Introduction to GACRC Teaching Cluster PHYS8602

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

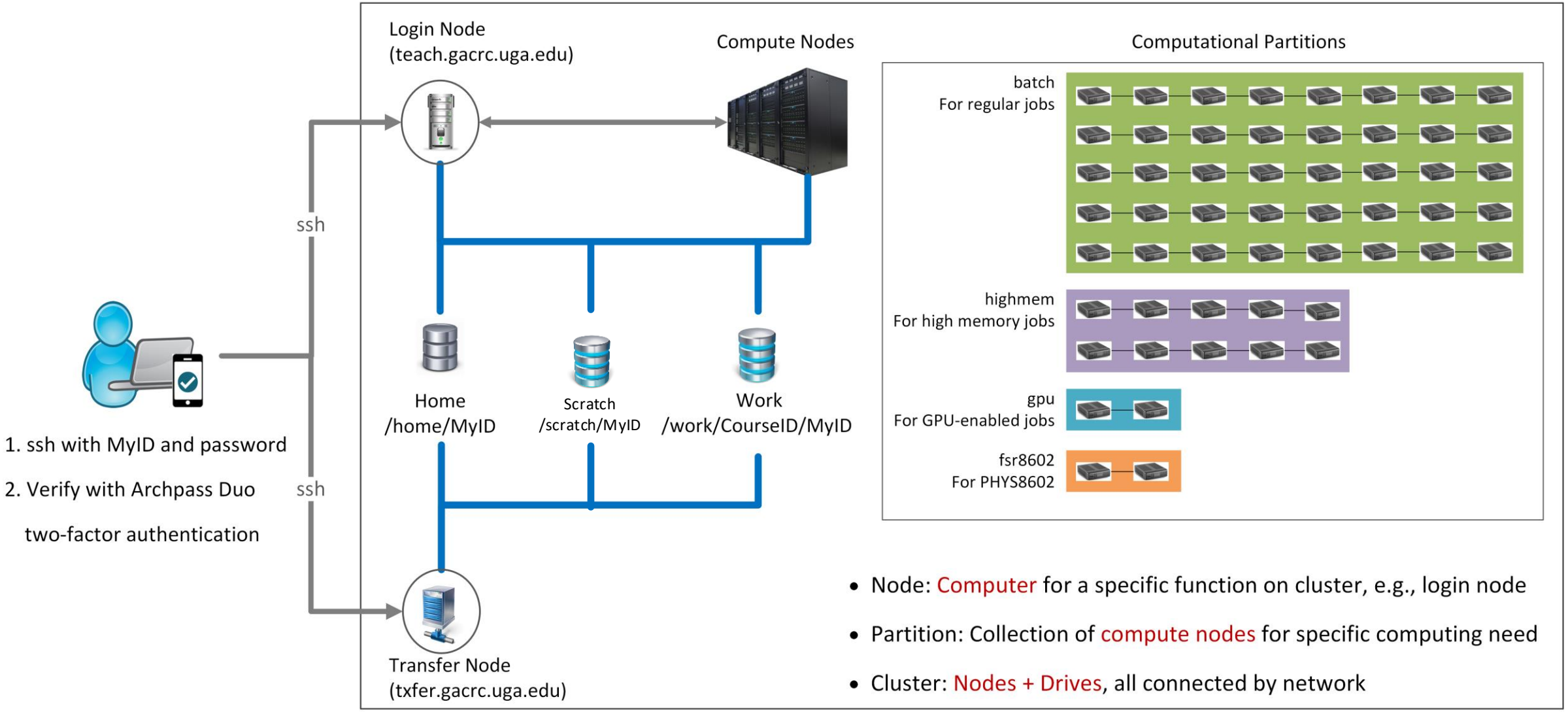
Wiki: http://wiki.gacrc.uga.edu

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



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:
  1. For batch or interactive 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/phys8602/MyID : Data storing space for individual user in a class
  3. /work/phys8602/instructor_data : Data shared with class by the instructors
- Partitions for your class: fsr8602

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/3.11.3-GCCcore-12.3.0
  3. Software names are case-sensitive!
     - `module spider pattern` : Search module names matching a pattern (case-insensitive)
     - `module load/unload moduleName` : Load/remove a module
     - `module avail` : List all available modules installed on the cluster
     - `module list` : List modules that are currently loaded
     - `module purge` : Remove all modules from your current 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. 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. Compile C code *mult.c* into a binary code
7. Make a job submission script in workDir : nano sub.sh
8. Submit a job from workDir : sbatch sub.sh
9. 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

