

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

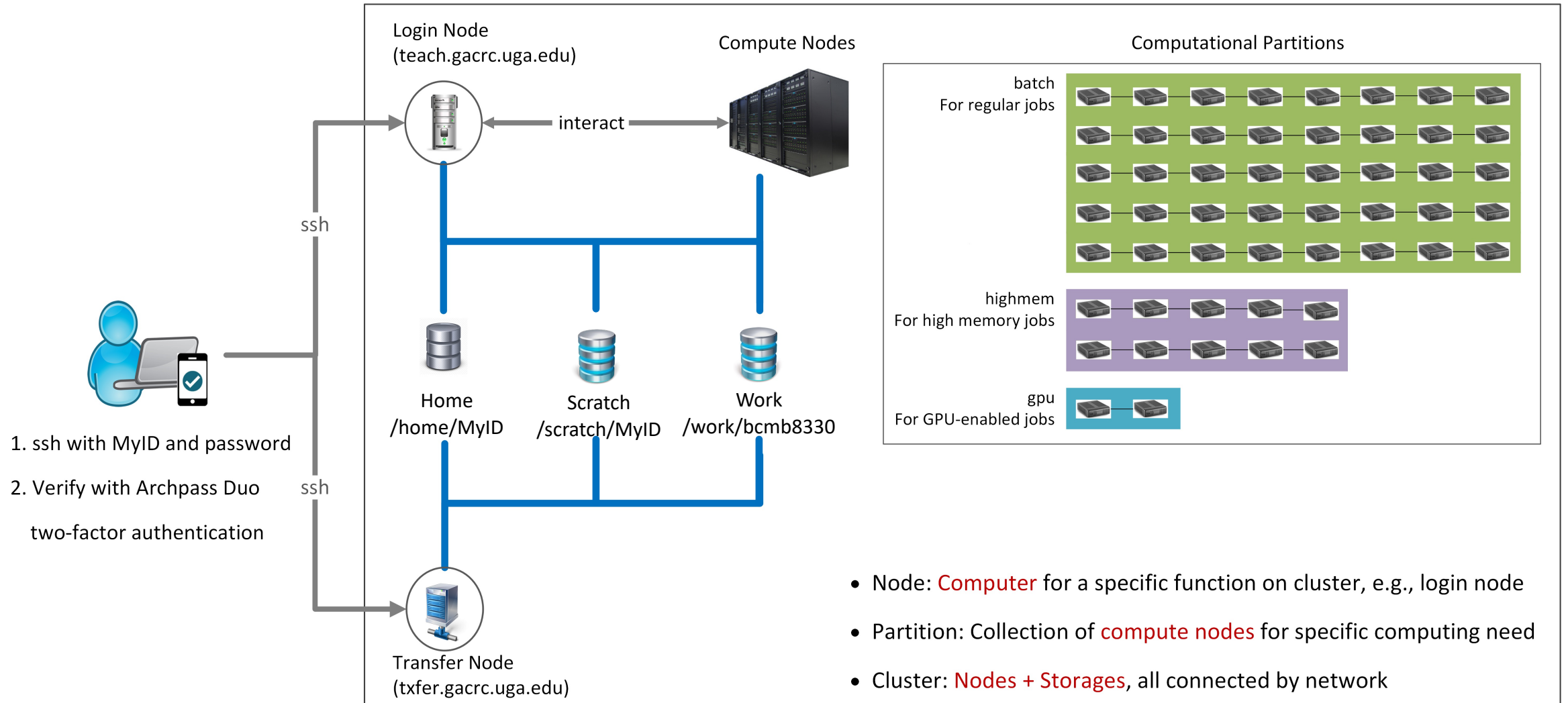
Wiki: <http://wiki.gacrc.uga.edu>

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



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/3.10.4**-GCCcore-11.3.0
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_mpi.sh`
7. Submit a job from workDir : `sbatch sub_mpi.sh`
8. Check job status : `sq --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](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:

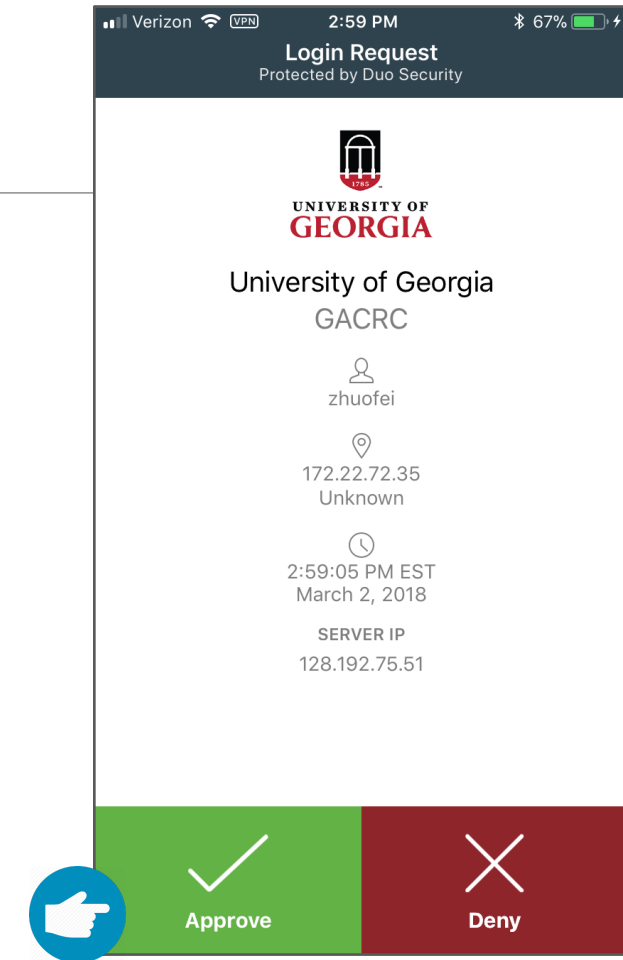
1. Duo Push to XXX-XXX-5758
2. Phone call to XXX-XXX-5758
3. Phone call to XXX-XXX-1925
- 4 5. SMS passcodes to XXX-XXX-5758 (next code starts with: 1)

