Introduction to GACRC Teaching Cluster PHYS4601/6601

Georgia Advanced Computing Resource Center (GACRC)

Enterprise Information Technology Services(EITS)

The University of Georgia

Outline

- GACRC
- Overview
- Working Environment
  - Two Nodes and Three Folders
  - Computational Partitions
  - Software
- Submit a Computational Batch Job
- 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

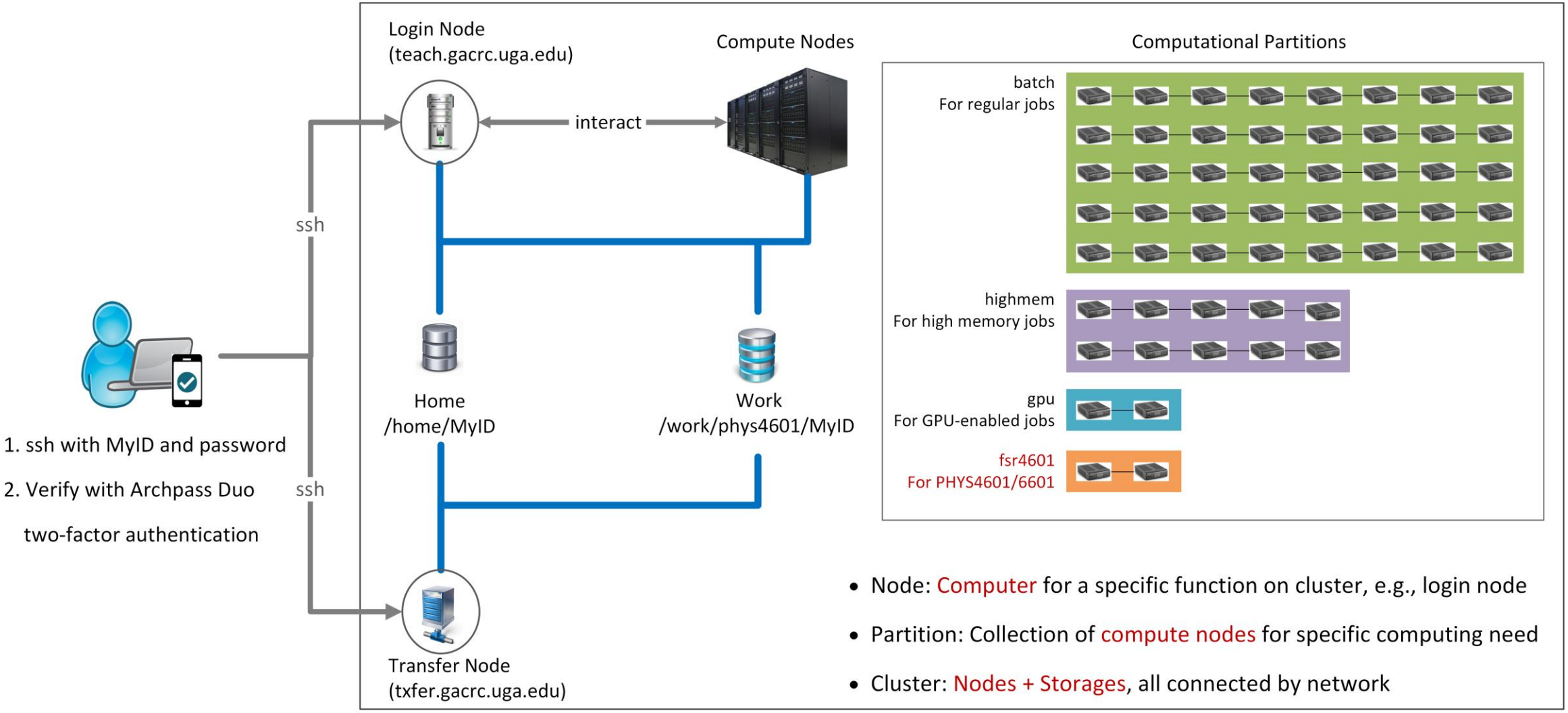
Wiki: http://wiki.gacrc.uga.edu

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 folders:
  1. /home/MyID : working space for running computational jobs
  2. /work/phys4601/MyID : data storing space for individual user in a class
  3. /work/phys4601/instructor_data : data shared with class by the instructors
- Partitions for PHYS4601/6601 class: fsr4601

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 Computational Batch Job

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

   ssh MyID@teach.gacrc.uga.edu
2. Create a working subdirectory for a job : mkdir workDir
3. Change directory to workDir : cd workDir
4. 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
5. Compile Fortran code *mult.f* into a binary code
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…

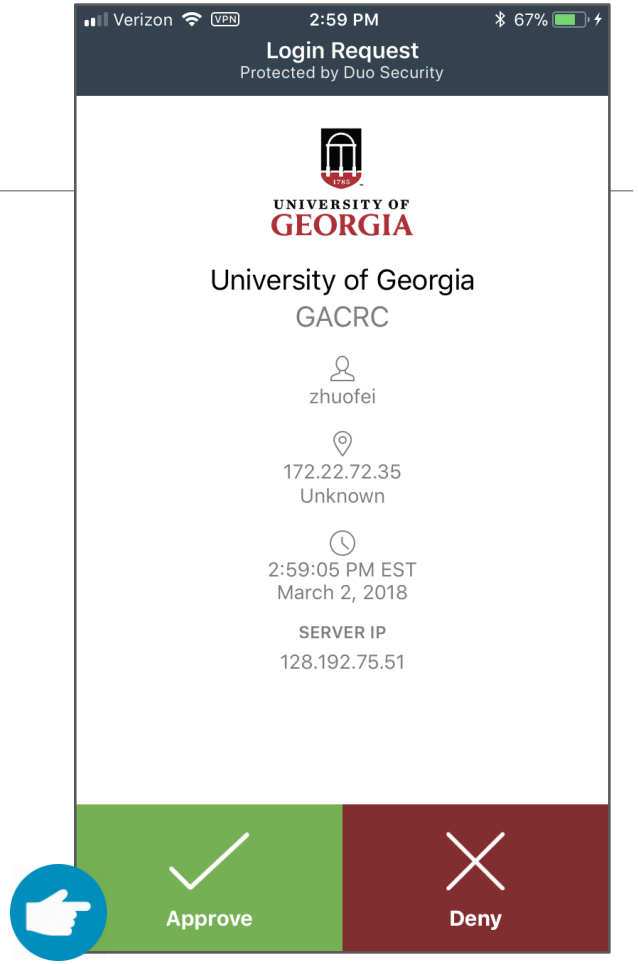
Password: ← 2. Enter your MyID password
When you enter password, no stars or dots will show as you are typing. Please type password carefully!

