.240.123
zhuofei@teach-sub1 ~$ ←  Logged on!
```

Step2 - 4: cd to /scratch dir, make and cd into workDir

```
zhuofei@teach-sub1 ~$ cd /scratch/zhuofei
zhuofei@teach-sub1 zhuofei$ mkdir workDir
zhuofei@teach-sub1 zhuofei$ cd workDir/
zhuofei@teach-sub1 workDir$ ls
zhuofei@teach-sub1 workDir$
```

← cd command to change directory

← mkdir command to create a subdirectory

← cd command to change directory

← ls command to list contents of directory

← it is empty in workDir!

Step 5: Transfer data from local computer to workDir - Mac/Linux

https://wiki.gacrc.uga.edu/wiki/Transferring_Files#Using_scp_2

1. Connect to Transfer node (txfer.gacrc.uga.edu) in Terminal from your local computer
2. Use scp command: scp (-r) [Source] [Target]
3. Enter your MyID password, then select Duo option to verify connection

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

```
scp ./file zhuofei@txfer.gacrc.uga.edu:/home/zhuofei/workDir
```

```
scp -r ./folder/ zhuofei@txfer.gacrc.uga.edu:/home/zhuofei/workDir
```

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

```
scp zhuofei@txfer.gacrc.uga.edu:/home/zhuofei/workDir/file .
```

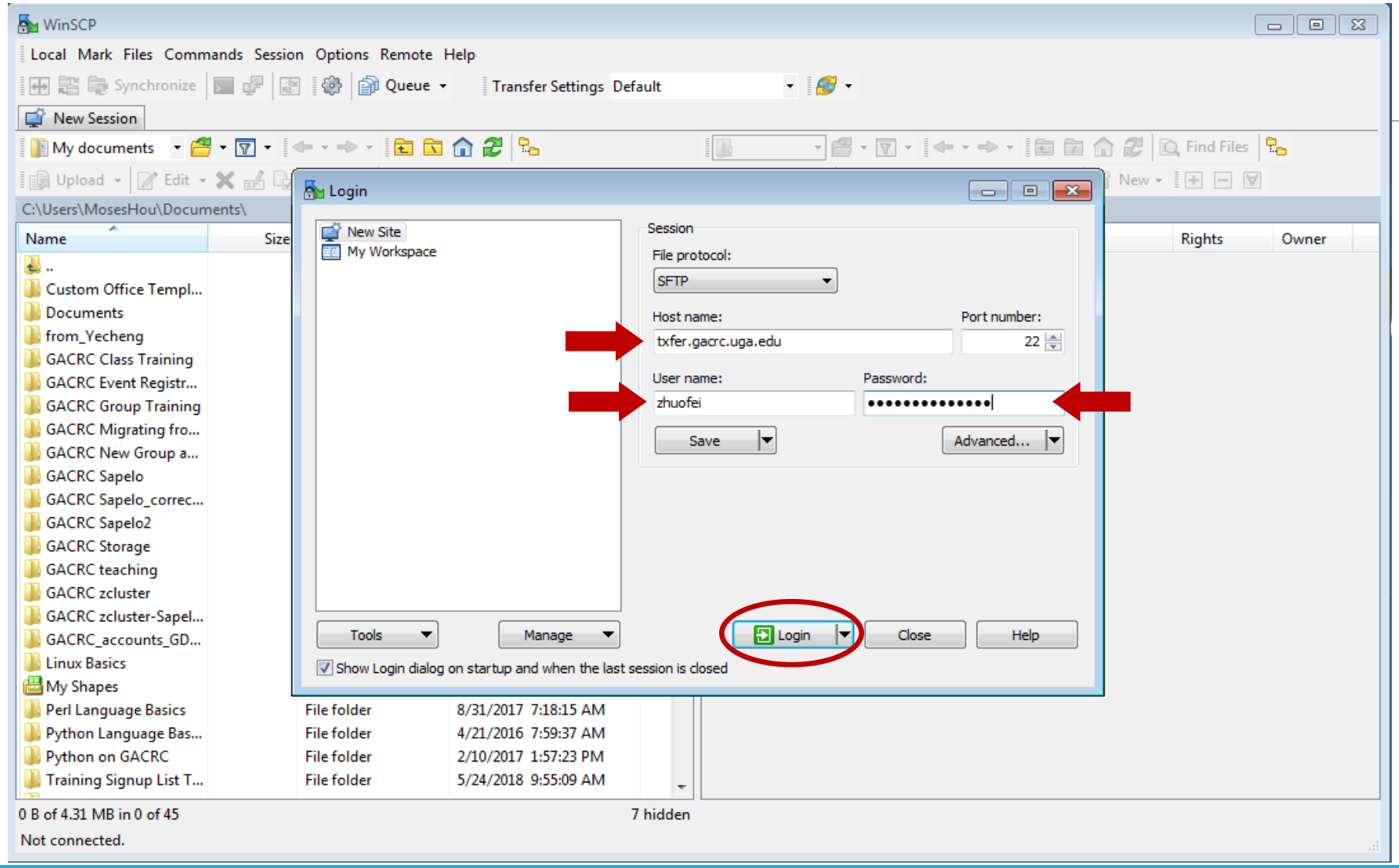
```