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/>

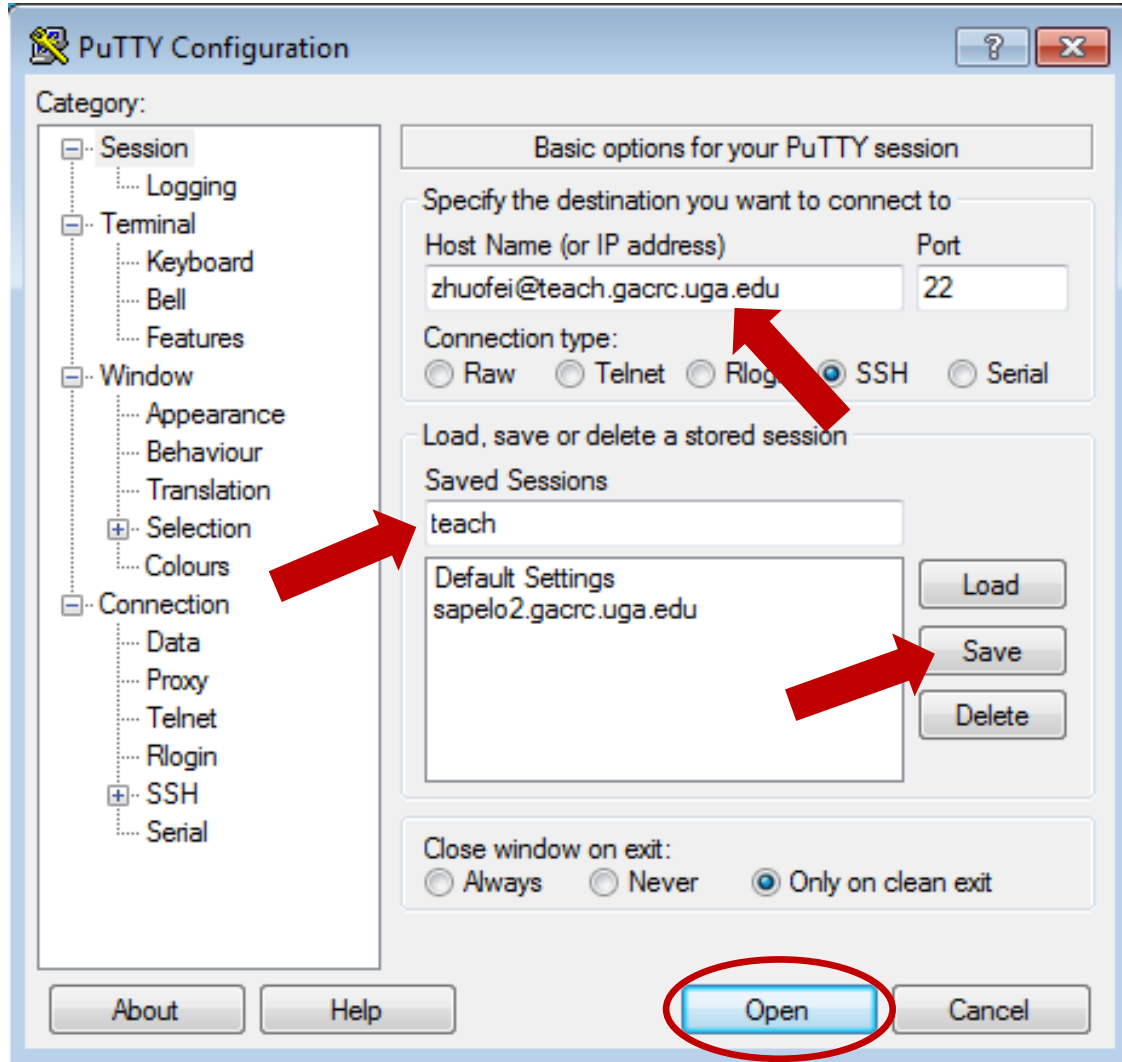
2. Detailed downloading and installation instructions:

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

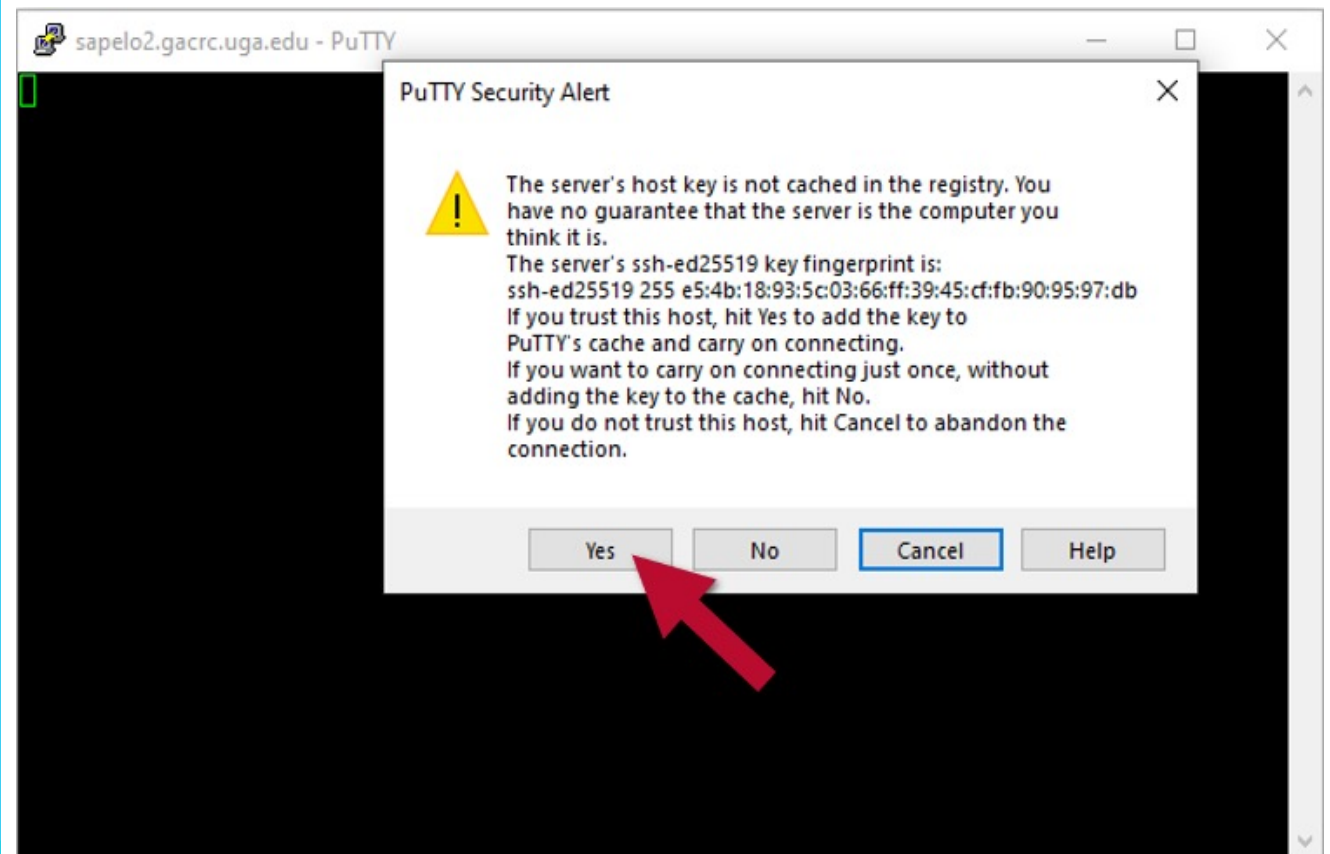
3. Detailed configuring and usage instructions:

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

Step1 (Cont.) - Windows using PuTTY

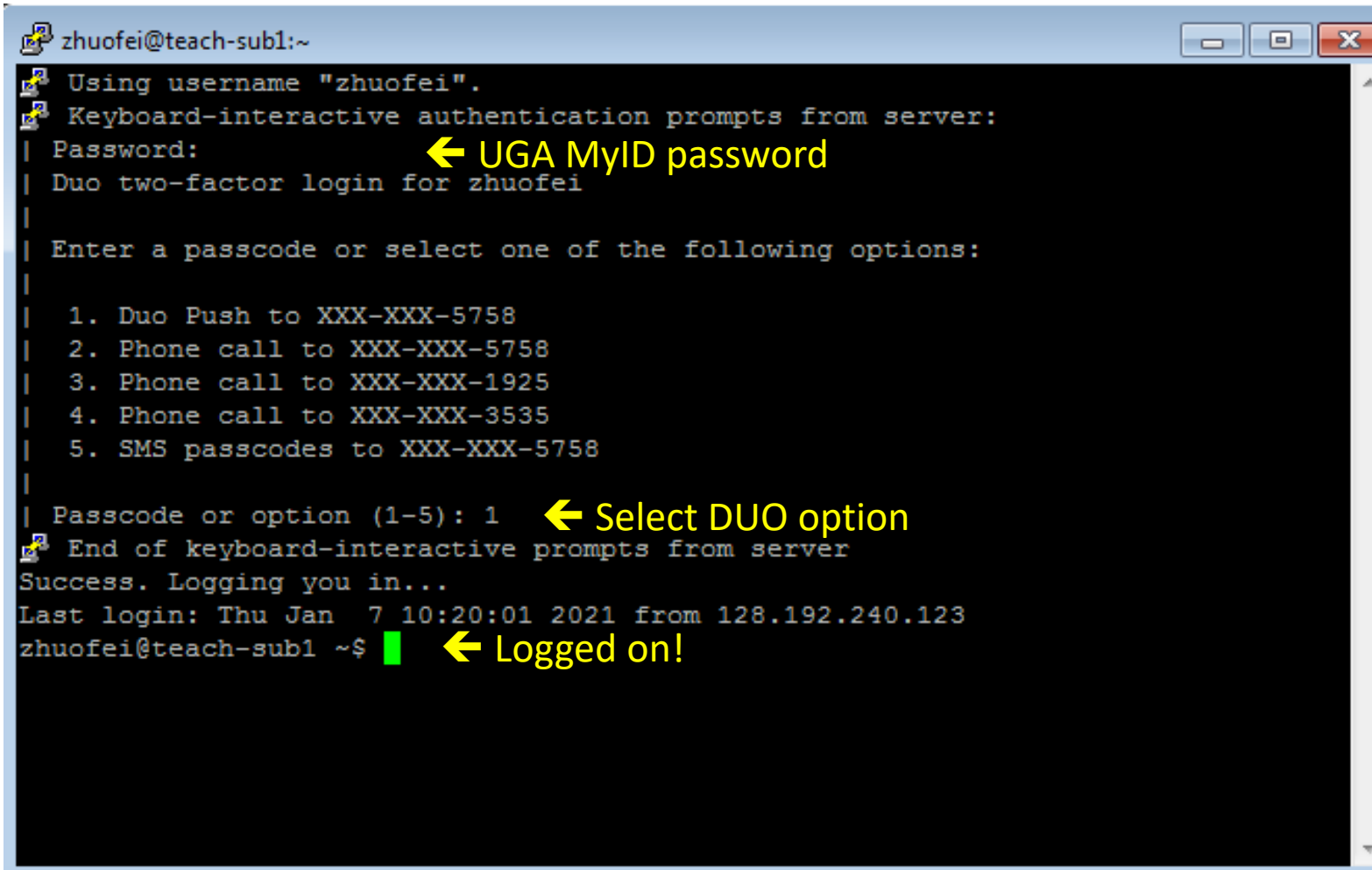


The first time you connect to login node, PuTTY will give you this security alert window. Please click "Yes"