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…

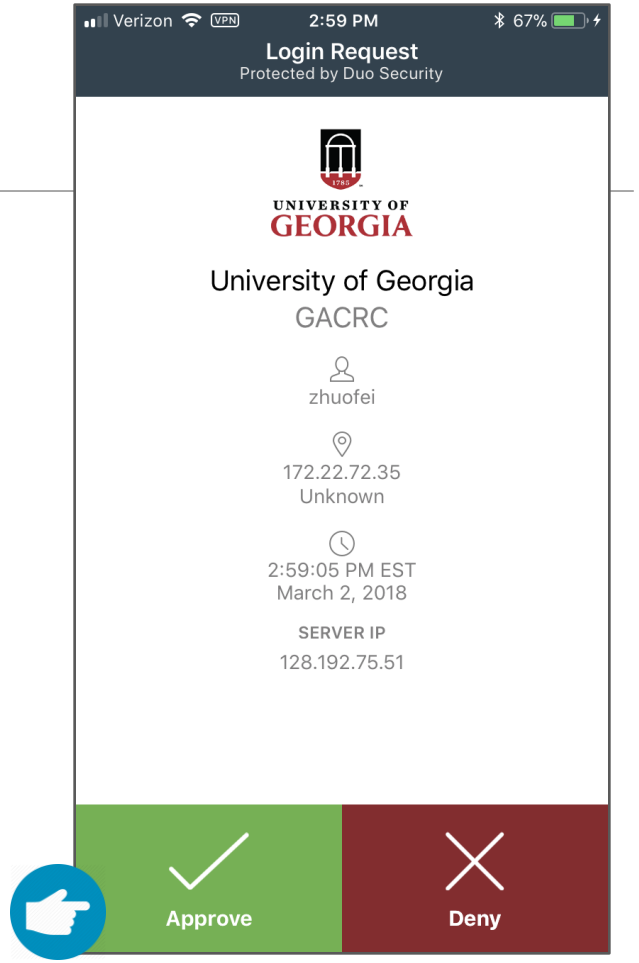
Password: ← 2. Enter your MyID password
When you enter password, no stars or dots will show as you are typing. Please type password carefully!