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

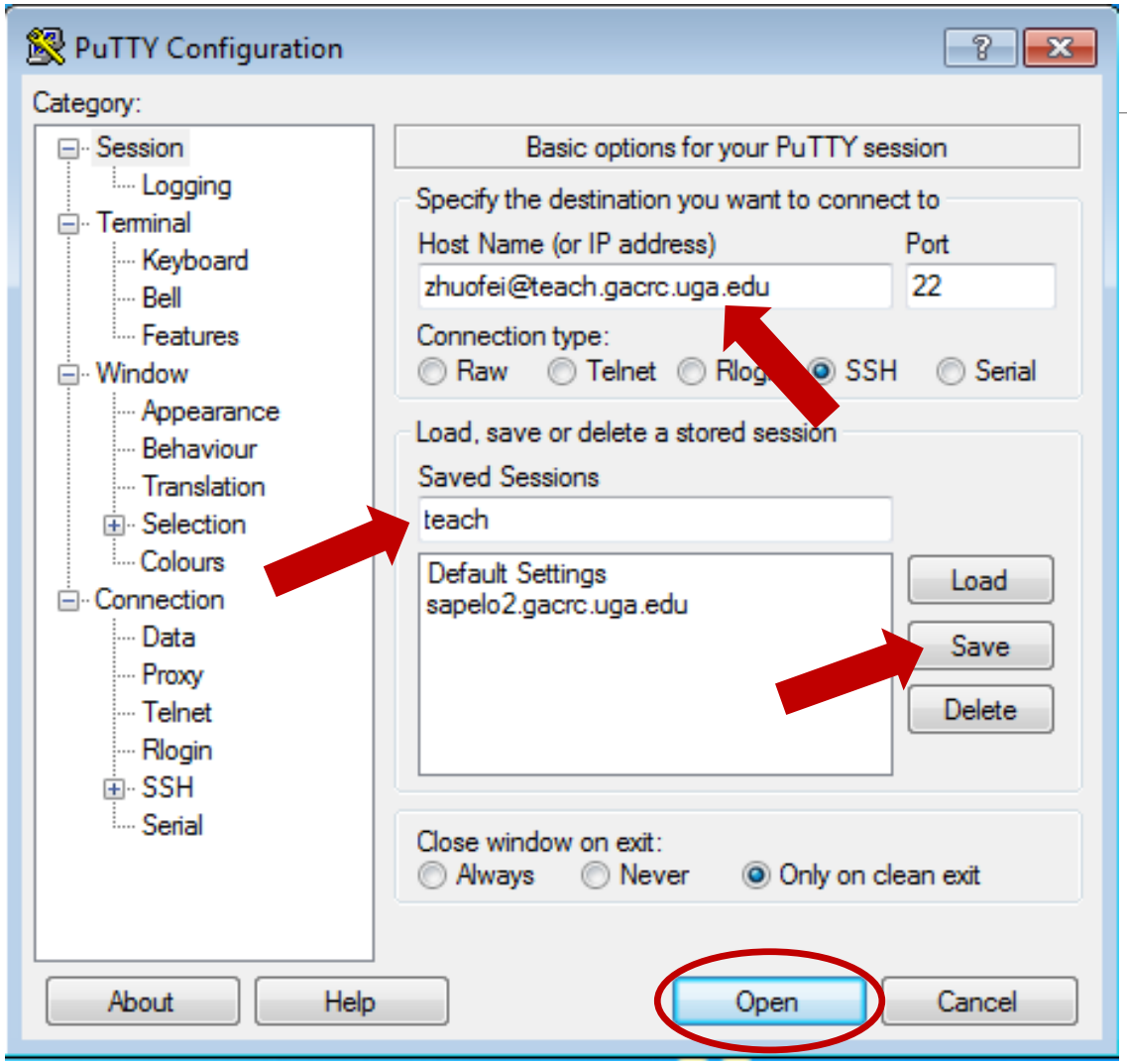
Step1 (Cont.) - Windows using PuTTY

1. Download and install PuTTY: https://www.putty.org/
2. Detailed downloading and installation instructions:

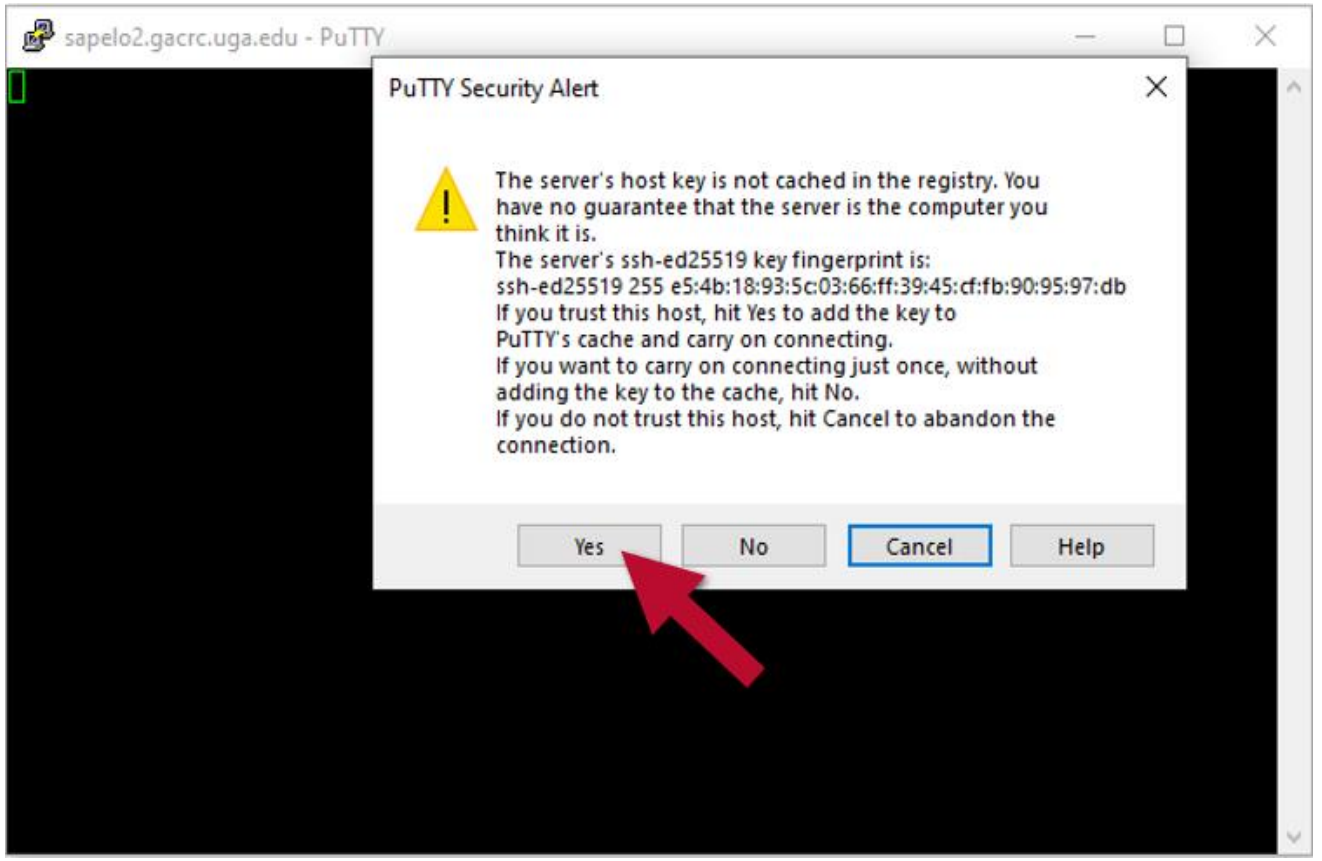
   https://wiki.gacrc.uga.edu/wiki/How_to_Install_and_Configure_PuTTY
3. Detailed configuring and usage instructions:

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

Step1 (Cont.) - Windows using PuTTY

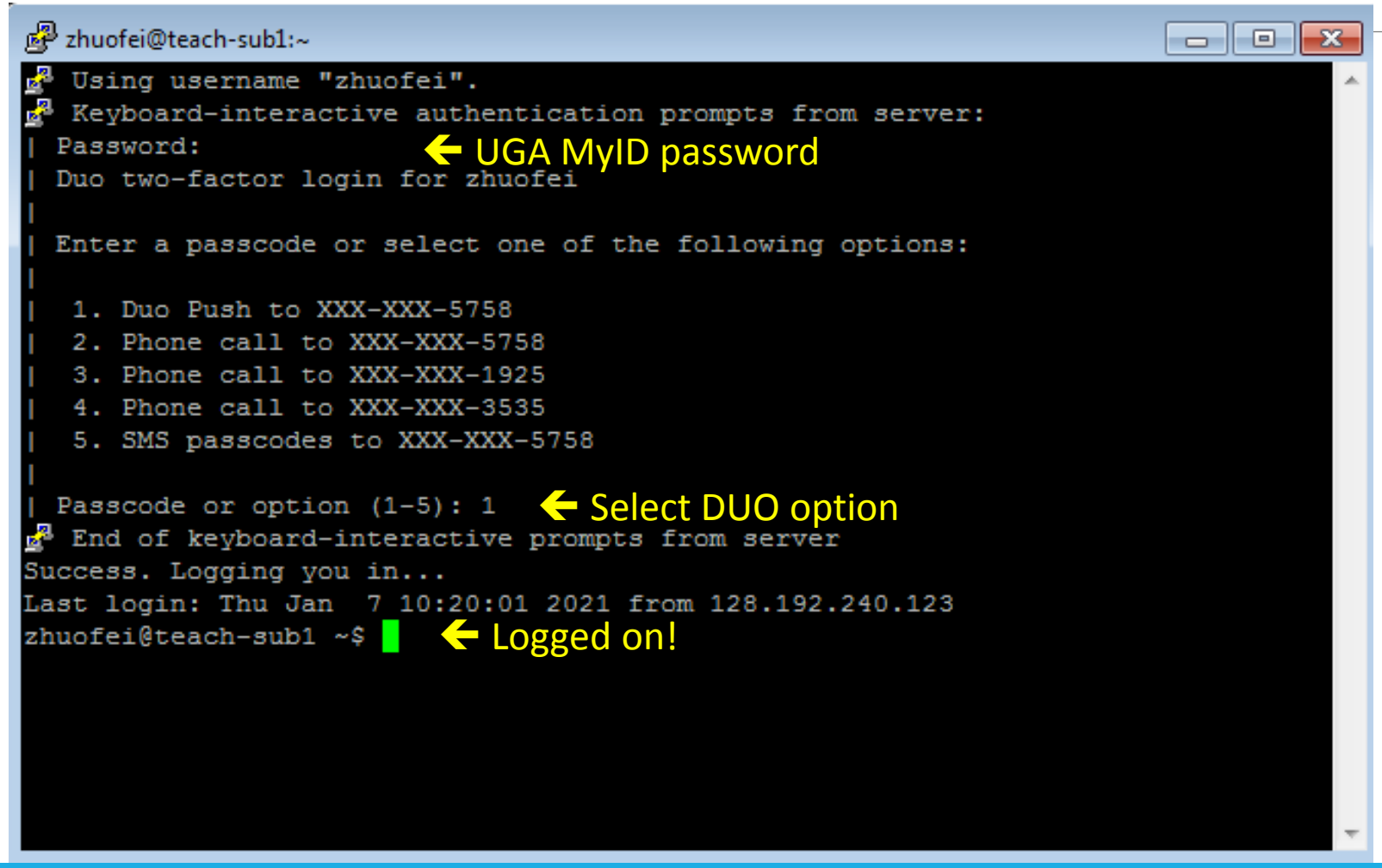


The first time you connect to login node, PuTTY will give you this security alert window. Please click "Yes"



Step1 (Cont.) - Windows using PuTTY

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



Step2 - 3: Create and change directory to workDir

```
[zhuofei@teach-sub1 ~]$ ls                    ← List folder contents
[zhuofei@teach-sub1 ~]$ mkdir workDir         ← Create a subdirectory
[zhuofei@teach-sub1 ~]$ ls
workDir
[zhuofei@teach-sub1 ~]$ cd workDir            ← Change directory
[zhuofei@teach-sub1 workDir]$ ls
[zhuofei@teach-sub1 workDir]$                 ← workDir is empty
```