Step1 (Cont.) - Windows using PuTTY

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 ← cd command to change directory
zhuofei@teach-sub1 zhuofei$ mkdir workDir ← mkdir command to create a subdirectory
zhuofei@teach-sub1 zhuofei$ cd workDir/ ← cd command to change directory
zhuofei@teach-sub1 workDir$ ls ← ls command to list contents of directory
zhuofei@teach-sub1 workDir$ ← 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 .
```

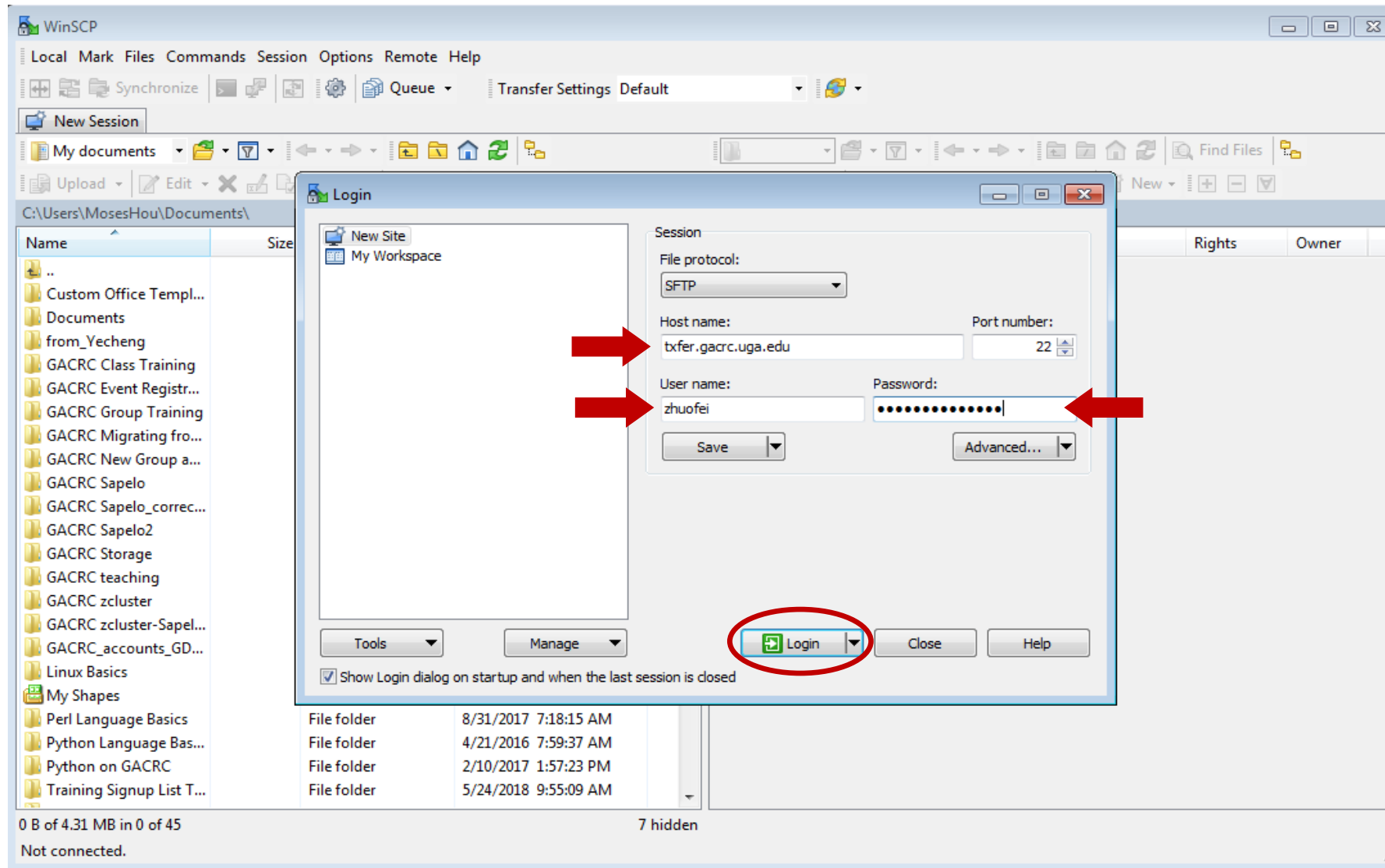
```
scp -r zhuofei@txfer.gacrc.uga.edu:/home/zhuofei/workDir/folder/ .
```

Step 5 (Cont.) - Windows using WinSCP

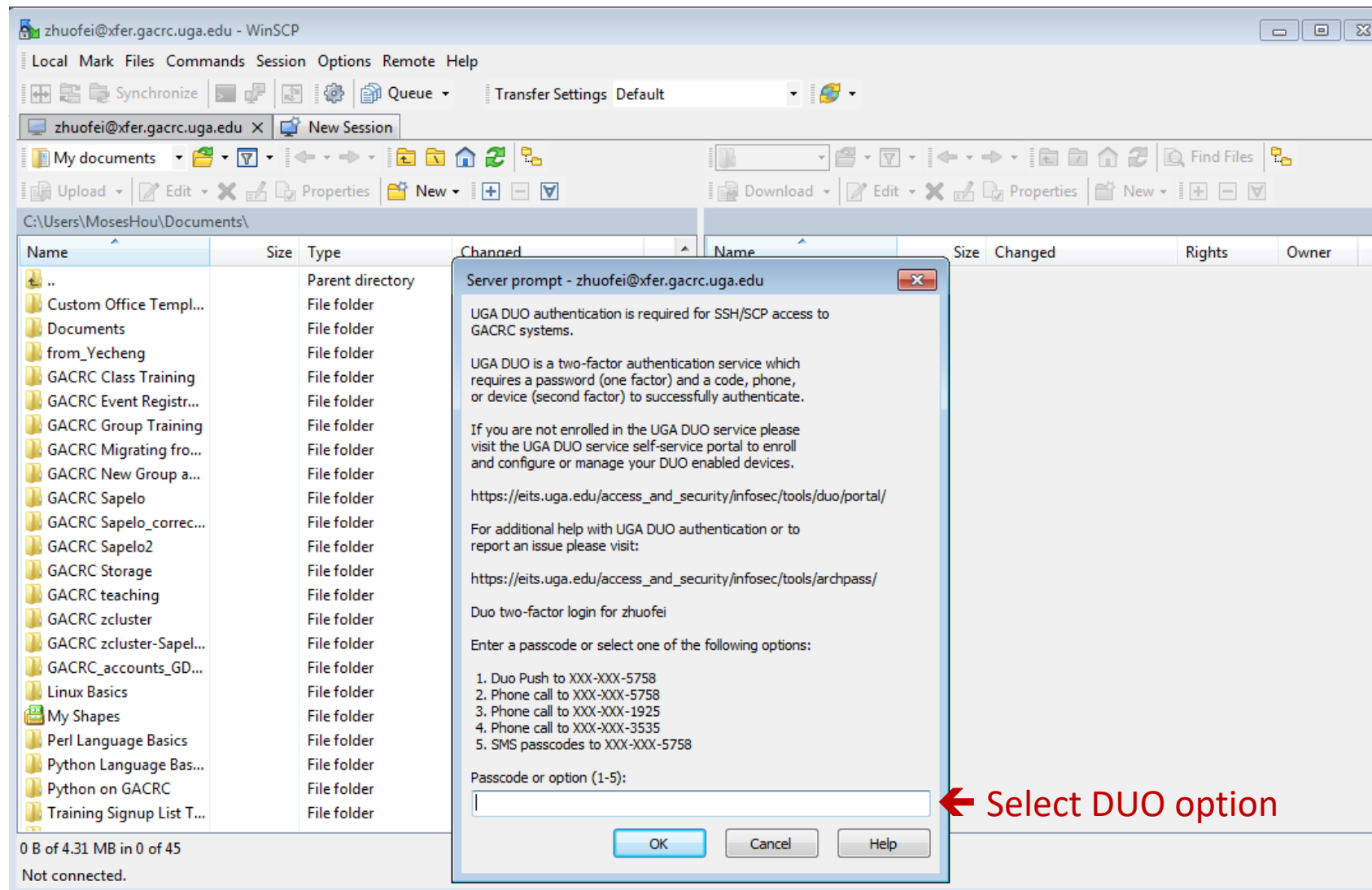
https://wiki.gacrc.uga.edu/wiki/Transferring_Files#Using_WinSCP_2

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



Step 5 (Cont.) - Windows using WinSCP

The screenshot shows the WinSCP interface with two panes. The left pane shows the local file system at `C:\Users\MosesHou\`, and the right pane shows the remote file system at `/home/zhuofei/`. Both paths are circled in red. A blue box with the text "Change paths on your local computer and transfer node" has arrows pointing to these two paths. A green double-headed arrow points from a blue box with the text "Drag to transfer files or folders" between the two panes. The status bar at the bottom shows "0 B of 0 B in 0 of 12" for the local pane and "27 hidden 0 B of 125 MB in 0 of 14" for the remote pane.

Name	Size	Type	Changed
..		Parent directory	7/10/2020 6:29:42 AM
Contacts		File folder	6/24/2020 5:30:50 AM
Desktop		File	1/6/2021 9:32:41 AM
Documents		File folder	11/18/2020 1:04:09 PM
Downloads		File folder	1/5/2021 6:40:34 AM
Favorites		File folder	6/24/2020 5:30:50 AM
Links		File folder	6/24/2020 5:30:50 AM
Music		File folder	6/24/2020 5:30:50 AM
Pictures		File folder	6/24/2020 5:30:50 AM
Saved Games		File folder	6/24/2020 5:30:50 AM
Searches		File folder	6/24/2020 5:30:50 AM
Tracing		File folder	6/24/2020 5:30:50 AM
Videos		File folder	6/24/2020 5:30:50 AM

Name	Size	Changed	Rights	Owner
..		12/22/2020 2:35:28 PM	rw-r--r--	root
class_test		9/5/2019 9:26:34 AM	rw-r--r--	zhuofei
CytoscapeConfigurati...		8/11/2020 10:47:52 AM	rw-r--r--	zhuofei
ens		10/13/2020 8:39:53 AM	rw-r--r--	zhuofei
intel		10/9/2020 10:03:39 AM	rw-r--r--	zhuofei
notification		8/17/2018 5:43:27 AM	rw-r--r--	zhuofei
scripts		8/8/2018 2:14:03 PM	rw-r--r--	zhuofei
term-account		1/4/2021 1:01:58 PM	rw-r--r--	zhuofei
templates		8/9/2018 8:18:34 AM	rw-r--r--	zhuofei
workDir		10/29/2020 9:00:13 AM	rw-r--r--	zhuofei
workDir_template		7/30/2020 12:17:24 PM	rw-r--r--	zhuofei
gcc-4.4.sif	128,788 KB	10/9/2020 10:25:27 AM	rw-r--r--	zhuofei
ling6570_config.sh	1 KB	11/19/2019 6:19:22 AM	rw-r--r--	zhuofei
ml-search-gacrc	3 KB	1/4/2021 1:03:39 PM	rw-r--r--	zhuofei
		9/25/2019 7:12:13 AM	rw-r--r--	zhuofei

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
```

