Introduction to GACRC Teaching Cluster PHYS8602

Georgia Advanced Computing Resource Center (GACRC)

EITS/University of Georgia

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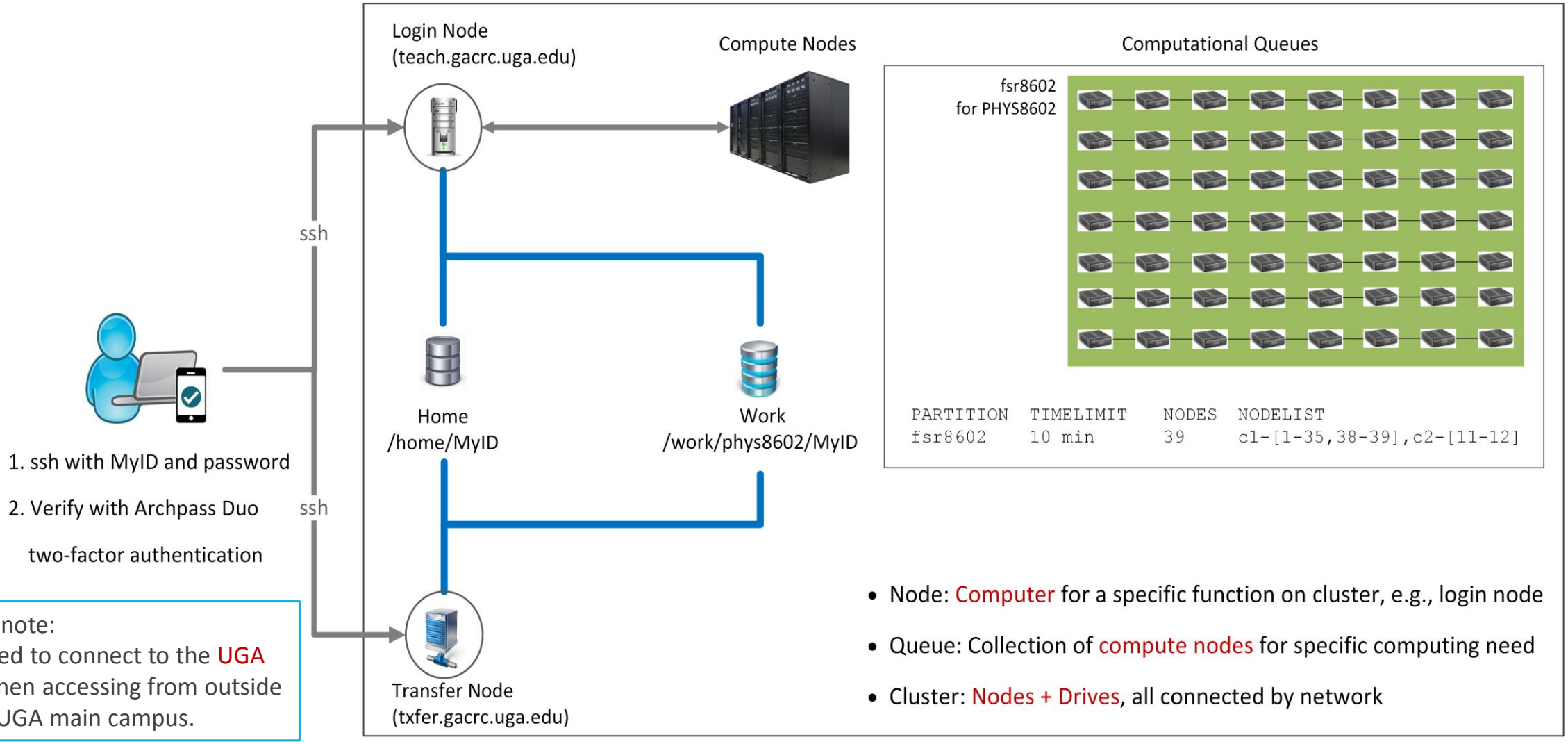
Outline

- GACRC
- Overview
- Computing Resources
  - Three Folders
  - Three Computational Queues
  - Software
- Submit Batch Job
- GACRC Wiki and Support

GACRC

- We are a high-performance-computing (HPC) center at UGA
- We 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
- http://wiki.gacrc.uga.edu (GACRC Wiki)
- https://wiki.gacrc.uga.edu/wiki/Getting_Help (GACRC Support)
- http://gacrc.uga.edu (GACRC Web)

Teaching Cluster



Please note:
You need to connect to the UGA VPN when accessing from outside of the UGA main campus.

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

Computing Resources

- Two Nodes:
  1. Login node (MyID@teach.gacrc.uga.edu): for submitting computational jobs
  2. Transfer node (MyID@txfer.gacrc.uga.edu): for transferring data files
- Three Directories:
  1. /home/MyID: working space for computational jobs
  2. /work/phys8602/MyID: data parking for individual user in the class
  3. /work/phys8602/instructor_data: data shared with class by the instructors
- Queue for your class: fsr8602

Computing Resources (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/2.7.14-foss-2016b
  3. Software names are case-sensitive!
     - `module avail` : List all available software modules installed on cluster
     - `module load` *`moduleName`* : Load a module into your working environment
     - `module list` : List modules currently loaded
     - `module unload` *`moduleName`* : Remove a module from working environment
     - `ml spider` *`pattern`* : Search module names matching a pattern (case-insensitive)

Submit 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 SSH File Transfer to connect Transfer node

   Transfer data on cluster to workDir : log on to Transfer node and then use cp or mv
5. Compile your source codes *phys8602_mult.c* into binary
6. Make a job submission script in workDir : nano ./phys8602_sub.sh
7. Submit a job from workDir : sbatch ./phys8602_sub.sh
8. Check job status : squeue or Cancel a job : scancel JobID

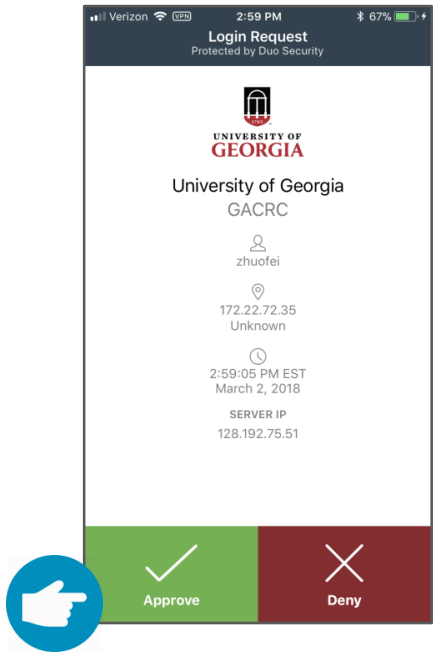
Step1: Log on to Login node - Mac/Linux using ssh

1. Open Terminal utility
2. Type command line: `ssh MyID@teach.gacrc.uga.edu`
3. You will be prompted for your MyID password
4. Teaching cluster access requires ID 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

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

Step1 (Cont.) - Mac/Linux

Using ssh in Terminal!