Step4: 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 .
```

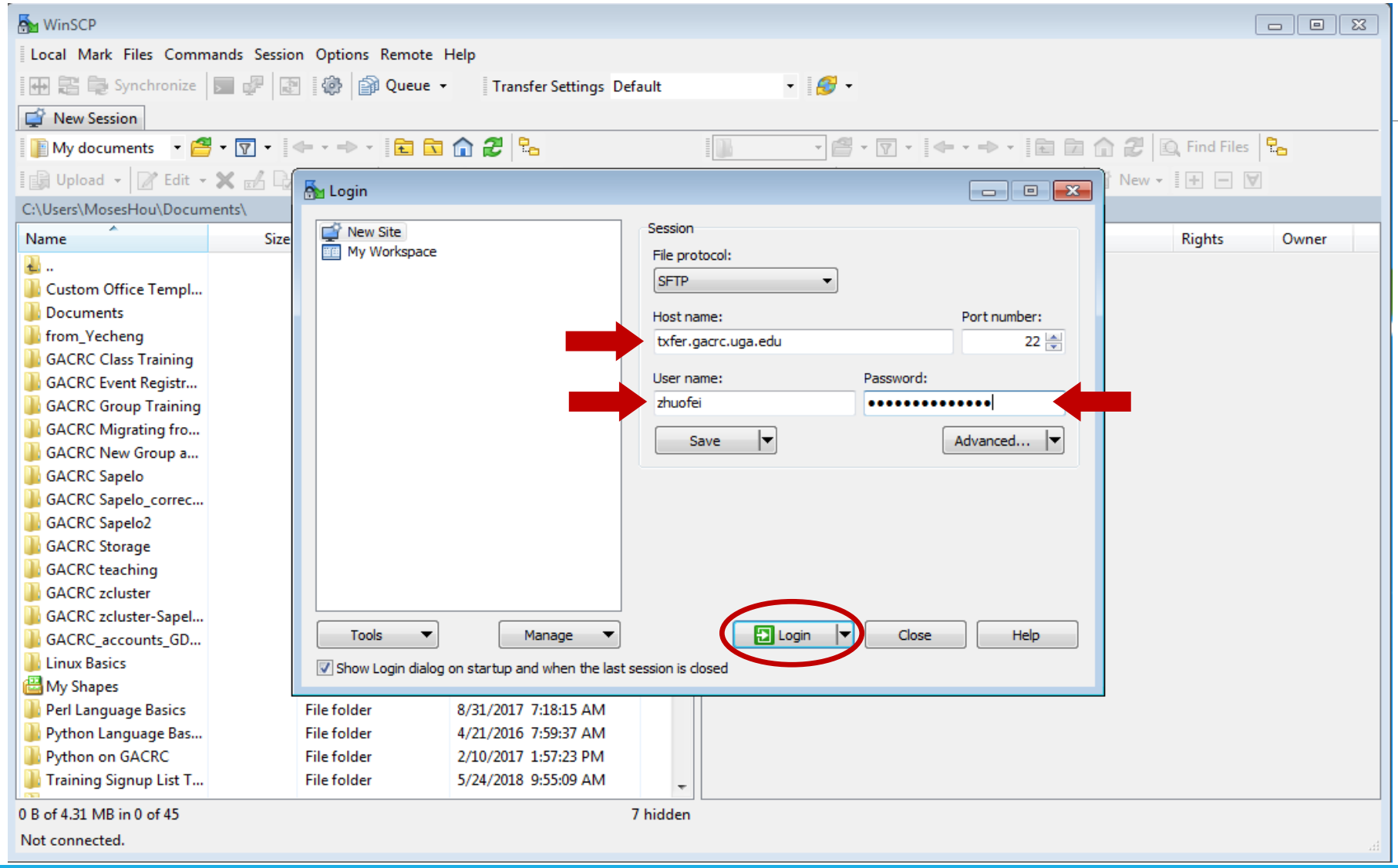
```
scp -r zhuofei@txfer.gacrc.uga.edu:/home/zhuofei/workDir/folder/ .
```

Step4 (Cont.) - Windows using WinSCP

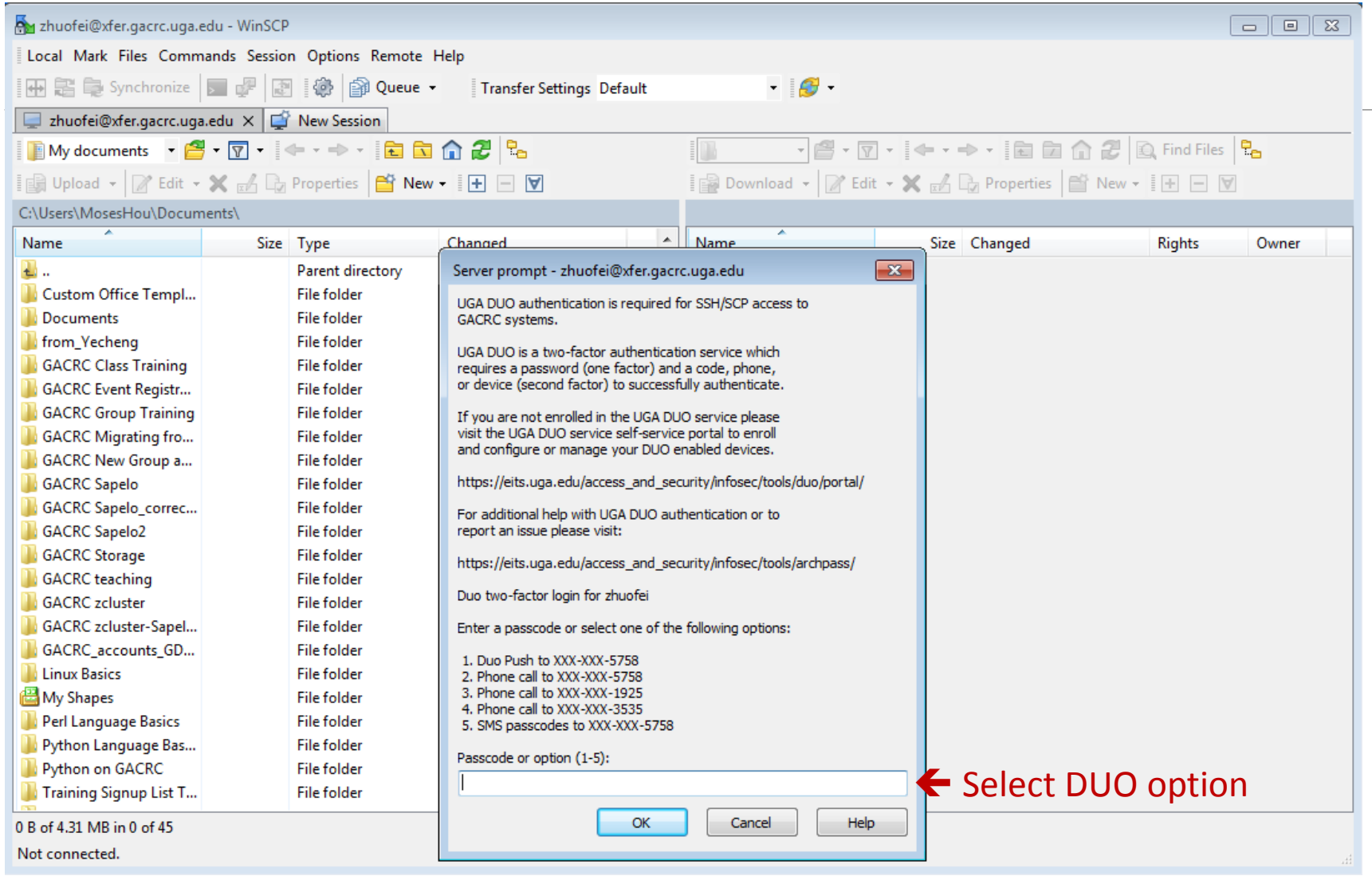
https://wiki.gacrc.uga.edu/wiki/Transferring_Files#Using_WinSCP_2

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

