Introduction to GACRC Teaching Cluster

PHYS8601

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

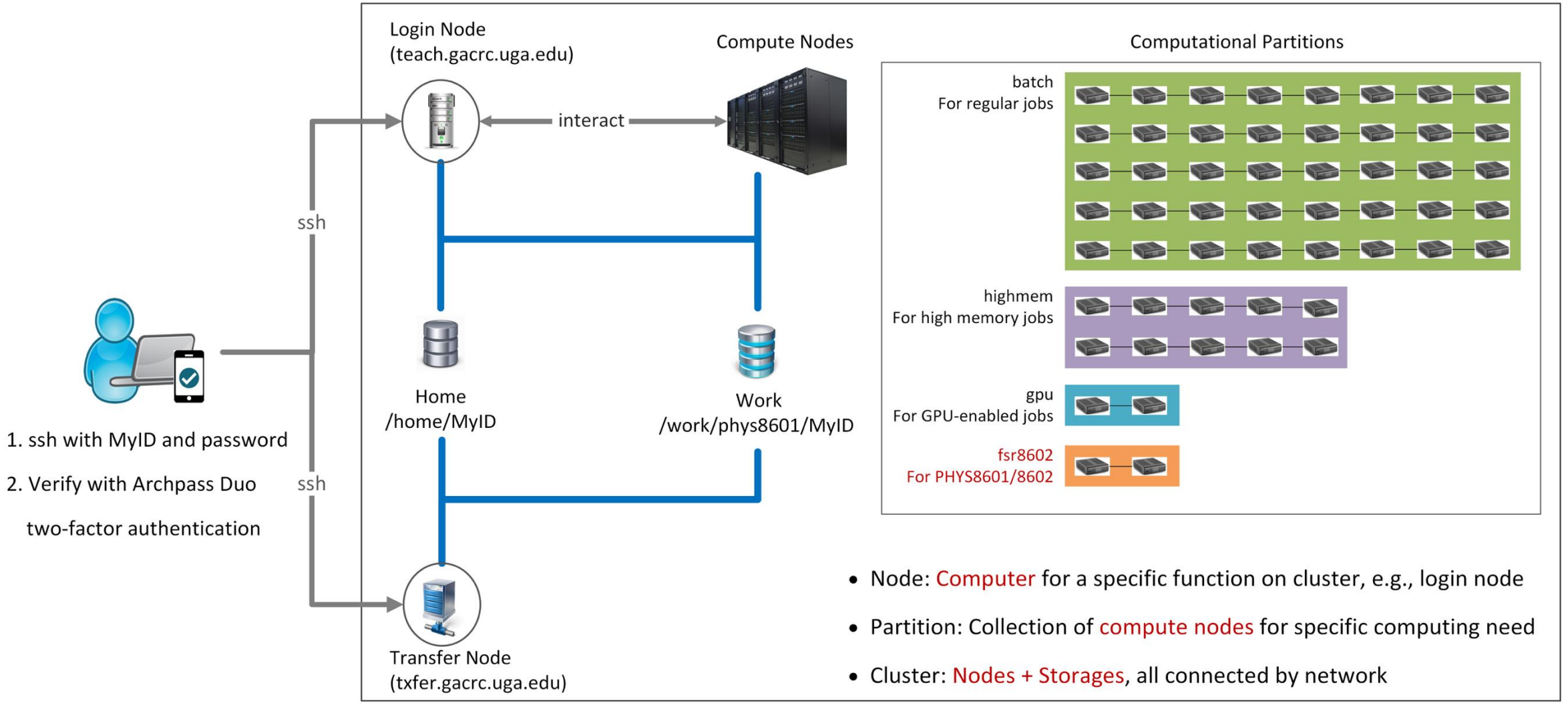
Wiki: http://wiki.gacrc.uga.edu

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/phys8601/MyID : data storing space for individual user in a class
  3. /work/phys8601/instructor_data : data shared with class by the instructors
- Partitions for PHYS8601/8602 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/3.12.3-GCCcore-13.3.0
  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. 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. 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 : 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://uga.teamdynamix.com/TDClient/3190/eitsclientportal/KB/?CategoryID=23825 on how to enroll.
2. If you are connecting from off-campus, please first connect to the UGA VPN, then connect to teach.gacrc.uga.edu. Information on how to use the VPN is available at https://uga.teamdynamix.com/TDClient/3190/eitsclientportal/KB/?CategoryID=23843