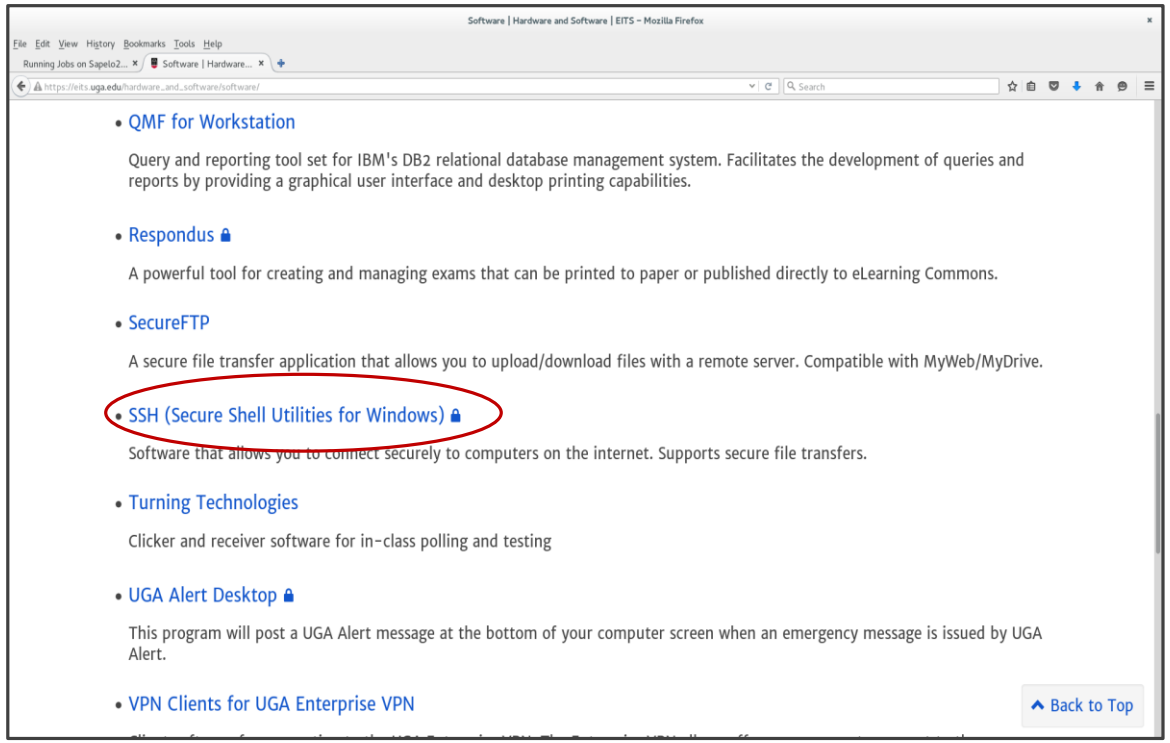


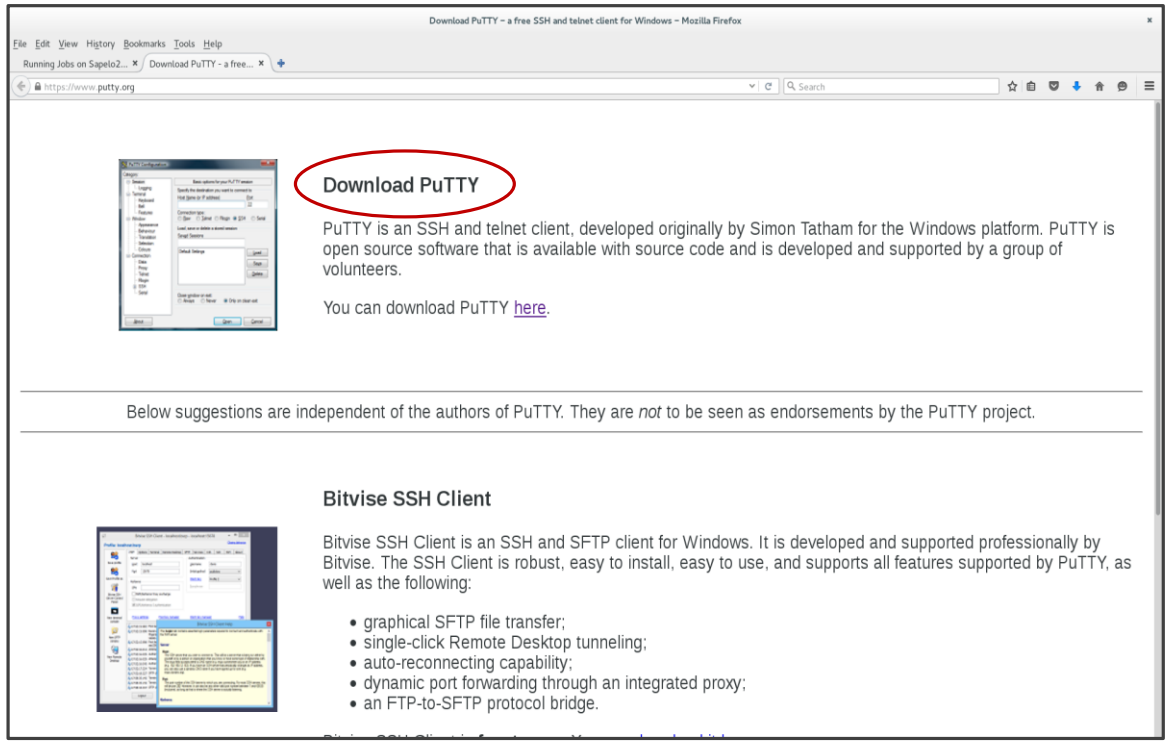
4. Verify login using Duo

```
ssh zhuofei@teach.gacrc.uga.edu        ← 1. Log on

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 login option 1
Success. Logging you in...
Last login: Fri Aug  3 11:24:43 2018 from 172.22.72.35
[zhuofei@teach ~]$                 ← 5. Logged on!
```