scp -r zhuofei@txfer.gacrc.uga.edu:/home/zhuofei/workDir/folder/ .
```

Step 5 (Cont.) - Windows using WinSCP

https://wiki.gacrc.uga.edu/wiki/Transferring_Files#Using_WinSCP_2

1. You need to connect to cluster's Transfer node (txfer.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_2

Step 5 (Cont.) - Windows using WinSCP



Step 5 (Cont.) - Windows using WinSCP

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zhuofei@xfer.gacrc.uga.edu - WinSCP

Local Mark Files Commands Session Options Remote Help

Synchronize | Queue | Transfer Settings Default

zhuofei@xfer.gacrc.uga.edu | New Session

My documents | Upload | Edit | Properties | New | Download | Find Files

C:\Users\MosesHou\Documents\

Name	Size	Type	Changed
..		Parent directory	
Custom Office Templ...		File folder	
Documents		File folder	
from_Yecheng		File folder	
GACRC Class Training		File folder	
GACRC Event Registr...		File folder	
GACRC Group Training		File folder	
GACRC Migrating fro...		File folder	
GACRC New Group a...		File folder	
GACRC Sapelo		File folder	
GACRC Sapelo_correc...		File folder	
GACRC Sapelo2		File folder	
GACRC Storage		File folder	
GACRC teaching		File folder	
GACRC zcluster		File folder	