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

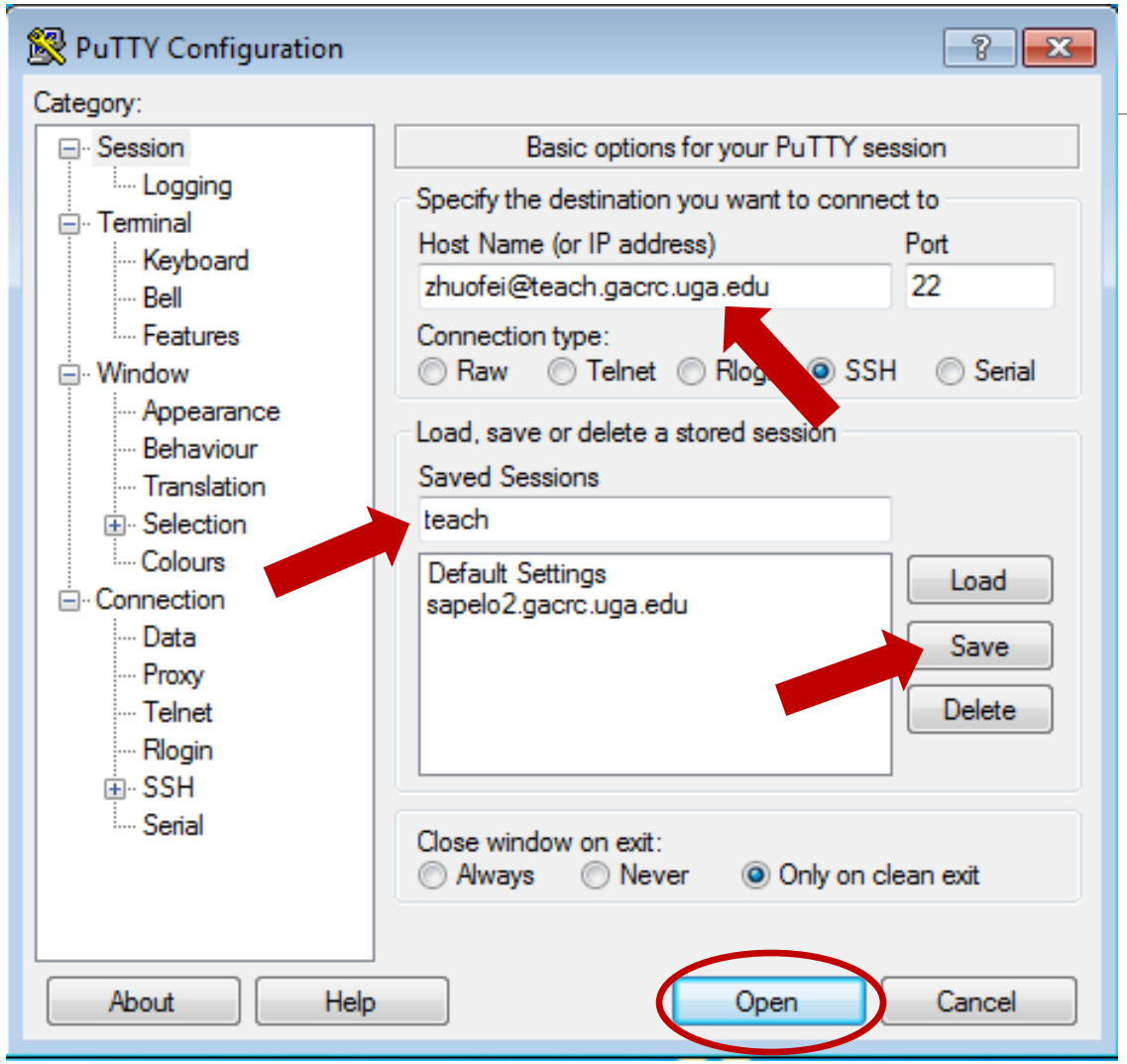
Step1 (Cont.) - Windows using PuTTY

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

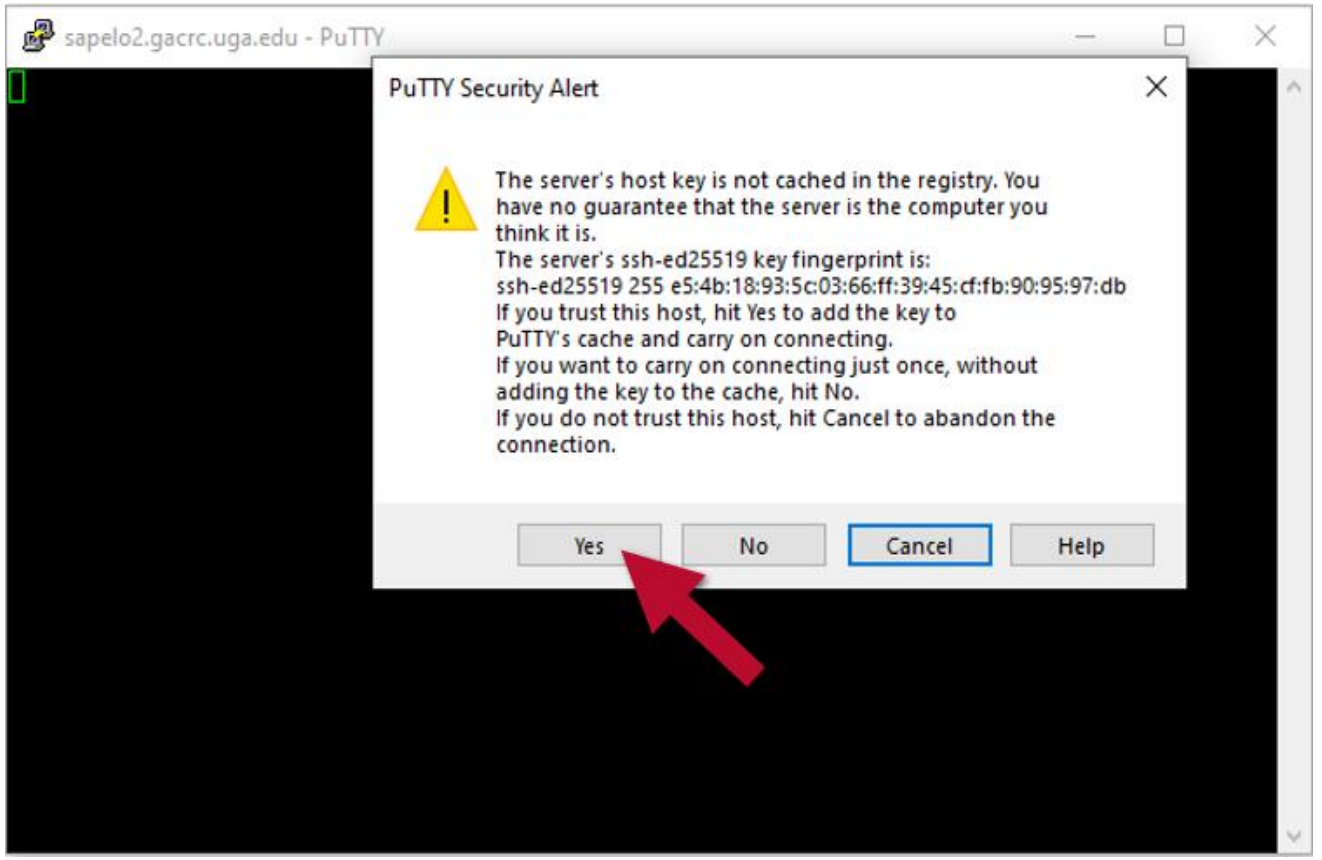
   https://wiki.gacrc.uga.edu/wiki/How_to_Install_and_Configure_PuTTY
3. Detailed configuring and usage instructions:

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

Step1 (Cont.) - Windows using PuTTY

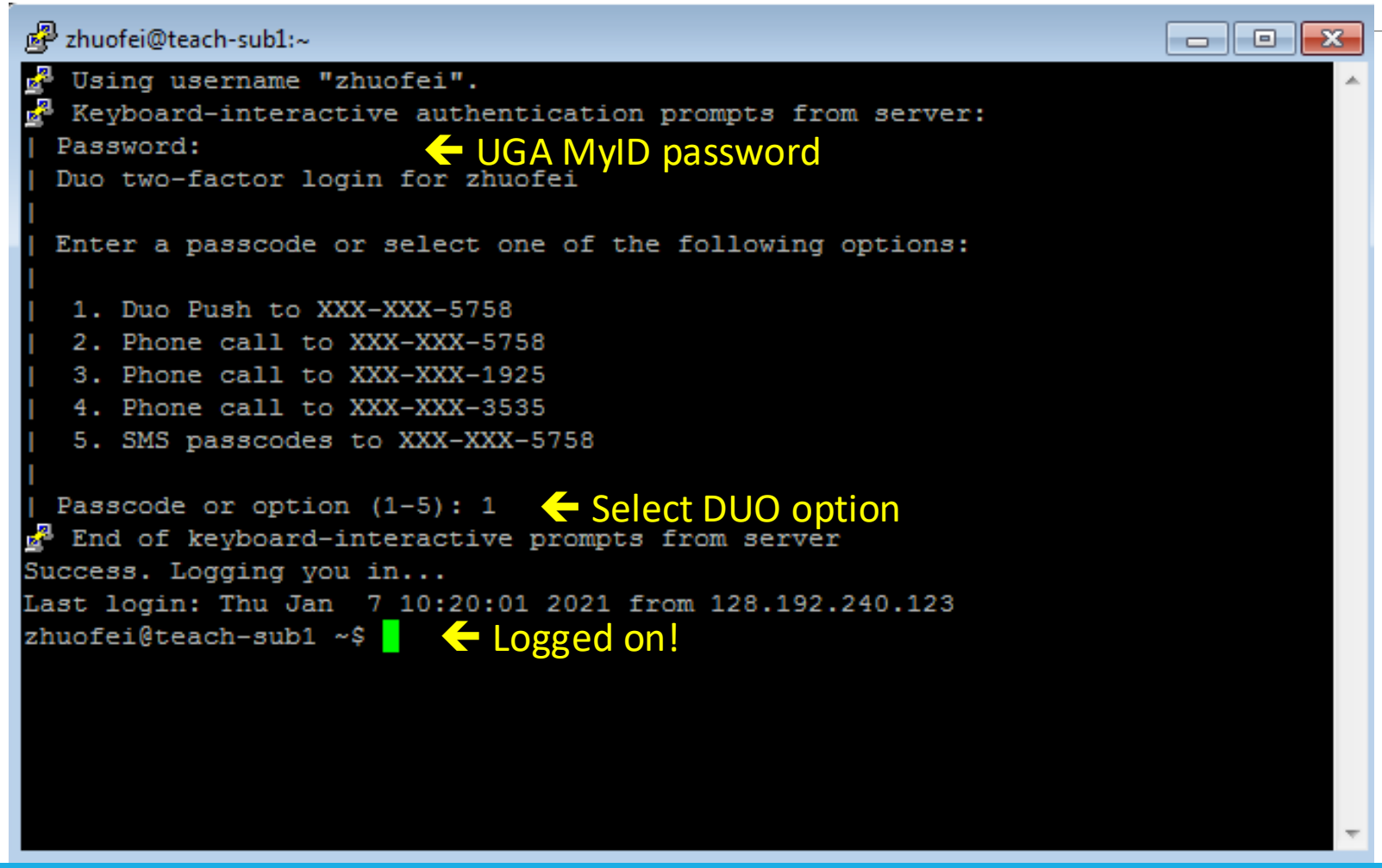


The first time you connect to login node, PuTTY will give you this security alert window. Please click "Yes"



Step1 (Cont.) - Windows using PuTTY

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



Step2 - 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$
```

← change directory to your scratch space

← create a working directory

← change directory to your working directory

← list contents of the directory

← it is an empty folder

Step5: 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/ .
```