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…

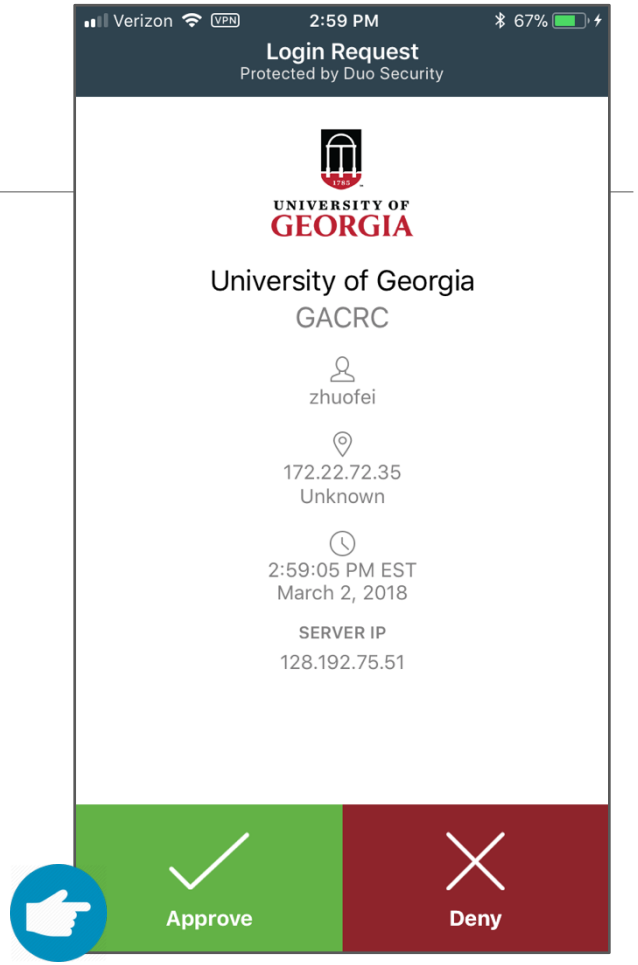
Password: ← 2. Enter your MyID password
When you enter password, no stars or dots will show as you are typing. Please type password carefully!

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.chiark.greenend.org.uk/~sgtatham/putty/latest.html

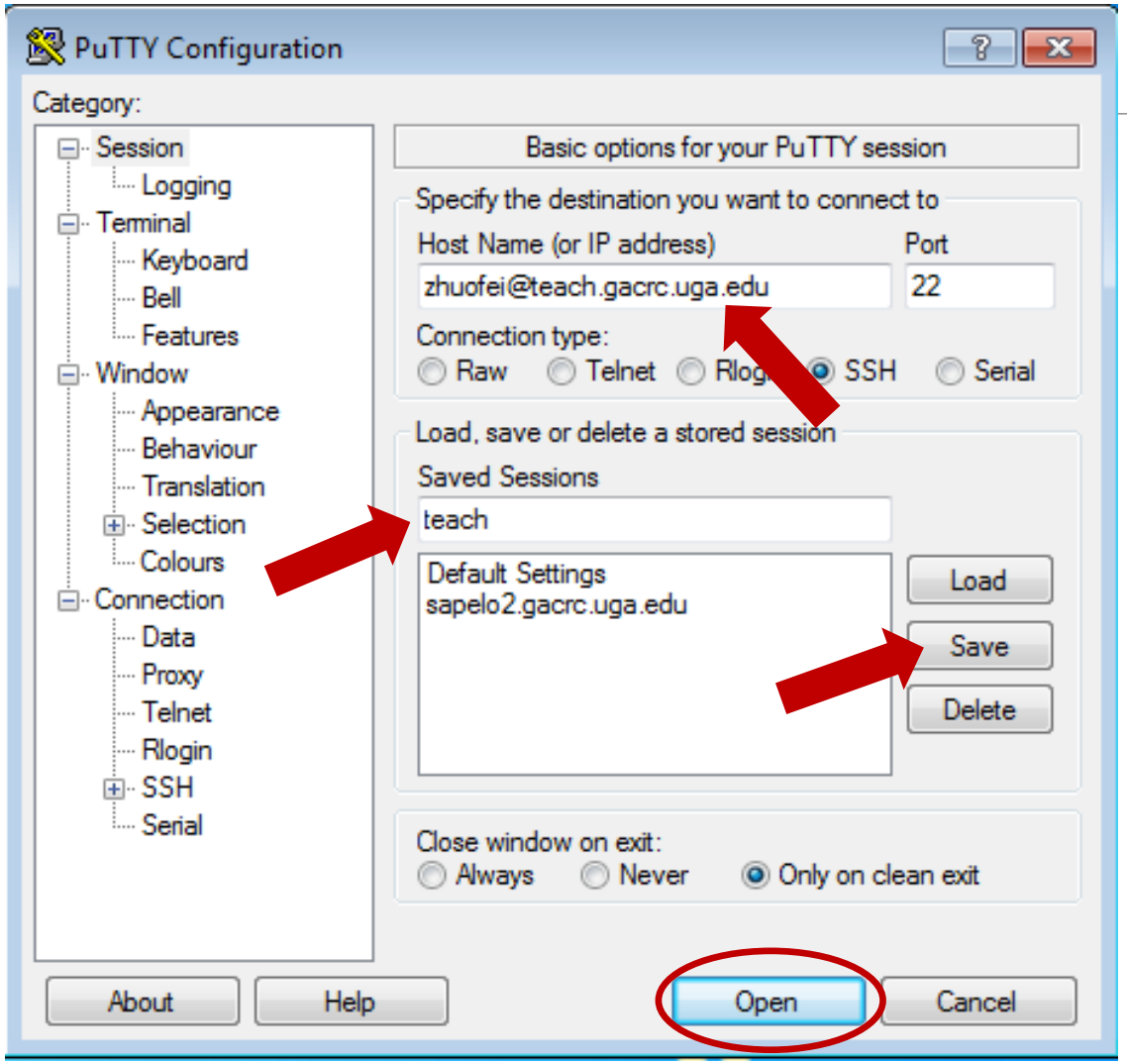
2. Detailed downloading and installation instructions:

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

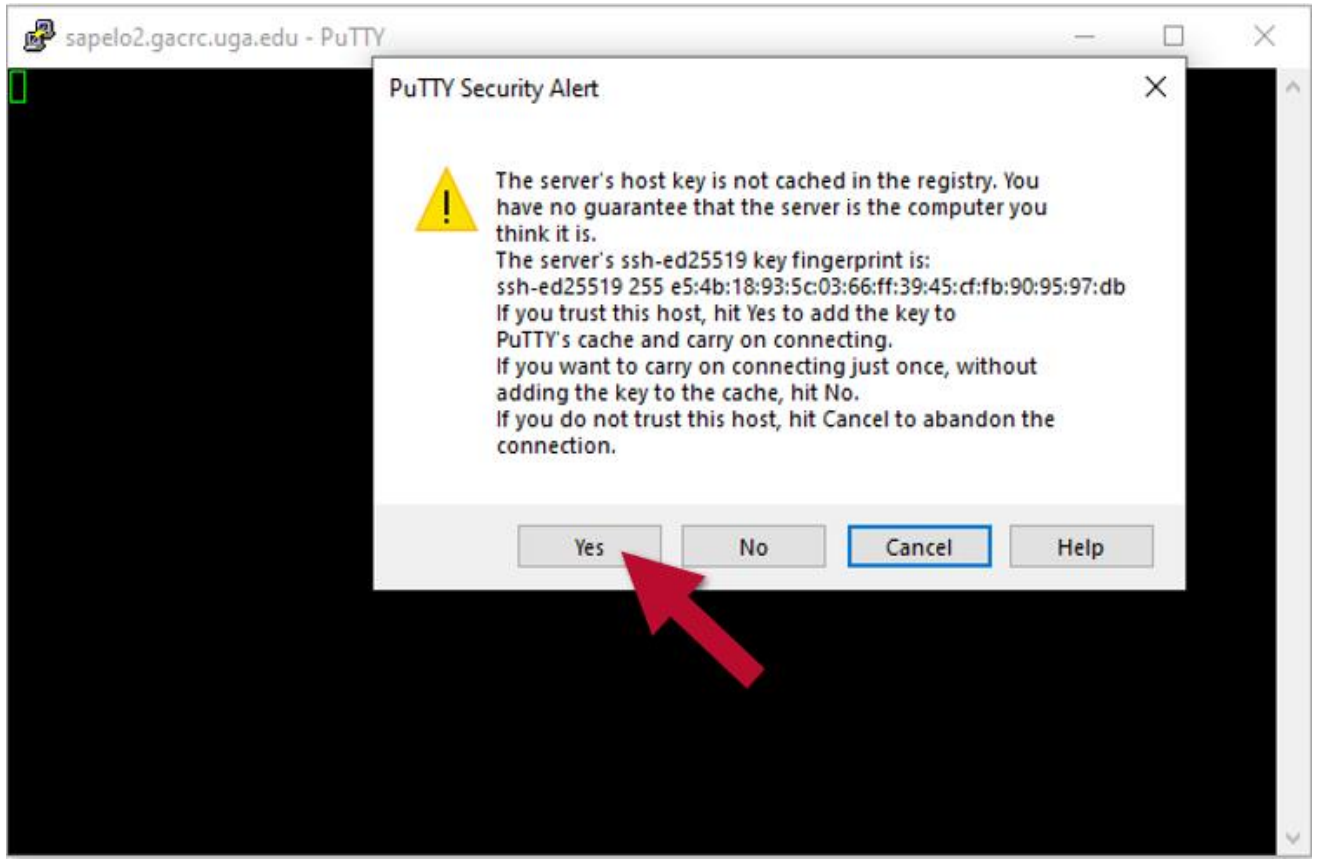
3. Detailed configuring and usage instructions:

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

Step1 (Cont.) - Windows using PuTTY

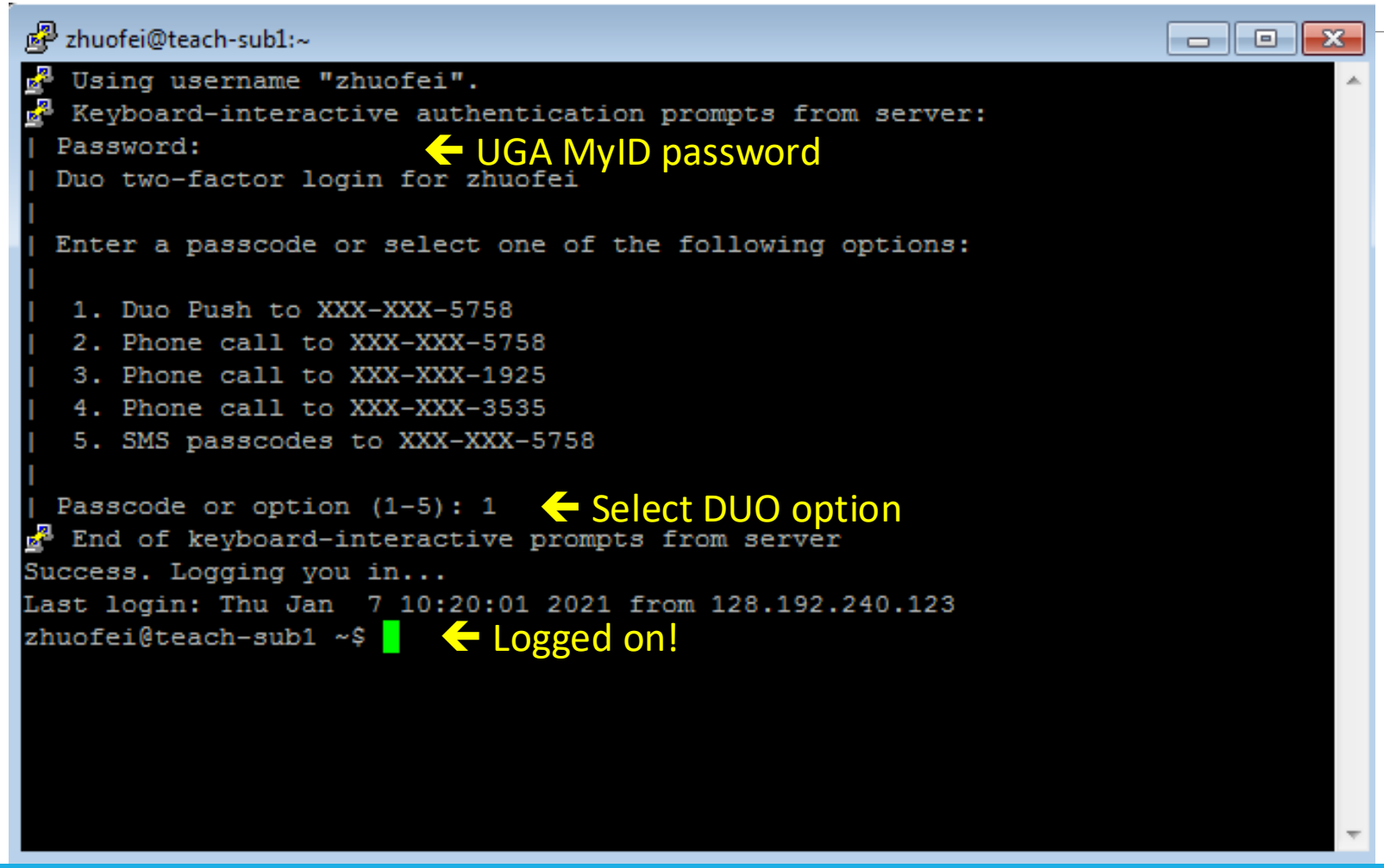


The first time you connect to login node, PuTTY will give you this security alert window. Please click "Yes"



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/MyID          ← 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!
```

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 .
```

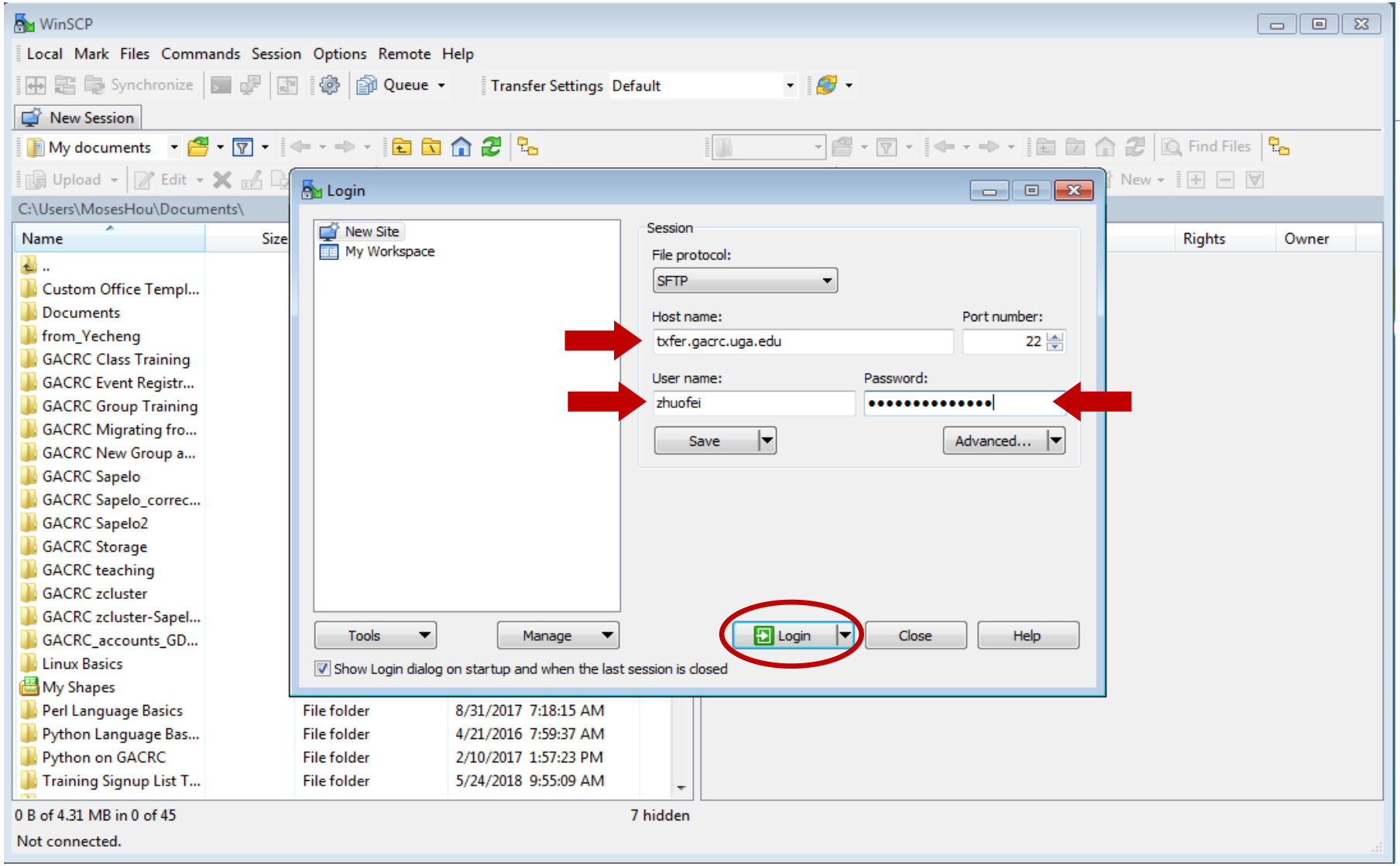
```
scp -r zhuofei@txfer.gacrc.uga.edu:/home/zhuofei/workDir/folder/ .
```