GACRC zcluster-Sapel...		File folder	
GACRC_accounts_GD...		File folder	
Linux Basics		File folder	
My Shapes		File folder	
Perl Language Basics		File folder	
Python Language Bas...		File folder	
Python on GACRC		File folder	
Training Signup List T...		File folder	

0 B of 4.31 MB in 0 of 45

Not connected.

Server prompt - zhuofei@xfer.gacrc.uga.edu

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/

Duo two-factor login for zhuofei

Enter a passcode or select one of the following options:

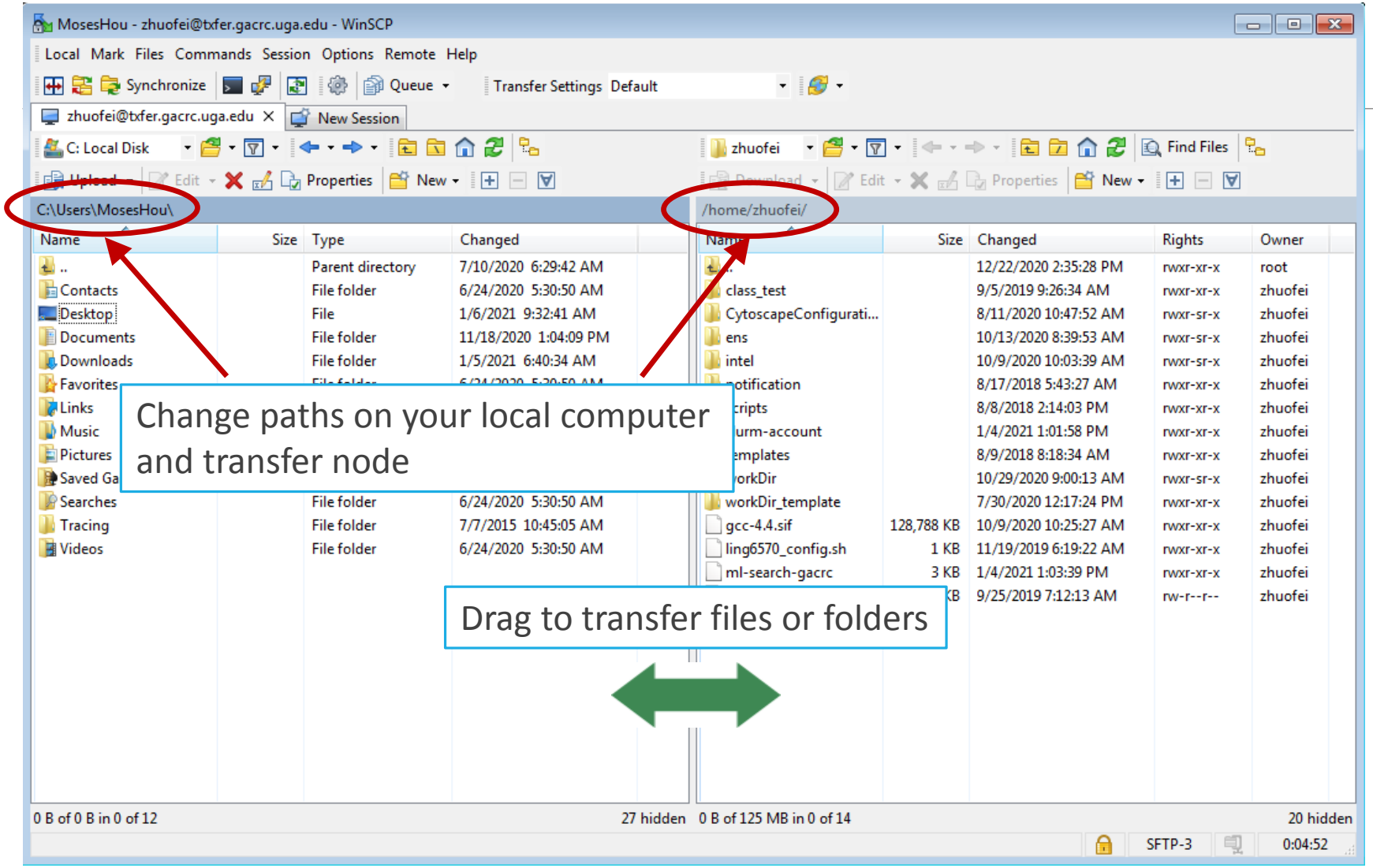
1. Duo Push to XXX-XXX-5758
2. Phone call to XXX-XXX-5758
3. Phone call to XXX-XXX-1925
4. Phone call to XXX-XXX-3535
5. SMS passcodes to XXX-XXX-5758

Passcode or option (1-5):

OK | Cancel | Help

← Select DUO option

Step 5 (Cont.) - Windows using WinSCP



Step 5 (Cont.): Transfer data on cluster to workDir

- Log on to Transfer node (txfer.gacrc.uga.edu)
  - ✓ Mac/Linux: ssh MyID@txfer.gacrc.uga.edu (page 9-10)
  - ✓ Windows: use PuTTY to log in MyID@txfer.gacrc.uga.edu (page 11-13)
- Directories you can access on transfer node:
  1. /home/MyID
  2. /scratch/MyID
  3. /work/bcmb8330/
- Transfer data between two folders on cluster using cp or mv, e.g.:

```
mv /work/bcmb8330/MyID/datafile /scratch/MyID/workDir
```

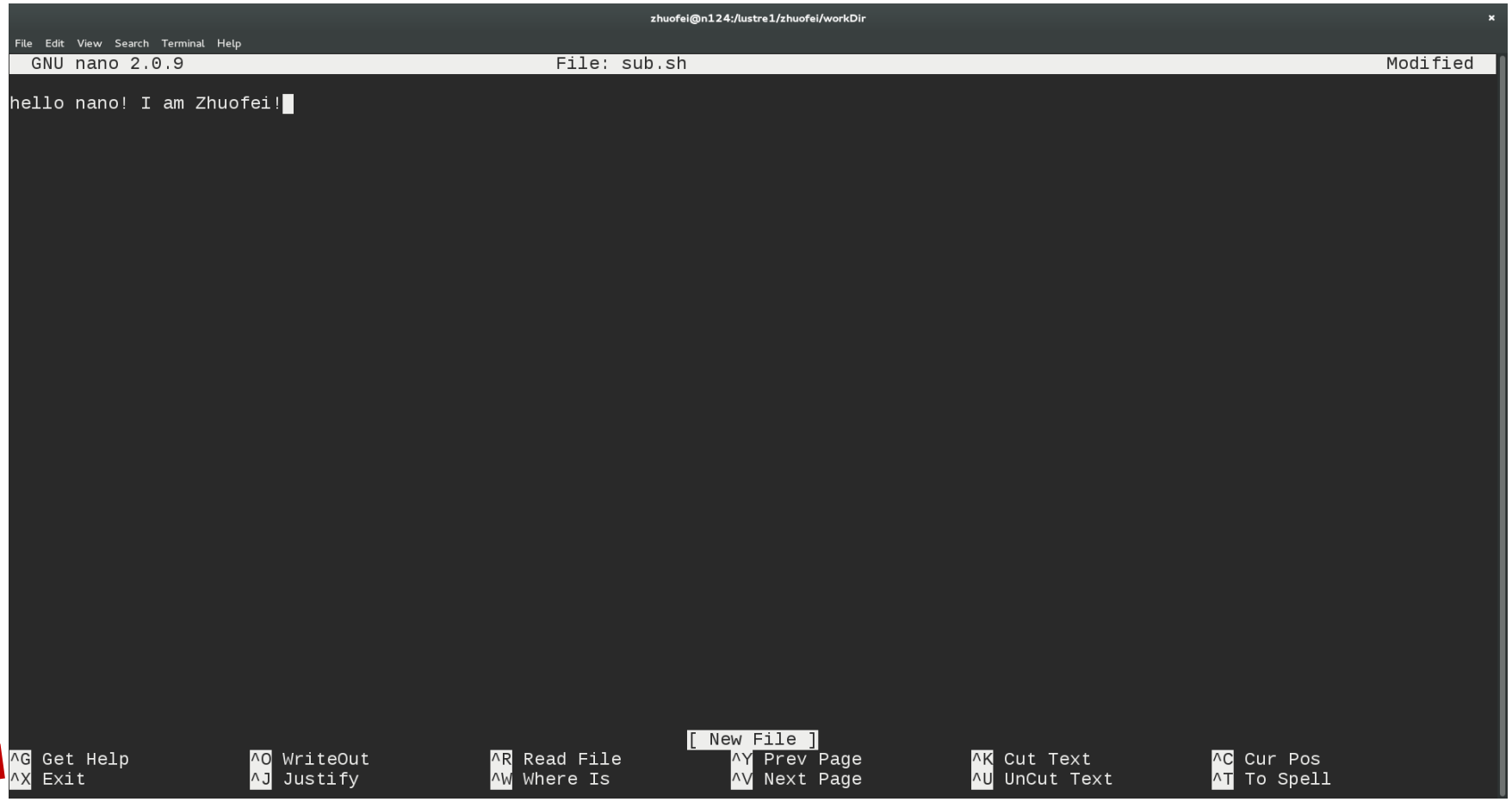
Step 6: Make a job submission script in workDir using nano

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