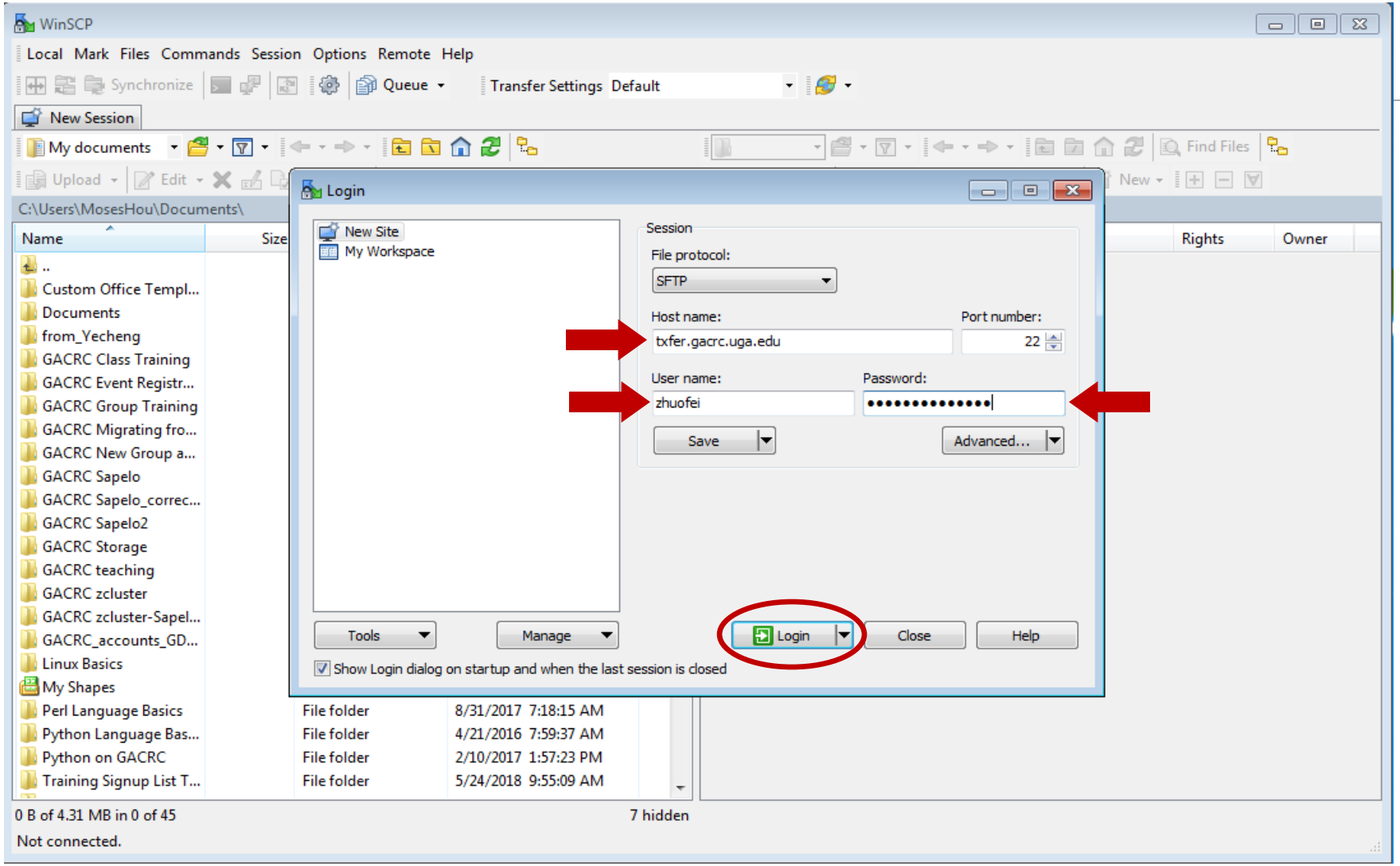
Step5 (Cont.) - Windows using WinSCP

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

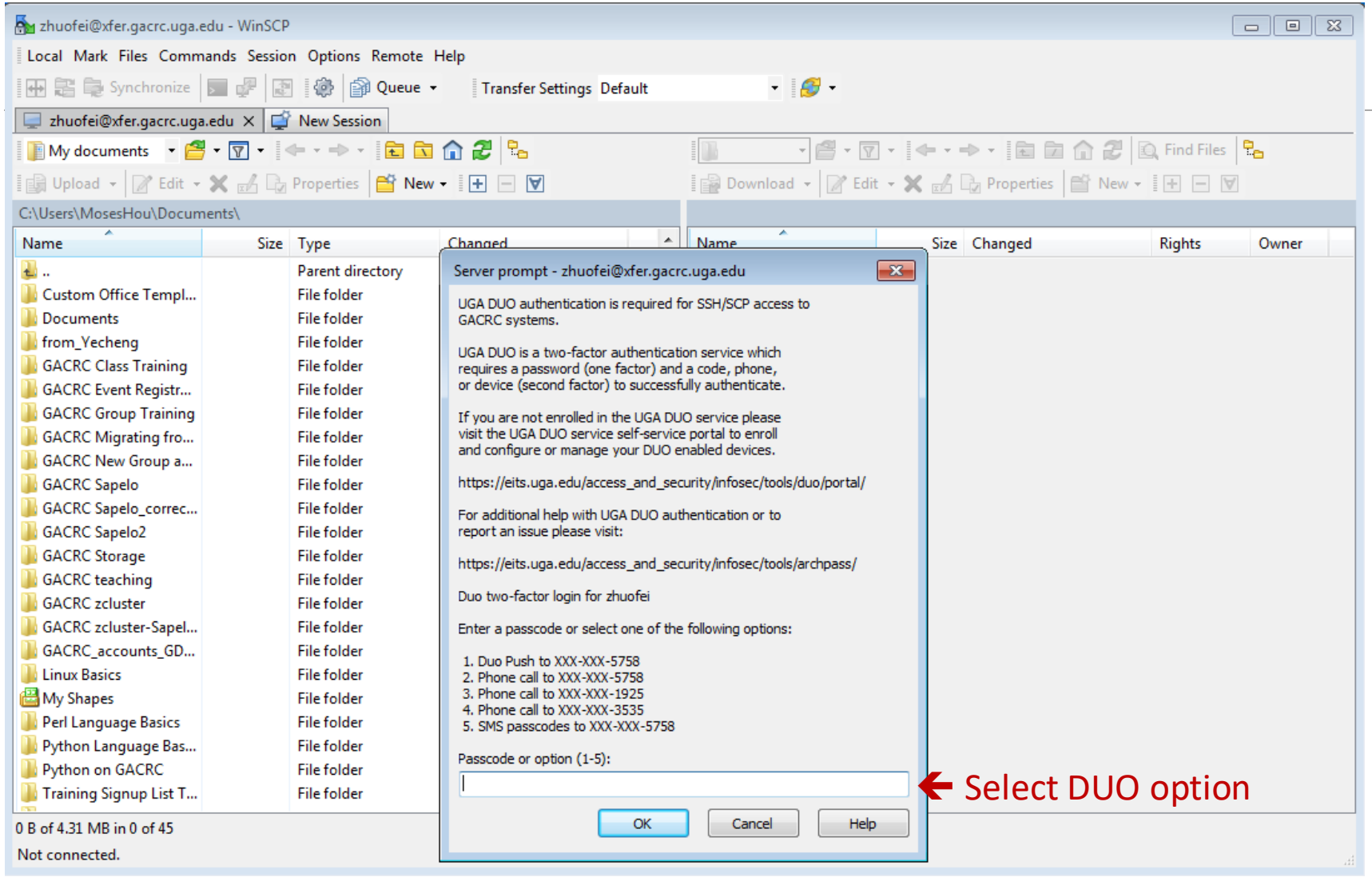
1. You need to connect to cluster's Transfer node (txfer.gacrc.uga.edu)
2. Use WinSCP on local computer
   - WinSCP can be downloaded from https://winscp.net/eng/index.php
   - Default installation procedure is simple
3. Alternative FileZilla https://wiki.gacrc.uga.edu/wiki/Transferring_Files#Using_FileZilla_2