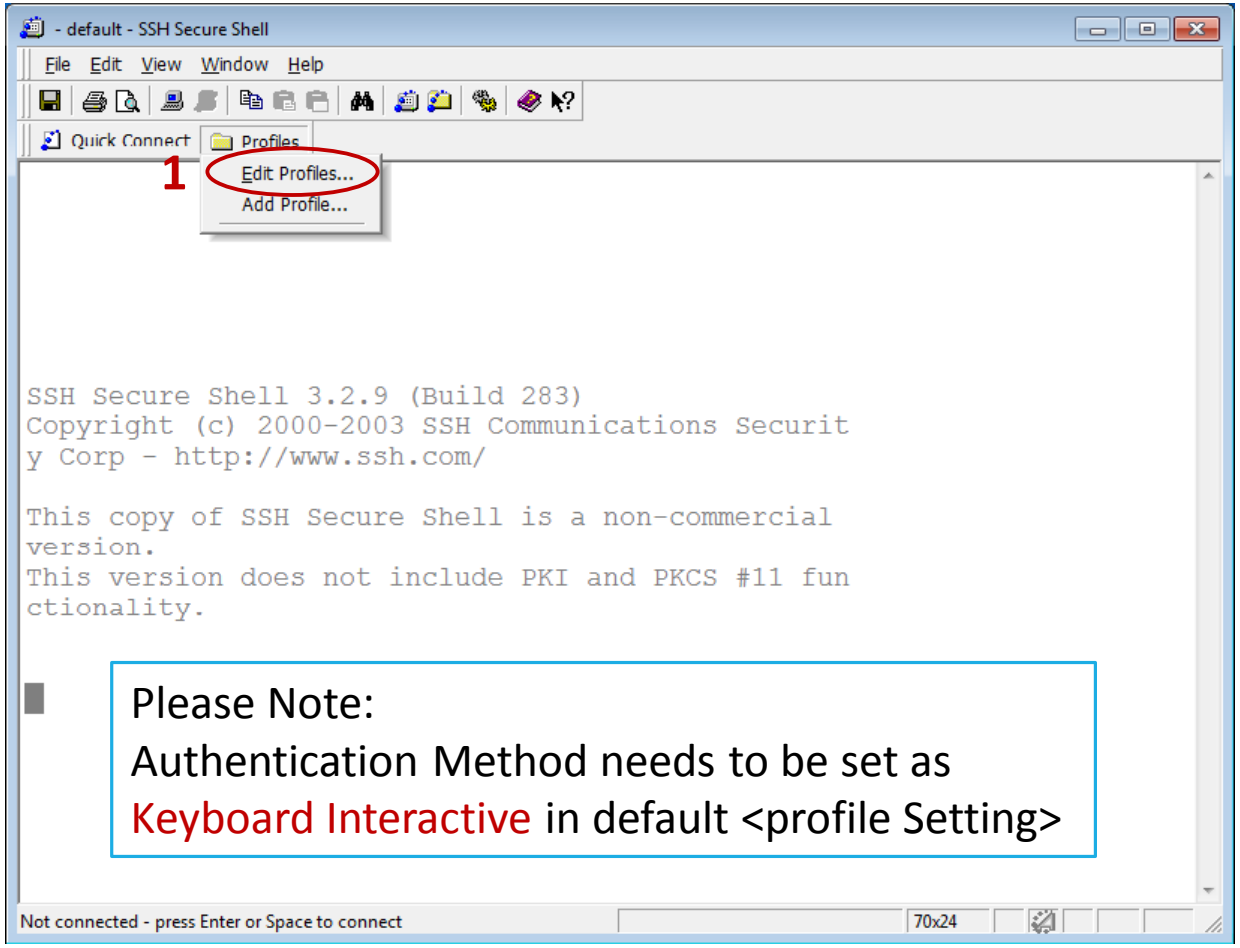
Step1 (Cont.) - Windows

1. Download and install SSH Secure Utilities: http://eits.uga.edu/hardware_and_software/software/
2. You can use PuTTY as an alternative: https://www.putty.org/

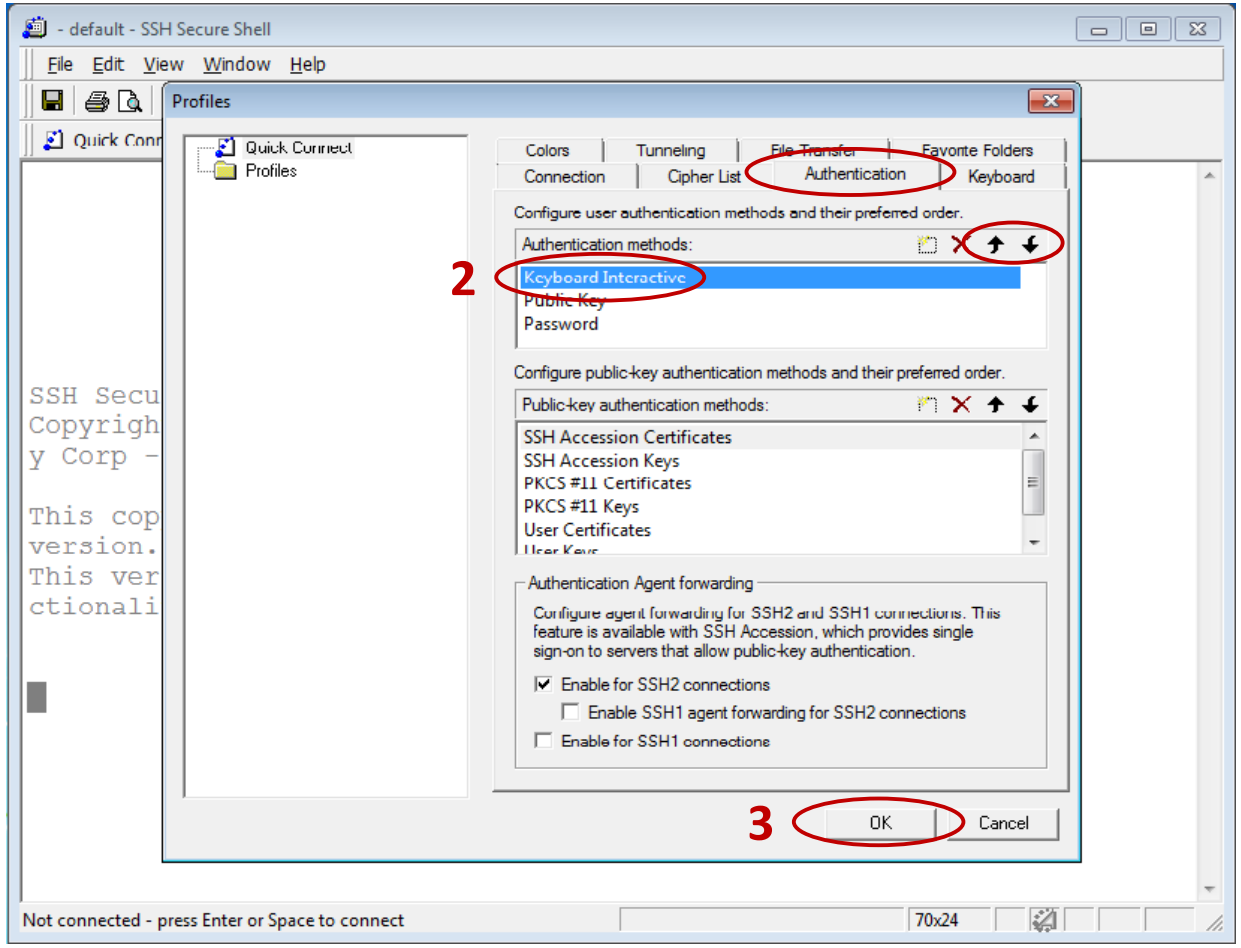




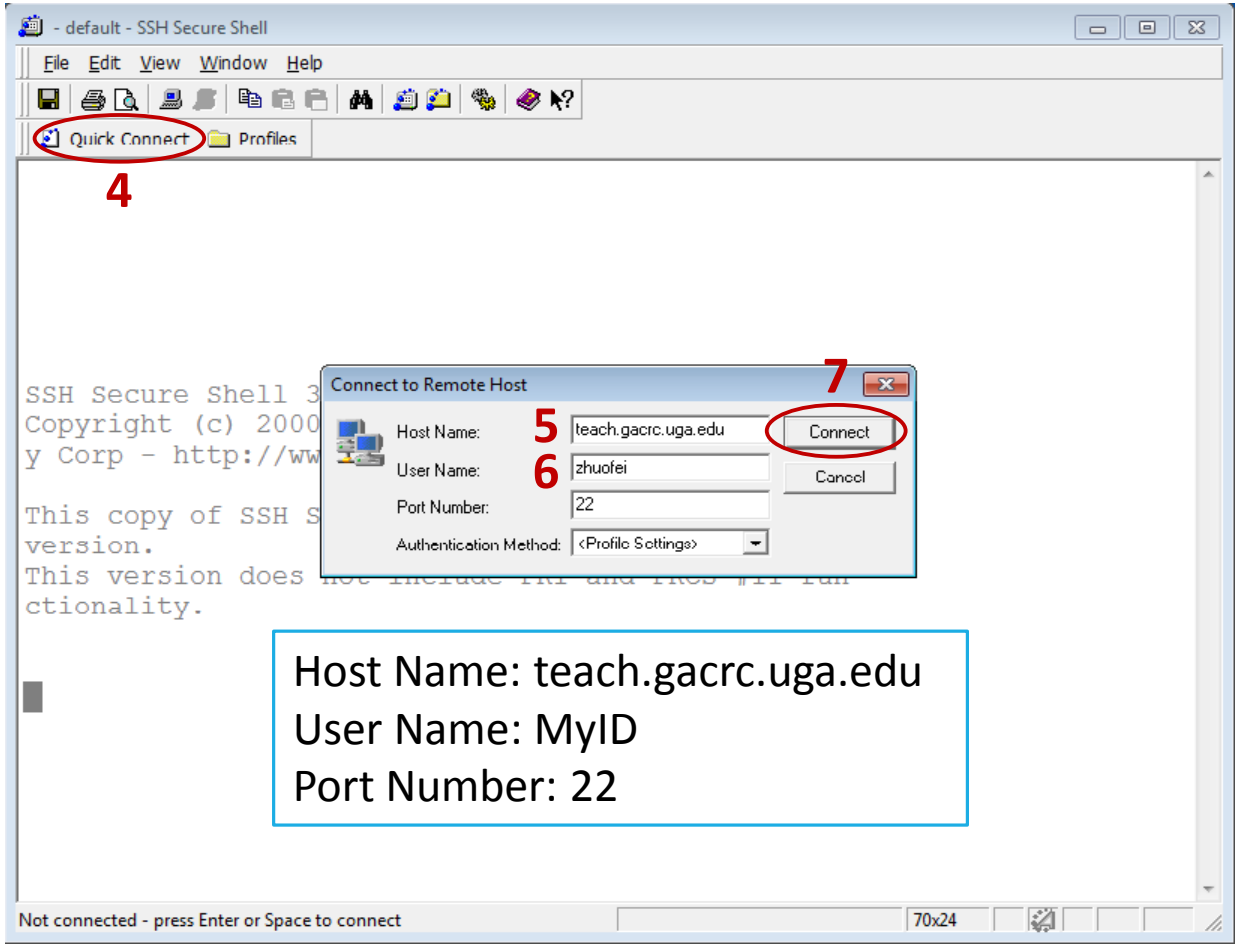
Step1 (Cont.) - Windows using SSH Secure Utilities