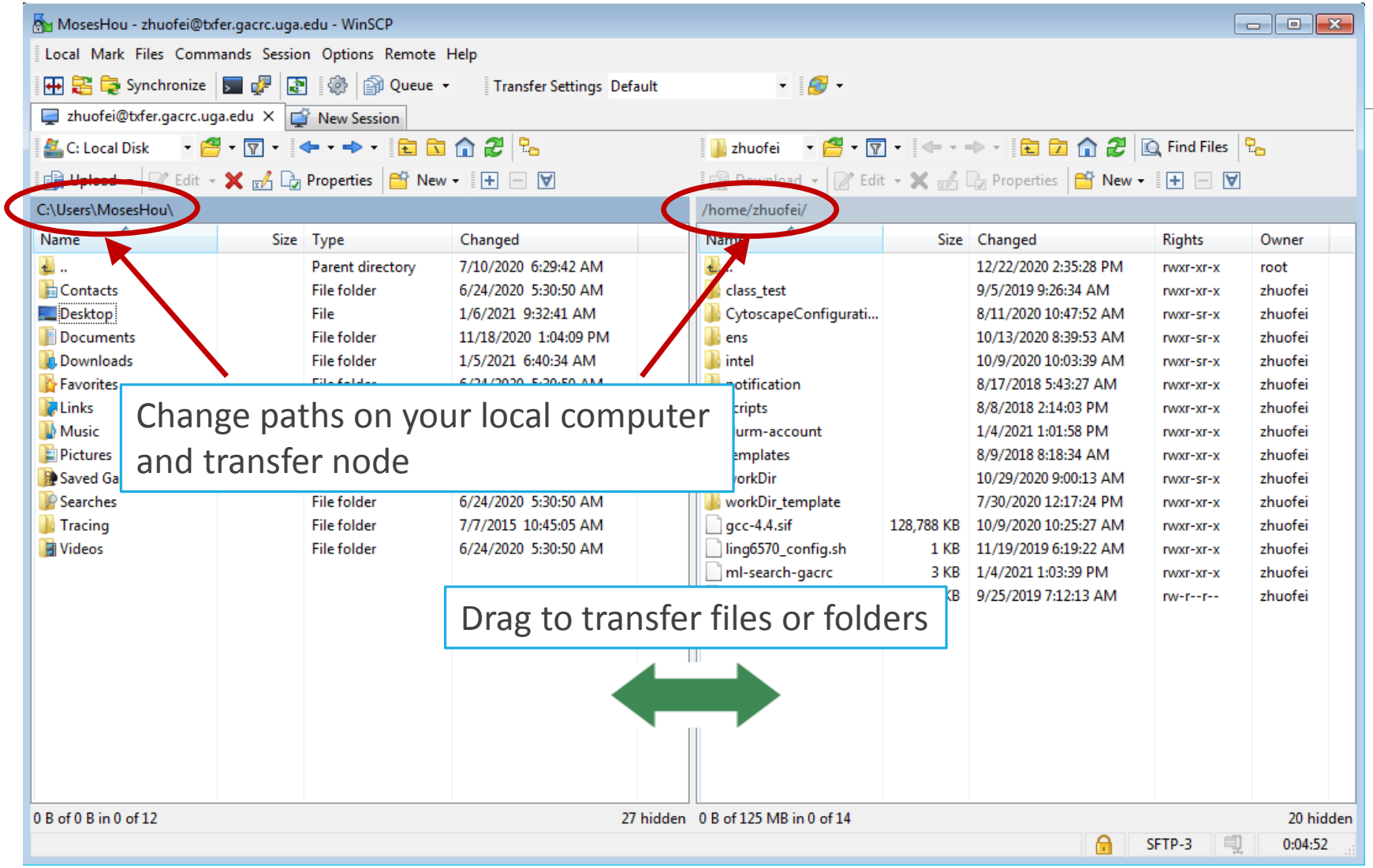
Step4 (Cont.) - Windows using WinSCP



Step4 (Cont.) - Windows using WinSCP



Step4 (Cont.) - Windows using WinSCP



Step4 (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 (Landing home)
  2. /work/phys4601/MyID
  3. /work/phys4601/instructor_data
- Transfer data between two folders on cluster using cp or mv, e.g.:

```
mv /work/phys4601/MyID/datafile /home/MyID/workDir
```

Step5: Compile Fortran code *mult.f* into a binary

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```
zhuofei@teach-sub1 workDir$ interact                          ← Start an interactive session
zhuofei@tcn26 workDir$ cp  /usr/local/training/phys4601/mult.f  .   ← Copy source code to your working dir
zhuofei@tcn26 workDir$ cat  mult.f                            ← Show contents of source code
      Program mult
C     Multiplies two integer numbers
      implicit none
      integer i,j,iprod
      i=3
      j=4
      open(1, file='output.txt')
      iprod=i*j
      write(1,10)i,j,iprod
10    format('The product of ', I2, ' and ', I2, ' is ', I3)
      close(1)
      end
zhuofei@tcn26 workDir$ module load  GCC/8.3.0                 ← Load GCC compiler module
zhuofei@tcn26 workDir$ gfortran  mult.f  -o  mult.x           ← Compile source code into a binary
zhuofei@tcn26 workDir$ ls
mult.f  mult.x                                                ← Binary is generated in your working dir
zhuofei@tcn26 workDir$ exit                                   ← Exit from interactive session
```

Step6: Make a job submission script *sub.sh using nano*

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```
zhuofei@teach-sub1 workDir$ cp  /usr/local/training/phys4601/sub.sh  .        ← Copy sub.sh to your working dir
zhuofei@teach-sub1 workDir$ cat  sub.sh                                      ← Show contents of sub.sh
#!/bin/bash
#SBATCH --job-name=test                 # Job name
#SBATCH --partition=fsr4601             # Submit job to fsr4601 partition
#SBATCH --ntasks=1                      # Single task job
#SBATCH --cpus-per-task=1               # Number of cores per task
#SBATCH --mem=2gb                       # Total memory for job
#SBATCH --time=00:01:00                 # Time limit hrs:min:sec; fsr4601 TIMELIMIT 1 min
#SBATCH --output=log.%j                 # Standard output and error log
#SBATCH --mail-user=MyID@uga.edu        # Where to send mail
#SBATCH --mail-type=ALL                 # Mail events (BEGIN, END, FAIL, ALL)

cd $SLURM_SUBMIT_DIR
module load GCC/8.3.0
time ./mult.x                           # run the binary code you compiled in step 5 in this job
zhuofei@teach-sub1 workDir$ nano sub.sh      ← Use nano modify sub.sh, e.g., email address
```

Step7: 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 12099
```

Tips: sub.sh is a job submission script for

1. specifying computing resources
2. loading compiler module using module load
3. running any Linux commands you want to run
4. running your binary code

Step7: Check job status using squeue

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

```
zhuofei@teach-sub1 workDir$ squeue --me
JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
12099    fsr4601      test   zhuofei  R       0:05      1 tcn18

zhuofei@teach-sub1 workDir$ squeue --me -l
Mon Jan 11 12:03:14 2021
JOBID PARTITION     NAME     USER    STATE       TIME TIME_LIMI  NODES NODELIST(REASON)
12099    fsr4601      test   zhuofei  RUNNING       0:11      1:00      1 tcn18
```