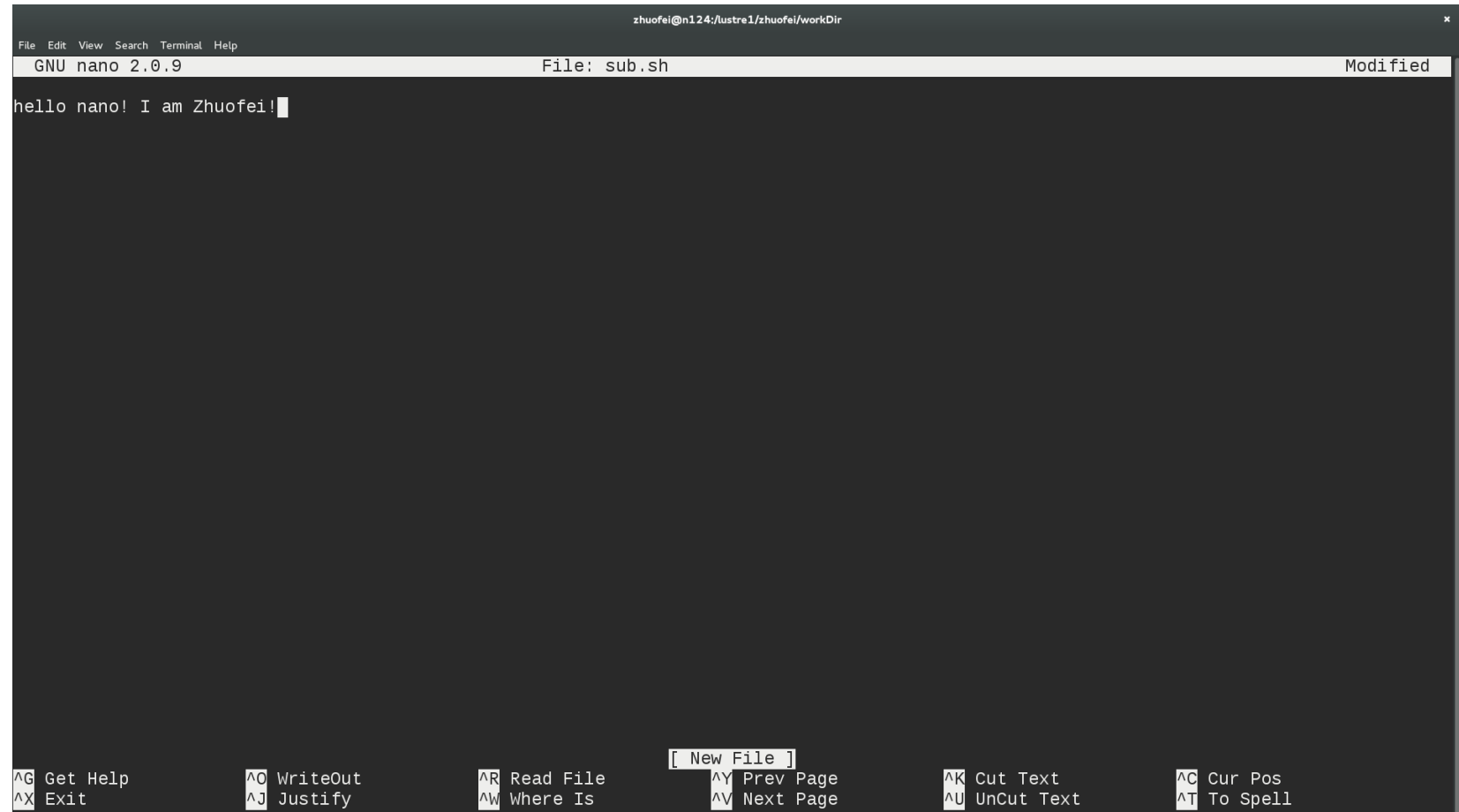
Step 6: Make a job submission script in workDir using nano