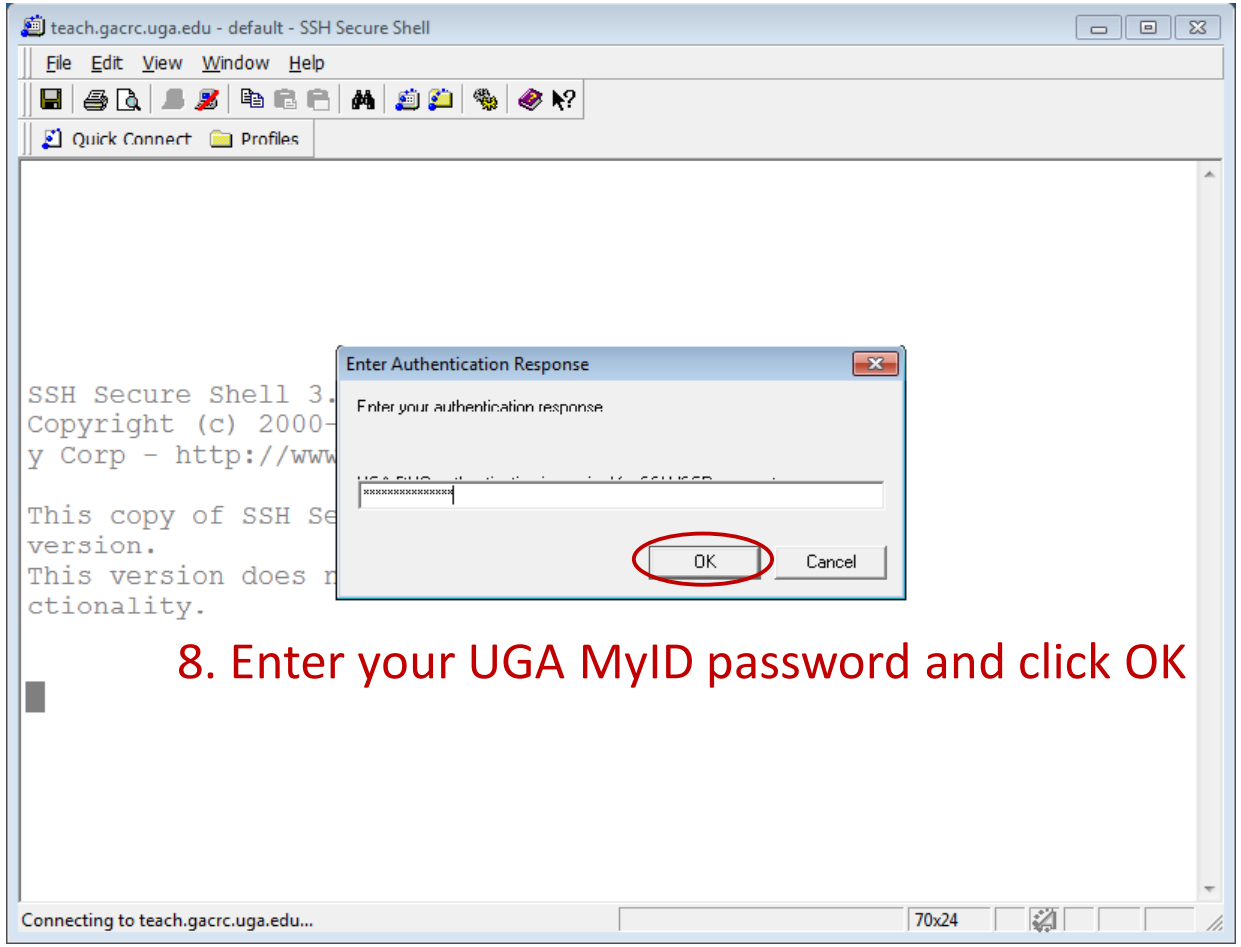
Please Note:
Authentication Method needs to be set as
Keyboard Interactive in default <profile Setting>