Job State: R for Running; PD for PenDing; F for Failed

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

Step7 (Cont.): Check job details using sacct-gacrc -X

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

```
$ sacct-gacrc -X

JobID    JobName      User  Partition   NodeList AllocNodes NTask NCPUS  ReqMem  MaxVMSize      State  CPUTime    Elapsed   Timelimit  ExitCode
------------ ---------- --------- ---------- ---------- ---------- ----- ----- ------- ---------- ---------- ---------- ---------- -------- ---------- ---------- ---------- ----------
174     testBLAST   zhuofei      batch       tcn18           1                4      20Gn                RUNNING  00:04:56   00:01:14   02:00:00        0:0
```

Step7 (Cont.): Check job details using scontrol show job

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

```
zhuofei@teach-sub1 workDir$ scontrol show job 12099
JobId=12099 JobName=test
   UserId=zhuofei(1772) GroupId=gacrc-instruction(21004) MCS_label=N/A
   ……
   JobState=RUNNING Reason=None Dependency=(null)
   Requeue=1 Restarts=0 BatchFlag=1 Reboot=0 ExitCode=0:0
   RunTime=00:00:23 TimeLimit=00:01:00 TimeMin=N/A
   ……
   Partition=fsr4601 AllocNode:Sid=10.31.32.252:92156
   NodeList=tcn18
   NumNodes=1 NumCPUs=1 NumTasks=1 CPUs/Task=1 ReqB:S:C:T=0:0:*:*
   MinCPUsNode=1 MinMemoryNode=2G MinTmpDiskNode=0
   Command=/home/zhuofei/workDir/sub.sh
   WorkDir=/home/zhuofei/workDir
   StdErr=/home/zhuofei/workDir/log.12099
   StdOut=/home/zhuofei/workDir/log.12099
   MailUser=zhuofei@uga.edu MailType=BEGIN,END,FAIL,REQUEUE,STAGE_OUT
```

Step7 (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

```
zhuofei@teach-sub1 workDir$ scancel 12099
zhuofei@teach-sub1 workDir$ squeue --me
JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
```

Step7 (Cont.): Check node info using sinfo

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

```
zhuofei@teach-sub1 workDir$ sinfo
PARTITION   AVAIL  TIMELIMIT  NODES  STATE NODELIST
batch*         up 7-00:00:00      1  down* tcn17
batch*         up 7-00:00:00     24   idle tcn[1-16,18-25]
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      2   idle tchmn[1-2]
fsr4601        up       1:00      1  down* tcn17
fsr4601        up       1:00     24   idle tcn[1-16,18-25]
fsr8602        up      10:00      1  down* tcn17
fsr8602        up      10:00     24   idle tcn[1-16,18-25]
```

idle = no cores in use; mix = some cores are still free; alloc = all cores are allocated

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: `scontrol show job JobID` for details of a running or pending jobs

Option 2: `seff` for details of computing resource usage of a finished job

Option 3: `sacct-gacrc` or `sacct-gacrc-v` for details of computing resource usage of a running or finished job

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

```
#SBATCH --mail-user=username@uga.edu
#SBATCH --mail-type=END,FAIL
```

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:

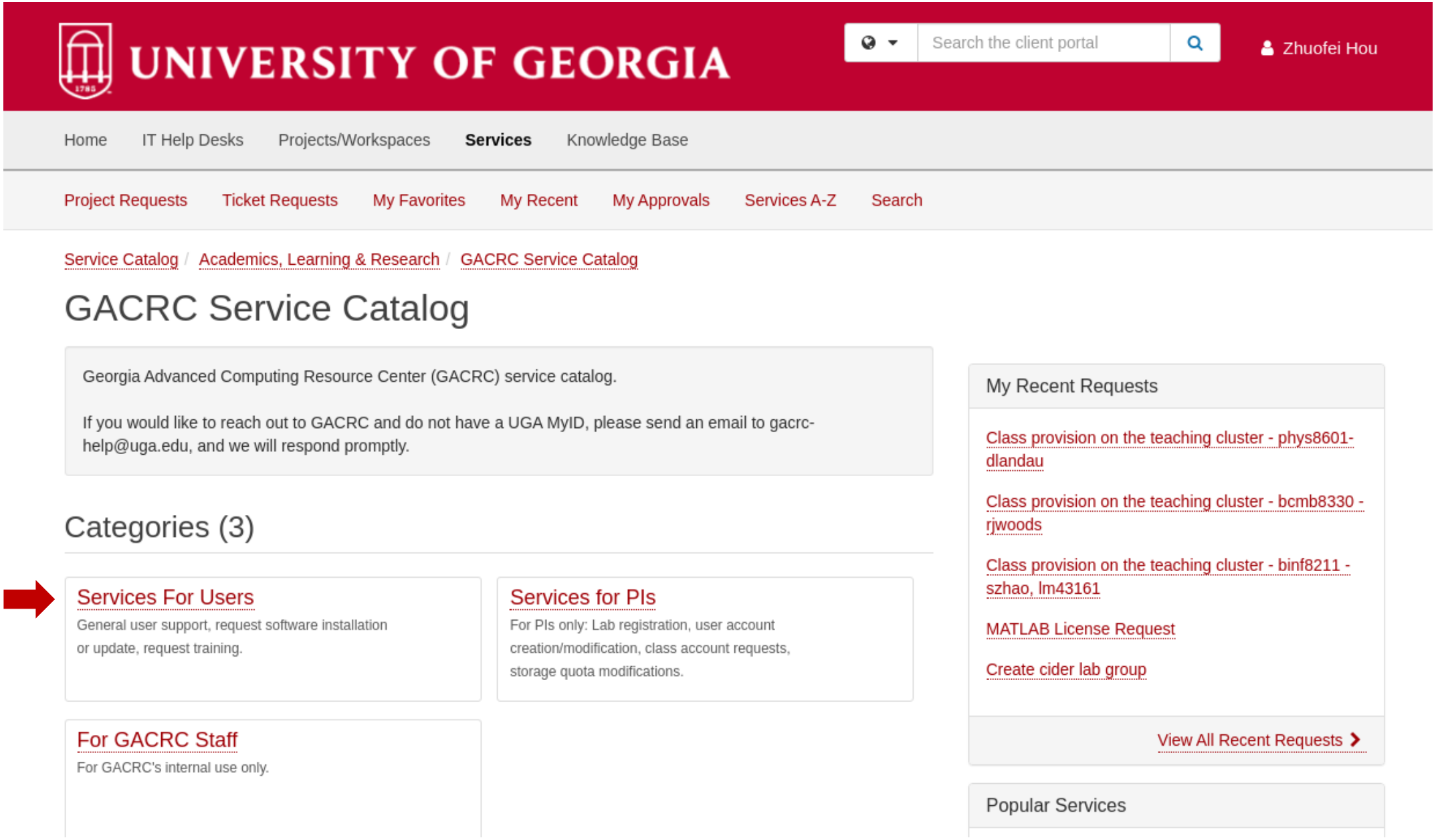
Please tell us details of your question or problem, including but not limited to:

- ✓ 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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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.
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For PIs only: Lab registration, user account creation/modification, class account requests, storage quota modifications.
For GACRC Staff
For GACRC's internal use only.
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Class provision on the teaching cluster - binf8211 - szhao, lm43161
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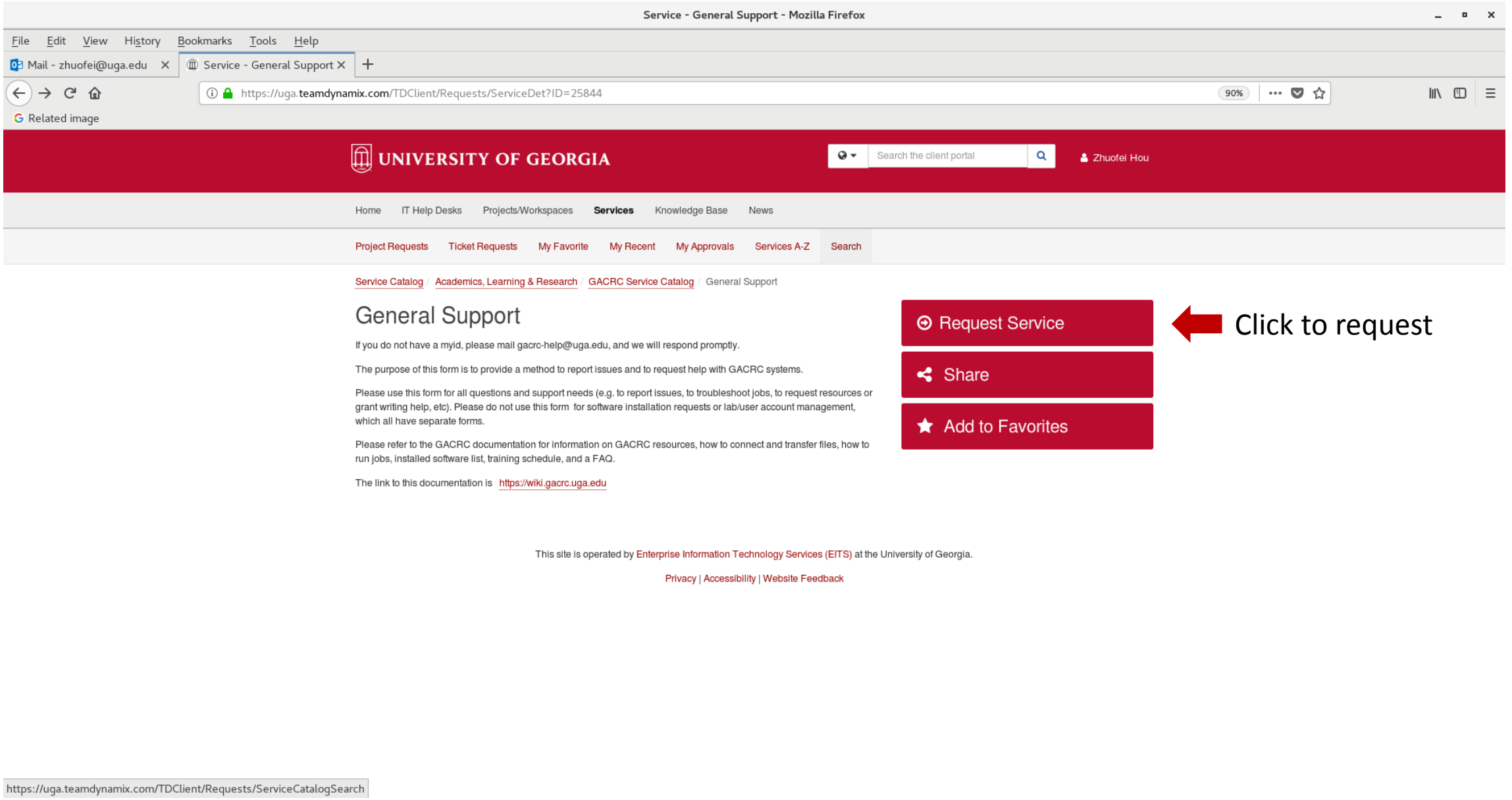
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General Support
If you do not have a myid, please mail gacrc-help@uga.edu, and we will respond promptly.
The purpose of this form is to provide a method to report issues and to request help with GACRC systems.
Please use this form for all questions 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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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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