Step4 (Cont.) - Windows using WinSCP

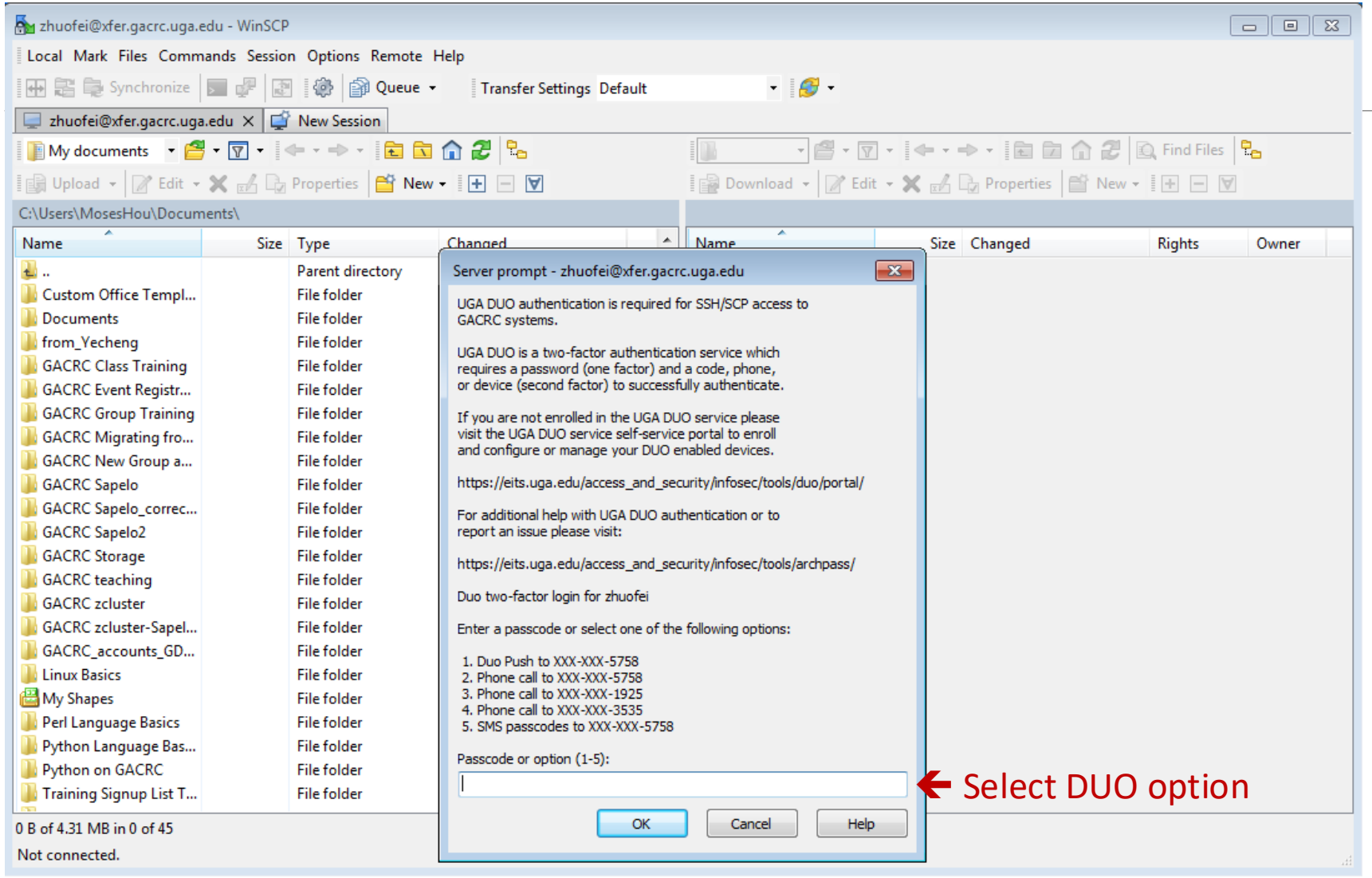
https://wiki.gacrc.uga.edu/wiki/Transferring_Files#Using_WinSCP_2