Step1 (Cont.) - Windows using SSH Secure Utilities

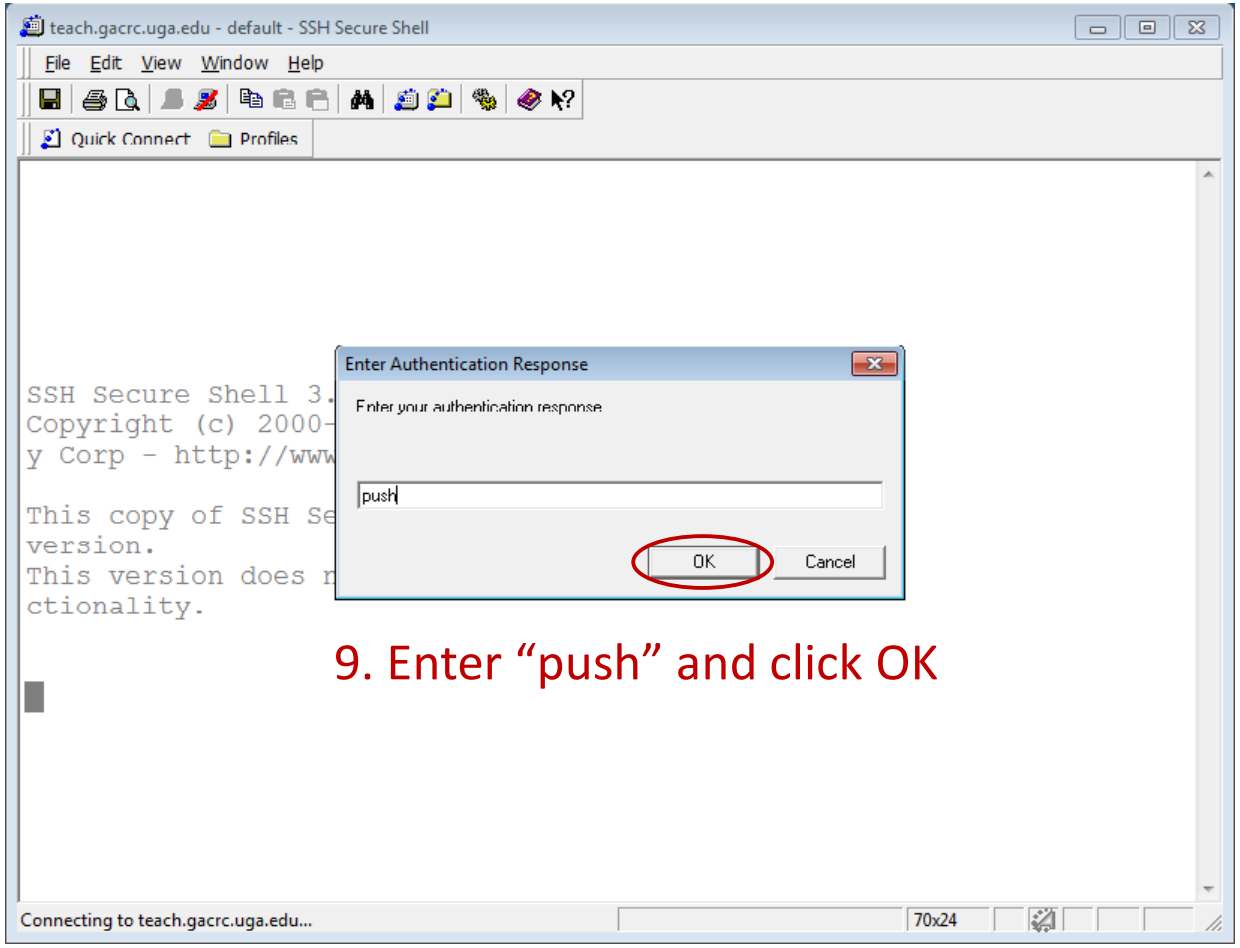


Host Name: teach.gacrc.uga.edu
User Name: MyID
Port Number: 22

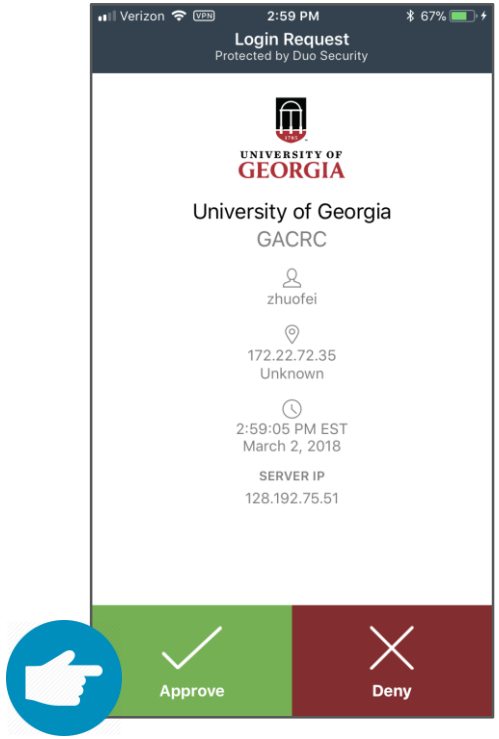


8. Enter your UGA MyID password and click OK

Step1 (Cont.) - Windows using SSH Secure Utilities

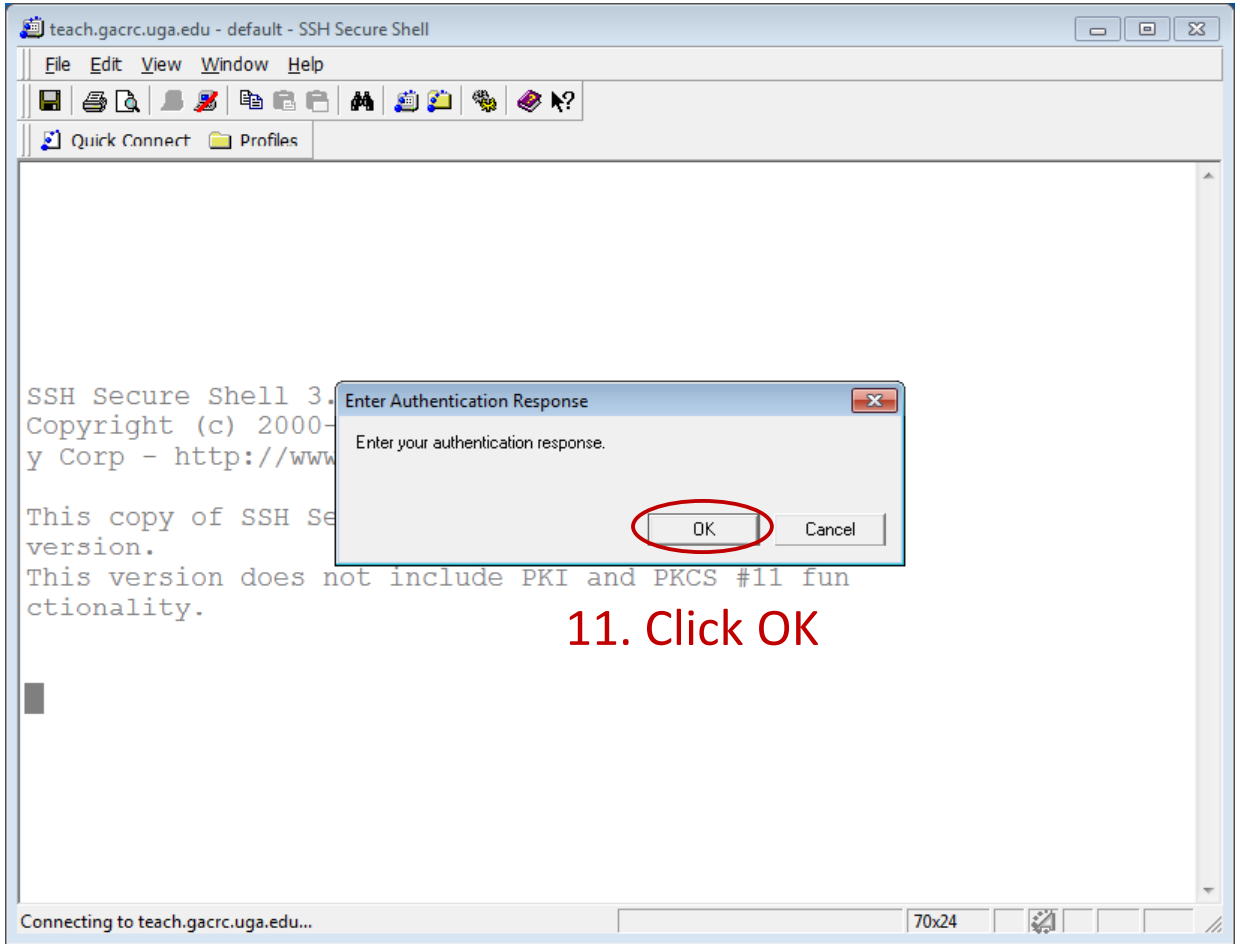


9. Enter “push” and click OK

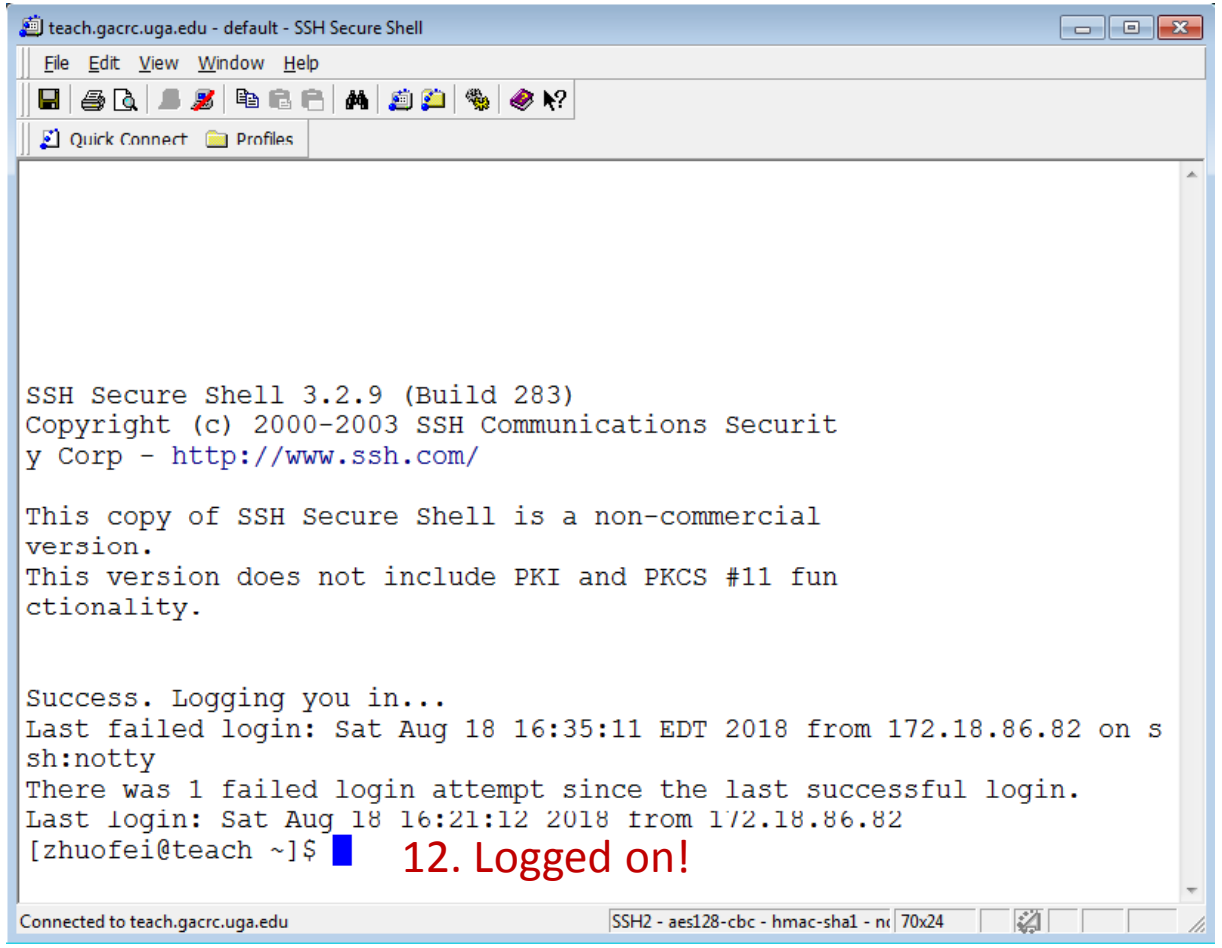


10. Verify login using Duo

Step1 (Cont.) - Windows using SSH Secure Utilities



11. Click OK



12. Logged on!

Step2 - 3: Create and change directory to workDir

```
[zhuofei@teach ~]$ ls                    ← ls command to list folder's contents
[zhuofei@teach ~]$ mkdir workDir         ← mkdir command to create a subdirectory
[zhuofei@teach ~]$ ls
workDir
[zhuofei@teach ~]$ cd workDir/           ← cd command to change directory
[zhuofei@teach workDir]$ ls
[zhuofei@teach workDir]$                 ← it is empty in workDir!
```

Step4: Transfer data from local computer to workDir - Mac/Linux

1. Connect to Transfer node (MyID@txfer.gacrc.uga.edu) in Terminal on local computer
2. Type scp command: scp (-r) [Source] [Target]
3. Once you input MyID password, scp command will send "push" to your Duo Enrolled mobile device for verification