```
$ 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



Step 6 (Cont.)

1. Copy sample job to workDir:

cp -r /usr/local/training/bcmb8330/* .

2. Job submission script:

sub.sh

3. Amber Wiki:

https://wiki.gacrc.uga.edu/wiki/AMBER-Sapelo2

```
#!/bin/bash
#SBATCH --job-name=Amber_test                # Job name
#SBATCH --partition=batch                    # Computational partition
#SBATCH --nodes=1                            # Number of compute nodes
#SBATCH --ntasks=10                          # MPI processes/rank number
#SBATCH --cpus-per-task=1                    # Number of CPU cores per task/MPI process
#SBATCH --mem-per-cpu=2gb                    # Memory per CPU core
#SBATCH --time=24:00:00                      # Time limit hrs:mins:secs
#SBATCH --output=minimization.%j.out         # Standard output log
#SBATCH --error=minimization.%j.err          # Standard error log
#SBATCH --mail-user=MyID@uga.edu             # Where to send mail
#SBATCH --mail-type=ALL                      # Mail events (BEGIN, END, FAIL, ALL)

ml Amber/18-fosscuda-2018b-AmberTools-18-patchlevel-10-8      # Load Amber module
source ${AMBERHOME}/amber.sh                 # Config software environment for Amber

cd $SLURM_SUBMIT_DIR                         # cd /scratch/MyID/workDir

# PMEMD: Job1: minimization, solvent
mpiexec --mca mpi_cuda_support 0 ${AMBERHOME}/bin/pmemd.MPI -O \
 -i min_solvent.in\
 -o min_solvent.out\
 -p gfp.parm7\
 -c gfp.rst7\
 -ref gfp.rst7\
 -r gfp_min_solvent.rst7
```

Step 7: Submit a job from workDir using sbatch

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

```
$ sbatch sub.sh
Submitted batch job 33780
```

Tips: sub.sh is a job submission script for

1. specifying computing resources
2. loading software using module load
3. running any Linux commands you want to run
4. running the Amber MPI command

Step 8: Check job status using squeue

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

```
$ squeue --me -l
Tue Jan 17 09:25:20 2023
JOBID PARTITION NAME     USER    STATE   TIME TIME_LIMI  NODES NODELIST(REASON)
33780 batch     Amber_te zhuofei RUNNING 0:23 1-00:00:00 1     tcn18

$ squeue -me
JOBID PARTITION NAME     USER    ST      TIME  NODES NODELIST(REASON)
33780 batch     Amber_te zhuofei R       2:15  1     tcn18
```

Common STATE: R for Running; PD for PenDing; TO for TimedOut; S for Suspended; F for FAILED

TIME: the elapsed time used by the job, not remaining time, not CPU time.

Step 8 (Cont.): Cancel job using scancel

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

```
$ squeue --me -l
Tue Jan 17 09:29:34 2023
JOBID PARTITION NAME      USER    STATE   TIME TIME_LIMI  NODES  NODELIST(REASON)
33780 batch     Amber_te  zhuofei RUNNING 4:37 1-00:00:00 1      tcn18

$ scancel 33780

$ squeue --me -l
Tue Jan 17 09:29:42 2023
JOBID PARTITION NAME      USER    STATE       TIME TIME_LIMI  NODES NODELIST(REASON)
33780 batch     Amber_te  zhuofei COMPLETI    4:44 1-00:00:00 1     tcn18

$ squeue --me -l
Tue Jan 17 09:29:45 2023
JOBID PARTITION NAME      USER    STATE       TIME TIME_LIMI  NODES NODELIST(REASON)
```