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

```
$ nano sub_mpi.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/gacrc/training/bcmb8330/* .
```

2. Job submission script:

```
sub_mpi.sh
```

3. Amber Wiki:

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

```
#!/bin/bash
#SBATCH --job-name=Amber_MPI
#SBATCH --partition=batch
#SBATCH --ntasks=10
#SBATCH --cpus-per-task=1
#SBATCH --mem-per-cpu=2gb
#SBATCH --time=24:00:00
#SBATCH --output=log.%j.out
#SBATCH --error=log.%j.err
#SBATCH --mail-user=MyID@uga.edu
#SBATCH --mail-type=ALL

cd $SLURM_SUBMIT_DIR

ml Amber/22.0-foss-2021b-AmberTools-22.3
source ${AMBERHOME}/amber.sh

# PMEMD: Job1: minimization, solvent
srun ${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
```

Job name
Computational partition
MPI processes/rank number
Number of CPU cores per task/MPI process
Memory per CPU core
Time limit hrs:mins:secs
Standard output log
Standard error log
Where to send mail
Mail events (BEGIN, END, FAIL, ALL)

cd /scratch/MyID/workDir

Load Amber module
Config software environment for Amber

Step 6 (Cont.)

1. Copy sample job to workDir:

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

2. Job submission script:

```
sub_gpu.sh
```

3. Amber Wiki:

<https://wiki.gacrc.uga.edu/wiki/AMBER->

[Sapelo2](https://wiki.gacrc.uga.edu/wiki/AMBER-Sapelo2)

```
#!/bin/bash
#SBATCH --job-name=Amber_GPU
#SBATCH --partition=gpu
#SBATCH --gres=gpu:P100:1
#SBATCH --ntasks=4
#SBATCH --cpus-per-task=1
#SBATCH --mem-per-cpu=2gb
#SBATCH --time=24:00:00
#SBATCH --output=log.%j.out
#SBATCH --error=log.%j.err
#SBATCH --mail-user=MyID@uga.edu
#SBATCH --mail-type=ALL

cd $SLURM_SUBMIT_DIR

ml Amber/22.0-foss-2021b-AmberTools-22.3-CUDA-11.4.1 # Load GPU Amber module
source ${AMBERHOME}/amber.sh # Config software environment for Amber

# PMEMD: Job1: minimization, solvent
$AMBERHOME/bin/pmemd.cuda -O \
-i min_solvent.in \
-o min_solvent.out \
-p gfp.parm7 \
-c gfp.rst7 \
-ref gfp.rst7 \
-r gfp_min_solvent.rst7
```