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
```

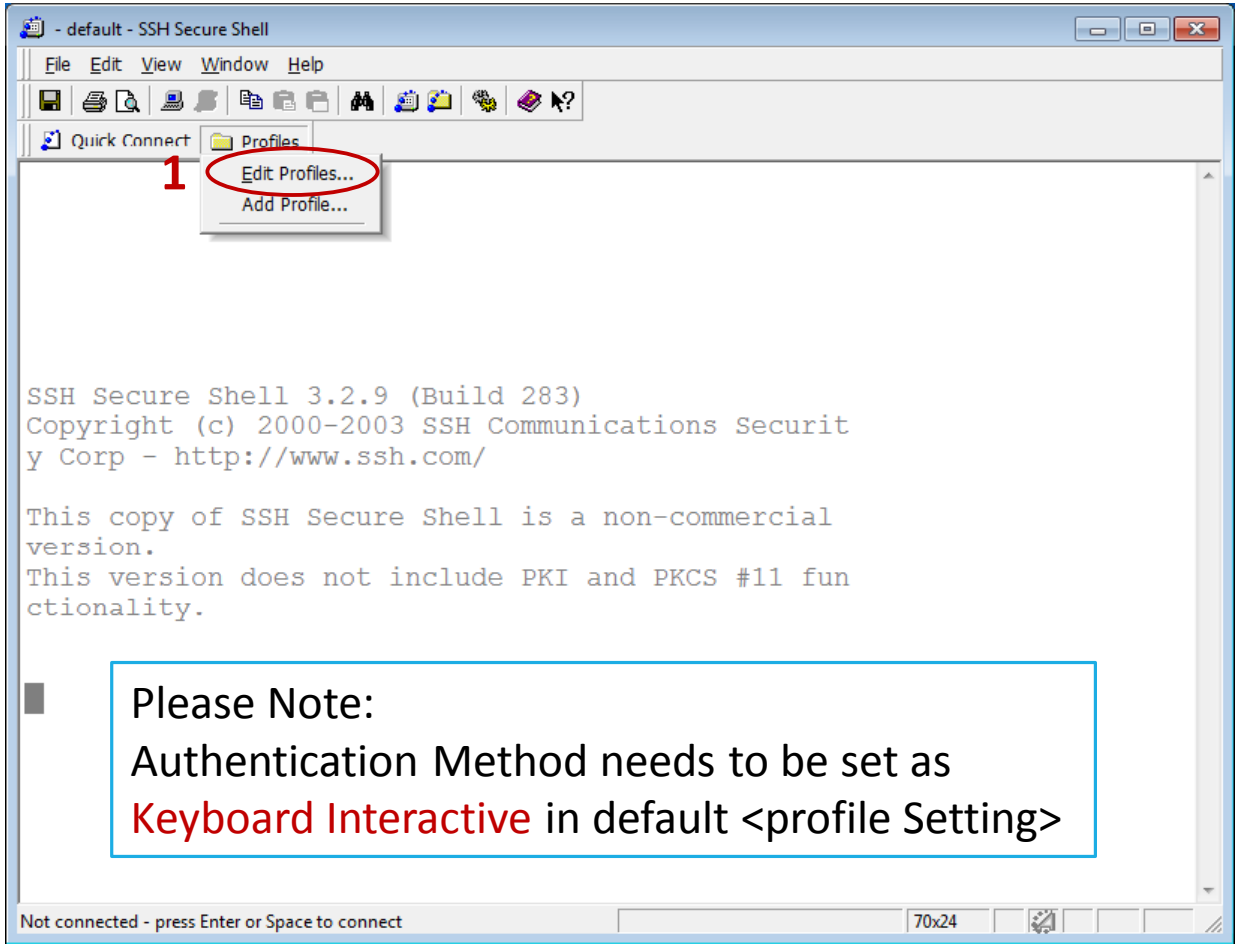
E.g. 2: use scp on local computer, from workDir on cluster ➔ Local

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

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

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

Step 4 (Cont.) - Windows using SSH Secure Utilities