Step5 (Cont.) - Windows using WinSCP

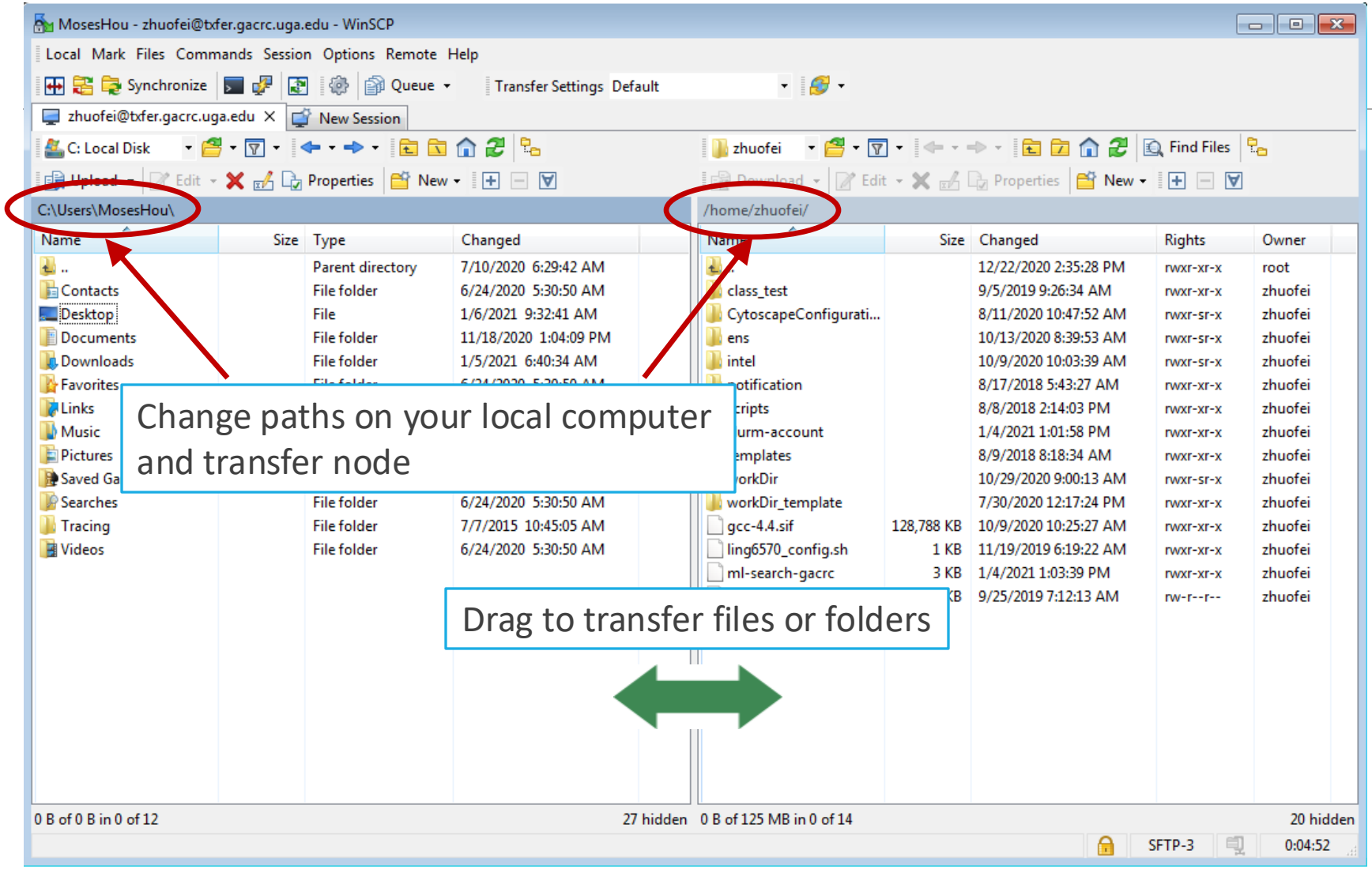
https://wiki.gacrc.uga.edu/wiki/Transferring_Files#Using_WinSCP_2