Job name
Computational partition
Request 1 P100 GPU device
Run 4 tasks
Number of CPU cores per task
Memory per CPU core
Time limit hrs:mins:secs
Standard output log
Standard error log
Where to send mail
Mail events (BEGIN, END, FAIL, ALL)

cd /scratch/MyID/workDir

Load GPU Amber module
Config software environment for Amber

PMEMD: Job1: minimization, solvent

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_mpi.sh  
Submitted batch job 5386
```

Tips: sub_mpi.sh is a job submission script for

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

Step 8: Check job status using sq --me

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

```
$ sq --me
```

JOBID	NAME	PARTITION	USER	NODES	CPUS	MIN_MEMORY	PRIORITY	TIME	TIME_LIMIT	STATE	NODELIST (REASON)
5386	Amber_MPI	batch	zhuofei	1	10	2G	992	1:23	1-00:00:00	RUNNING	rb1-3

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

```
$ sq --me
```

JOBID	NAME	PARTITION	USER	NODES	CPUS	MIN_MEMORY	PRIORITY	TIME	TIME_LIMIT	STATE	NODELIST (REASON)
5386	Amber_MPI	batch	zhuofei	1	10	2G	992	1:23	1-00:00:00	RUNNING	rb1-3

```
$ scancel 5386
```

```
$ sq --me
```

JOBID	NAME	PARTITION	USER	NODES	CPUS	MIN_MEMORY	PRIORITY	TIME	TIME_LIMIT	STATE	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
5385	Amber_MPI	zhuofei	batch	1	10	20G	01:44:00	00:10:24	1-00:00:00	COMPLETED	0:0	rb1-3
5386	Amber_MPI	zhuofei	batch	1	10	20G	01:28:20	00:08:50	1-00:00:00	CANCELLED+	0:0	rb1-3

```
$ seff 5385 # seff is useful if you wan to check computing resources used by a COMPLETED job
```

Job ID: 5385

Cluster: gacrc-teach

User/Group: zhuofei/gacrc-instruction

State: COMPLETED (exit code 0)

Nodes: 1

Cores per node: 10

CPU Utilized: 01:39:53

CPU Efficiency: 96.04% of 01:44:00 core-walltime

Job Wall-clock time: 00:10:24

Memory Utilized: 1.59 GB (estimated maximum)

Memory Efficiency: 7.95% of 20.00 GB (2.00 GB/core)

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
allnodes	up	infinite	1	mix	rb1-11
allnodes	up	infinite	11	idle	rb1-[1-10,12]
batch	up	2-00:00:00	8	idle	rb1-[3-10]
highmem	up	7-00:00:00	2	idle	rb1-[1-2]
interactive	up	7-00:00:00	1	mix	rb1-11
interactive	up	7-00:00:00	1	idle	rb1-12
fsr4601	up	1:00	8	idle	rb1-[3-10]
fsr8602	up	10:00	8	idle	rb1-[3-10]

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: `sq --me` 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_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](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	<code>interact</code>
Start an interactive session with X forwarding	<code>interact --x11</code>

<code>interact</code>	<code>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</code>
<code>interact --x11</code>	<code>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</code>

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!



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](#)

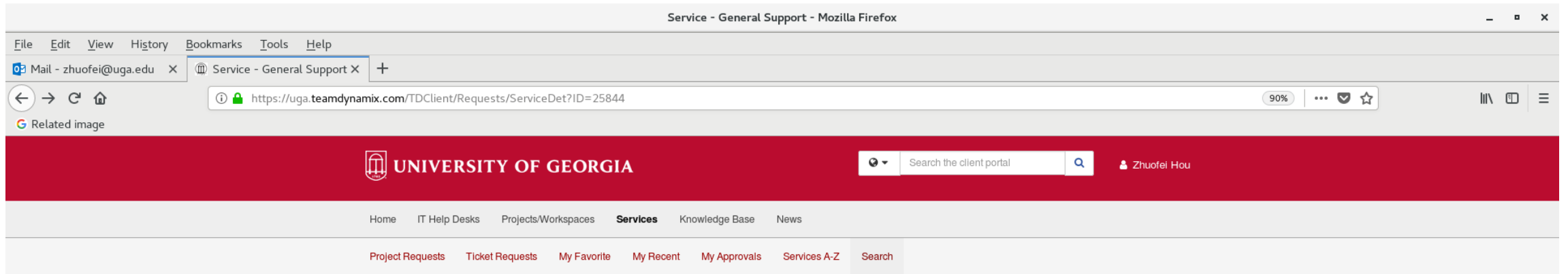
[Class provision on the teaching cluster - binf8211 - szhao, lm43161](#)

[MATLAB License Request](#)

[Create cider lab group](#)

[View All Recent Requests >](#)

Popular Services



[Service Catalog](#) / [Academics, Learning & Research](#) / [GACRC Service Catalog](#) / General Support

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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