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

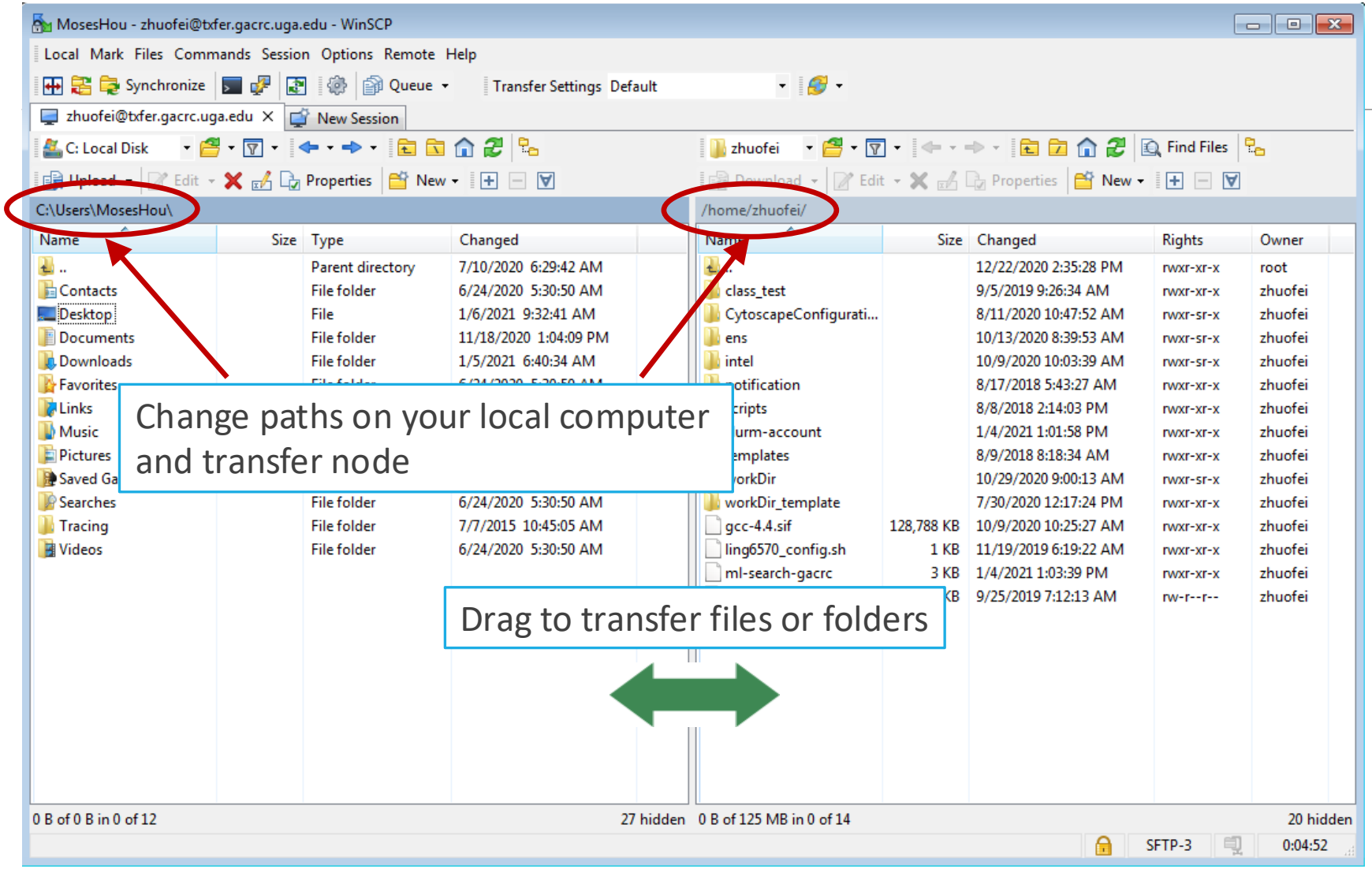
Step4 (Cont.) - Windows using WinSCP



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/phys8601/MyID
  3. /work/phys8601/instructor_data
- Transfer data between two folders on cluster using cp or mv, e.g.:

```
mv /work/phys8601/MyID/datafile /home/MyID/workDir
```

Step5: 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/training/phys8601/mult.c  .   ← Copy source code to current 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/13.3.0                ← 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
```

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

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```
zhuofei@teach-sub1 workDir$ cp  /usr/local/training/phys8601/sub.sh  .        ← Copy sub.sh to current 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 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 to current job submission location

module load GCC/13.3.0                           # Load GCC compiler module

time ./mult.x                                    # Run the binary

Zhuofei@teach-sub1 workDir$ nano sub.sh          ← Use nano to 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 281
```