Step5 (Cont.) - Windows using WinSCP



Step5 (Cont.) - Windows using WinSCP



Step5 (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 (page 5):
  1. /home/MyID (Landing folder)
  2. /scratch/MyID (Job working space)
  3. /work/phys8602/MyID
  4. /work/phys8602/instructor_data
- Transfer data between two folders on cluster using cp or mv, e.g.:

```
mv /work/phys8602/MyID/datafile /home/MyID/workDir
```

Step6: Compile C code *mult.c* into a binary

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```
zhuofei@teach-sub1 workDir$ interact                                  ← Start an interactive session
zhuofei@tcn26 workDir$ cp  /usr/local/gacrc/training/phys8602/mult.c  .  ← Copy source code to your working dir
zhuofei@tcn26 workDir$ cat  mult.c
/* Program mult
 * Multiple two integer numbers */
#include <stdio.h>
int main(void)
{
  int i=3, j=4, iprod;
  FILE *fp;
  fp = fopen("output.txt","w");
  iprod=i*j;
  fprintf(fp, "The product of %d and %d is %d\n", i,j,iprod);
  fclose(fp);
  return 0;
}
zhuofei@tcn26 workDir$ module load  GCC/12.3.0                        ← Load GCC compiler module
zhuofei@tcn26 workDir$ gcc  mult.c  -o  mult.x                        ← Compile source code into a binary
zhuofei@tcn26 workDir$ ls
mult.c  mult.x                                                        ← Binary is generated in your working dir
zhuofei@tcn26 workDir$ exit                                           ← Exit from interactive session
```

Step7: Make a job submission script *sub.sh using nano*

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```
zhuofei@teach-sub1 workDir$ cp  /usr/local/gacrc/training/phys8602/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=fsr8602             # Submit job to fsr8602, which is PHYS8602 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=00:10:00                 # Time limit hrs:min:sec; fsr8602 TIMELIMIT 10 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 $SLURM_SUBMIT_DIR                    # Change directory to current job working folder
module load GCC/12.3.0                  # Load GCC compiler module
time ./mult.x                           # run the binary you compiled in step 6
sleep 30                                # sleep 30 seconds
Zhuofei@teach-sub1 workDir$ nano sub.sh     ← Use nano to make modifications to sub.sh, e.g., email address
```

Step8: 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 17755
```

Tips: sub.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 your binary code

Step9: Check job status using squeue

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

```
zhuofei@teach-sub1 workDir$ sq --me

JOBID   NAME   PARTITION USER NODES CPUS MIN_MEMORY PRIORITY TIME TIME_LIMIT STATE   NODELIST(REASON)

17755   test   fsr8602    zhuofei 1  1    2G         21       0:05 10:00      RUNNING    rb1-3
```

Step9 (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 17755

zhuofei@teach-sub1 workDir$ sq --me

JOBID  NAME  PARTITION USER NODES CPUS MIN_MEMORY PRIORITY TIME TIME_LIMIT STATE  NODELIST(REASON)
```

Step9 (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
------------ -------------- --------- ---------- ----- ----- -------- ---------- ---------- ---------- --------------- --------- ---------------
17755           test   zhuofei    fsr8602        1      1        2G   00:00:23   00:00:23   00:10:00     CANCELLED+      0:0          rb1-3
17756           test   zhuofei    fsr8602        1      1        2G   00:00:31   00:00:31   00:10:00      COMPLETED      0:0          rb1-3