Step8 (Cont.): Check job details using sacct-gacrc -X and seff

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

```
$ sacct-gacrc -X
JobID        JobName      User       Partition NNode NCPUS   ReqMem  CPUTime   Elapsed  Timelimit    State ExitCode  NodeList
------------ ------------ --------- ---------- ----- ----- -------- ---------- ---------- ---------- -------- ---------- ---------- ----------
33780        Amber_test   zhuofei    batch     1     10      2Gc      02:31:28  00:04:44 1-00:00:00 CANCELLED+  0:0   tcn18
33798        Amber_test   zhuofei    batch     1     10      2Gc      00:34:40  00:03:28 1-00:00:00 COMPLETED    0:0   tcn18

$ seff 33798              # Check computing resources used by a COMPLETED job
Job ID: 33798
Cluster: gacrc-teach
User/Group: zhuofei/ gacrc-instruction
State: COMPLETED (exit code 0)
Nodes: 1
Cores per node: 10
CPU Utilized: 00:34:25
CPU Efficiency: 99.28% of 00:34:40 core-walltime
Job Wall-clock time: 00:03:28
Memory Utilized: 363.66 MB
Memory Efficiency: 1.78% of 20.00 GB
```

Step 8 (Cont.): Check node info using sinfo

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

```
$ sinfo
PARTITION    AVAIL  TIMELIMIT  NODES  STATE NODELIST
batch*          up 7-00:00:00      1  drain tcn17
batch*          up 7-00:00:00      4    mix tcn[18-21]
batch*          up 7-00:00:00     20   idle tcn[1-16,22-25]
interactive     up 7-00:00:00      5   idle tcn[26-30]
gpu             up 7-00:00:00      1   idle tcgn1
highmem         up 7-00:00:00      1   idle tchmn2
highmem         up 7-00:00:00      1   down tchmn1
fsr4601         up       1:00      1  drain tcn17
fsr4601         up       1:00      4    mix tcn[18-21]
fsr4601         up       1:00     20   idle tcn[1-16,22-25]
fsr8602         up      10:00      1  drain tcn17
fsr8602         up      10:00      4    mix tcn[18-21]
fsr8602         up      10:00     20   idle tcn[1-16,22-25]
```

Obtain Job Details

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

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

Option 2: sacct-gacrc -X 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
```

Run 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	interact
Start an interactive session with X forwarding	interact --x11

interact	srun --pty --cpus-per-task=1 --job-name=interact --ntasks=1 --nodes=1 --partition=inter_p --time=12:00:00 --mem=2GB /bin/bash -l
interact --x11	srun --pty --cpus-per-task=1 --job-name=interact --ntasks=1 --nodes=1 --partition=inter_p --time=12:00:00 --mem=2GB --x11 /bin/bash -l

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

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

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

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

Transfer File:

https://wiki.gacrc.uga.edu/wiki/Transferring_Files#The_File_Transfer_node_for_the_teaching_cluster_.28txfer.gacrc.uga.edu.29

Sample Job Scripts:

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

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

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 partition 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!

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Search the client portal

Zhuofei Hou

Home | IT Help Desks | Projects/Workspaces | **Services** | Knowledge Base

Project Requests | Ticket Requests | My Favorites | My Recent | My Approvals | Services A-Z | Search

Service Catalog / Academics, Learning & Research / GACRC Service Catalog

GACRC Service Catalog

Georgia Advanced Computing Resource Center (GACRC) service catalog.

If you would like to reach out to GACRC and do not have a UGA MyID, please send an email to gacrc-help@uga.edu, and we will respond promptly.

Categories (3)

Services For Users
General user support, request software installation or update, request training.

Services for PIs
For PIs only: Lab registration, user account creation/modification, class account requests, storage quota modifications.

For GACRC Staff
For GACRC's internal use only.

My Recent Requests

- Class provision on the teaching cluster - phys8601-dlandau
- Class provision on the teaching cluster - bcmb8330 - rjwoods
- Class provision on the teaching cluster - binf8211 - szhao, lm43161
- MATLAB License Request
- Create cider lab group

View All Recent Requests

Popular Services

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

Related image

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Search the client portal

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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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https://uga.teamdynamix.com/TDClient/Requests/ServiceCatalogSearch

Need Support? http://help.gacrc.uga.edu