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 sq --me

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)
281   test fsr8602   zhuofei  1    1   2G         21       0:04 10:00      RUNNING  rb1-3
```

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 281
JobId=281 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=00:00:08 TimeLimit=00:10:00 TimeMin=N/A
   ……
   Partition=fsr8602 AllocNode:Sid=10.31.32.252:92156
   NodeList=rb1-3
   NumNodes=1 NumCPUs=1 NumTasks=1 CPUs/Task=1 ReqB:S:C:T=0:0:*:*
   MinCPUsNode=1 MinMemoryNode=2G MinTmpDiskNode=0
   Command=/scratch/zhuofei/workDir/sub.sh
   WorkDir=/scratch/zhuofei/workDir
   StdErr=/scratch/zhuofei/workDir/log.281
   StdOut=/scratch/zhuofei/workDir/log.281
   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 281
zhuofei@teach-sub1 workDir$ sq -me
JOBID NAME PARTITION USER NODES CPUS MIN_MEMORY PRIORITY TIME TIME_LIMIT STATE    NODELIST(REASON)
```

Step7 (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
283	test	zhuofei	fsr8602	1	1	2G	00:00:10	00:00:10	00:10:00	COMPLETED	0:0	rb1-3

```
seff 283        ← Check computing resources used by a COMPLETED job
Job ID: 283
Cluster: gacrc-teach
User/Group: zhuofei/gacrc-instruction
State: COMPLETED (exit code 0)
Cores: 1
CPU Utilized: 00:00:10
CPU Efficiency: 100.00% of 00:00:10 core-walltime
Job Wall-clock time: 00:00:10
Memory Utilized: 42.45 MB
Memory Efficiency: 2.07% of 2.00 GB
```

Step7 (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      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      1    mix rb1-11
interactive     up 7-00:00:00      1   idle rb1-12
franklin_gpu    up 7-00:00:00      1    mix b8-6
franklin_gpu    up 7-00:00:00      1   idle b8-7
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_the_teaching_cluster#How_to_check_resource_utilization_of_a_running_or_finished_job

Option 1: sq --me for details of 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_the_teaching_cluster#How_to_open_an_interactive_session

https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_the_teaching_cluster#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=interactive --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=interactive --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:

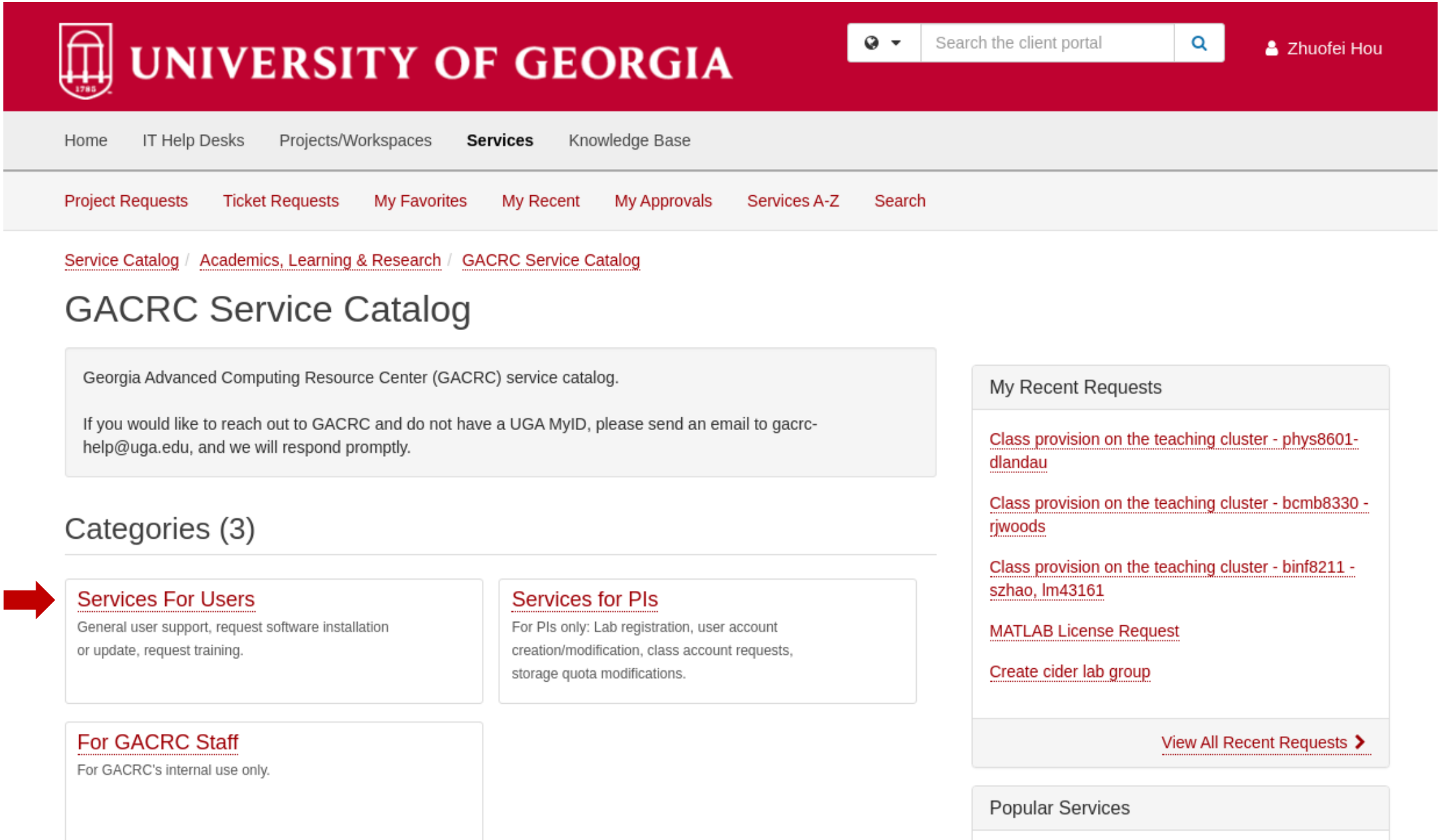
Please tell us details of your question or problem, including but not limited to:

- ✓ 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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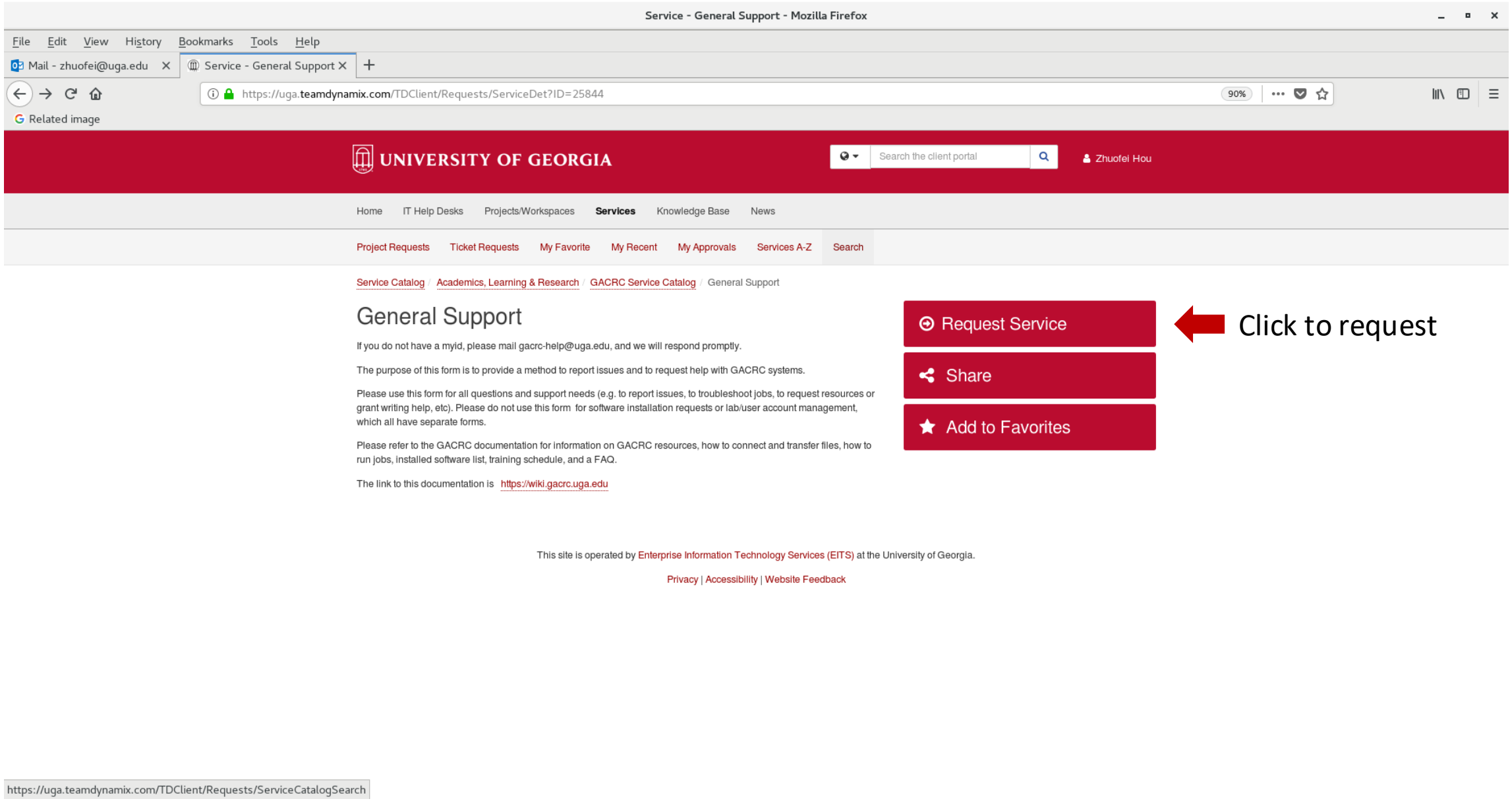
GACRC Service Catalog
Georgia Advanced Computing Resource Center (GACRC) service catalog.
If you would like to reach out to GACRC and do not have a UGA MyID, please send an email to gacrc-help@uga.edu, and we will respond promptly.
Categories (3)
Services For Users
General user support, request software 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
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Mail - zhuofei@uga.edu
Service - General Support
https://uga.teamdynamix.com/TDClient/Requests/ServiceDet?ID=25844
90%
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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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https://uga.teamdynamix.com/TDClient/Requests/ServiceCatalogSearch

Thank You!

Telephone Support

EITS Help Desk: 706-542-3106

Monday – Friday: 7:30 a.m. – 6:30 p.m.

Saturday: closed

Sunday: 1:30 p.m. – 6:30 p.m.

Georgia Advanced Computing Resource Center

101-108 Computing Services building

University of Georgia

Athens, GA 30602

https://gacrc.uga.edu/