$ seff  17756        # Check computing resources used by a COMPLETED job
Job ID: 17756
Cluster: gacrc-teach
User/Group: zhuofei/gacrc-instruction
State: COMPLETED (exit code 0)
Cores: 1
CPU Utilized: 00:00:01
CPU Efficiency: 3.23% of 00:00:31 core-walltime
Job Wall-clock time: 00:00:31
Memory Utilized: 700.00 KB
Memory Efficiency: 0.03% of 2.00 GB
```

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
allnodes        up   infinite      1  down*    c4-23
allnodes        up   infinite     14   idle    b8-[6-7],rb1-[1-12]
batch           up 7-00:00:00      8   idle    rb1-[3-10]
gpu             up 7-00:00:00      1  down*    c4-23
highmem         up 7-00:00:00      2   idle    rb1-[1-2]
interactive     up 7-00:00:00      2   idle    rb1-[11-12]
franklin_gpu    up 7-00:00:00      2   idle    b8-[6-7]
fsr4601         up       1:00      8   idle    rb1-[3-10]
fsr8602         up      10:00      8   idle    rb1-[3-10]
```

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_Sapelo2#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
```

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

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 >

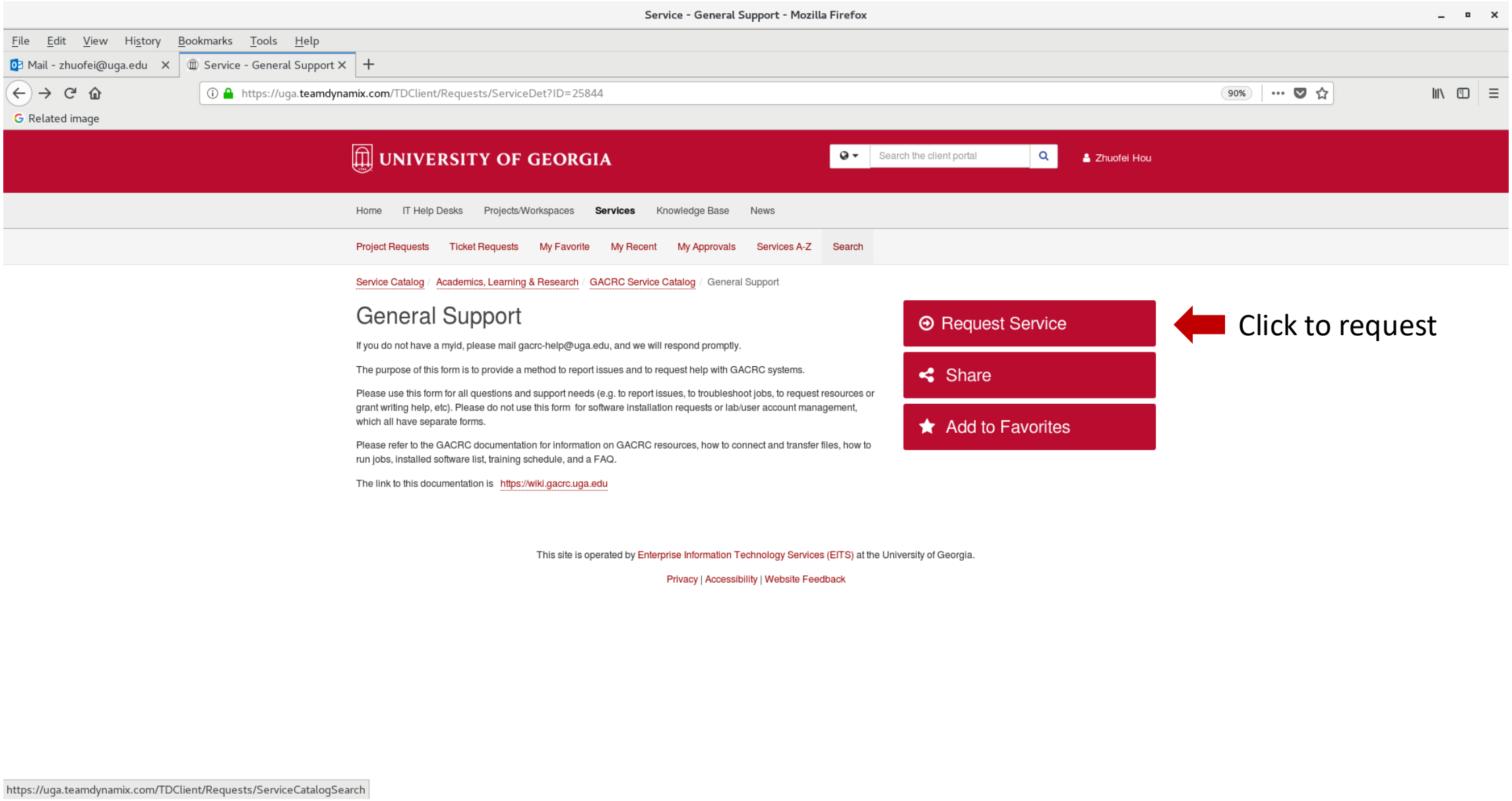
Popular Services

- 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
90%
Related image
UNIVERSITY OF GEORGIA
Search the client portal
Zhuofei Hou
Home IT Help Desks Projects/Workspaces Services Knowledge Base News
Project Requests Ticket Requests My Favorite My Recent My Approvals Services A-Z Search
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
Request Service
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Privacy | Accessibility | Website Feedback
https://uga.teamdynamix.com/TDClient/Requests/ServiceCatalogSearch

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