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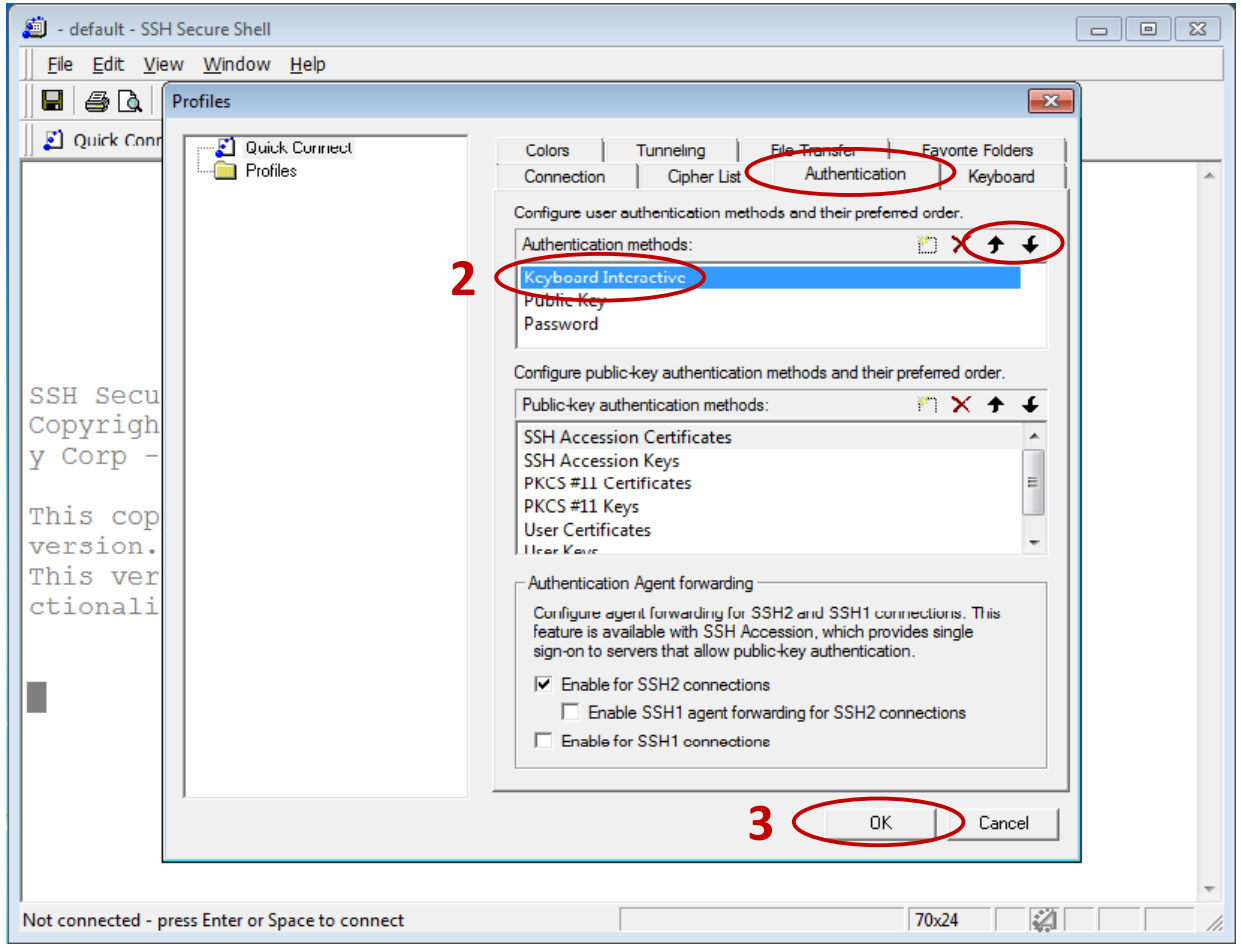
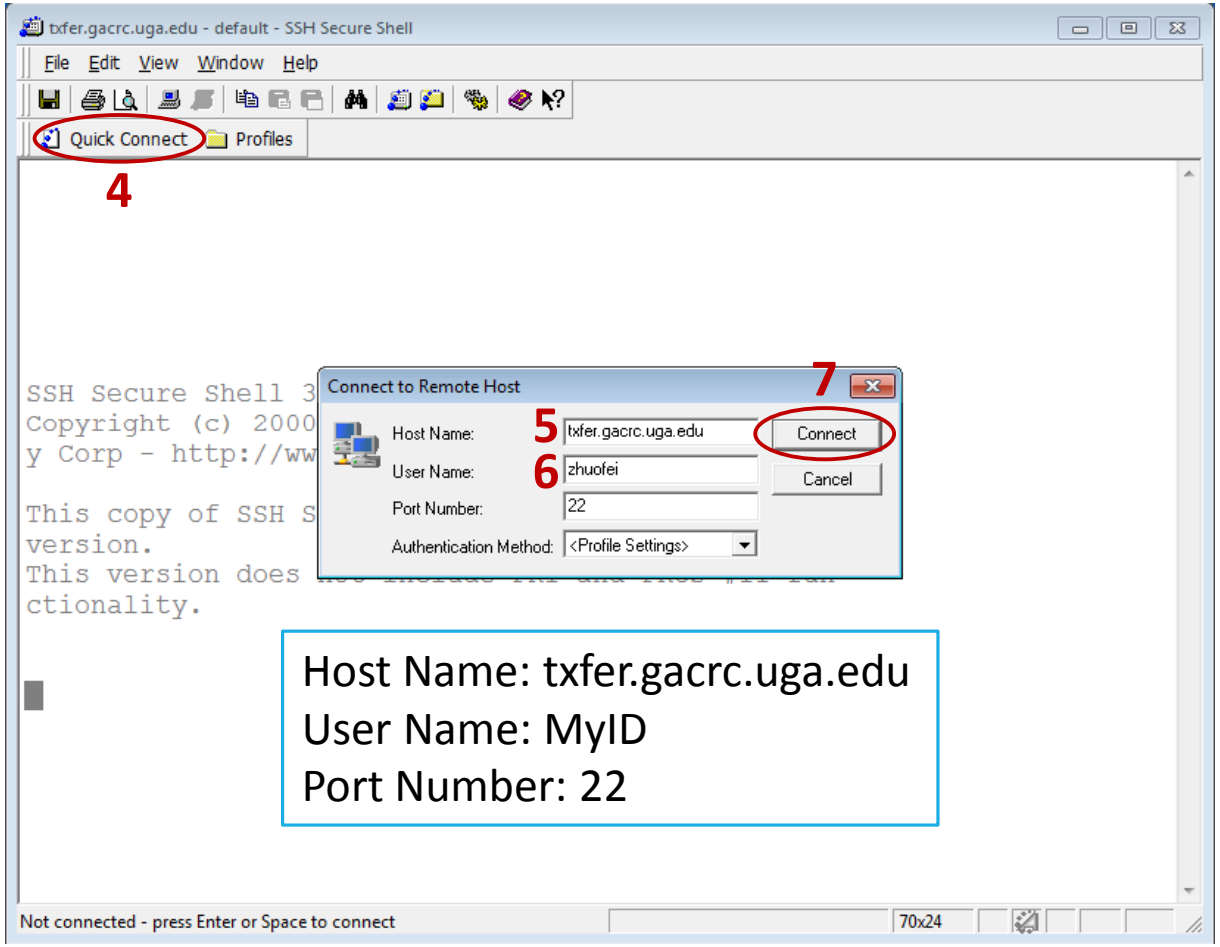
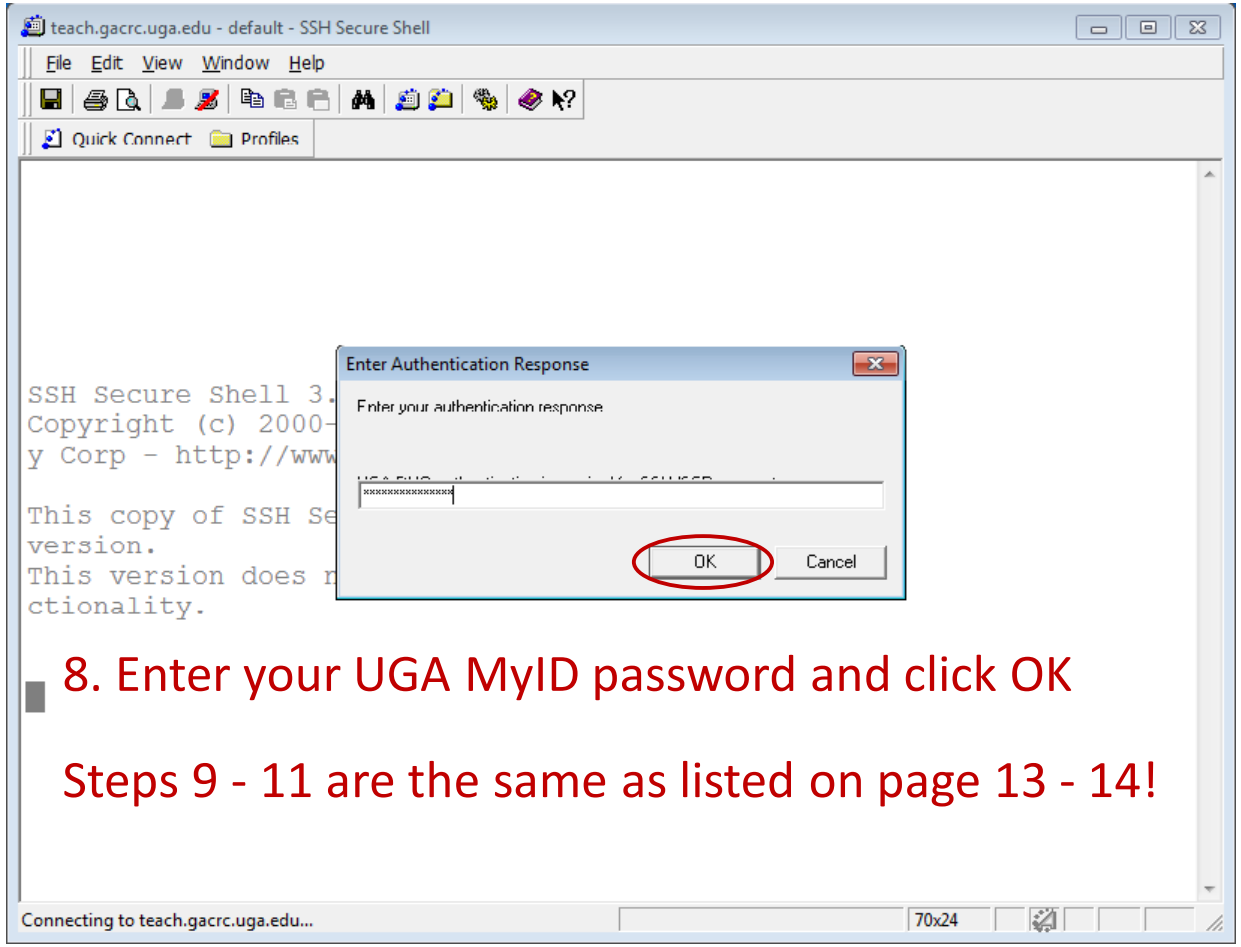


Step4 (Cont.) - Windows using SSH Secure Utilities



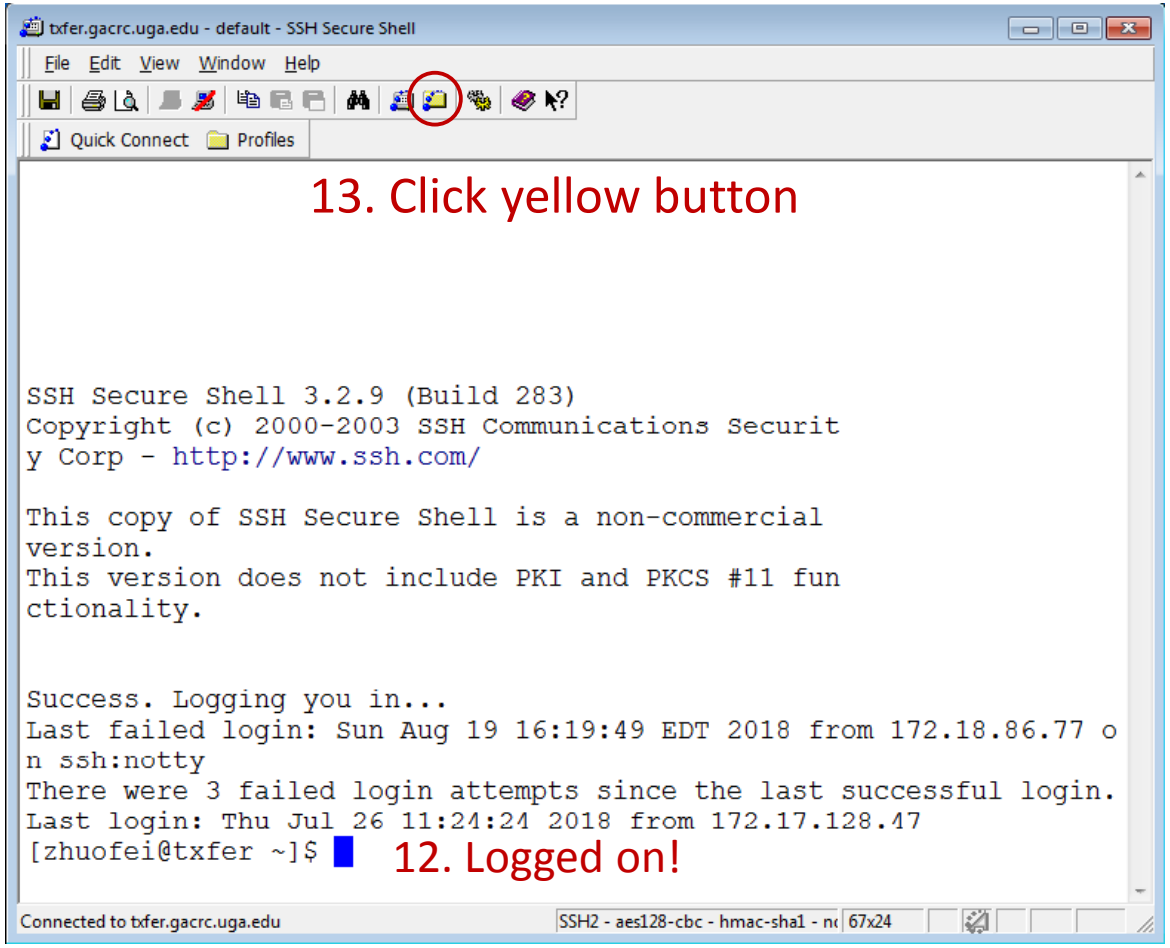
Host Name: txfer.gacrc.uga.edu
User Name: MyID
Port Number: 22

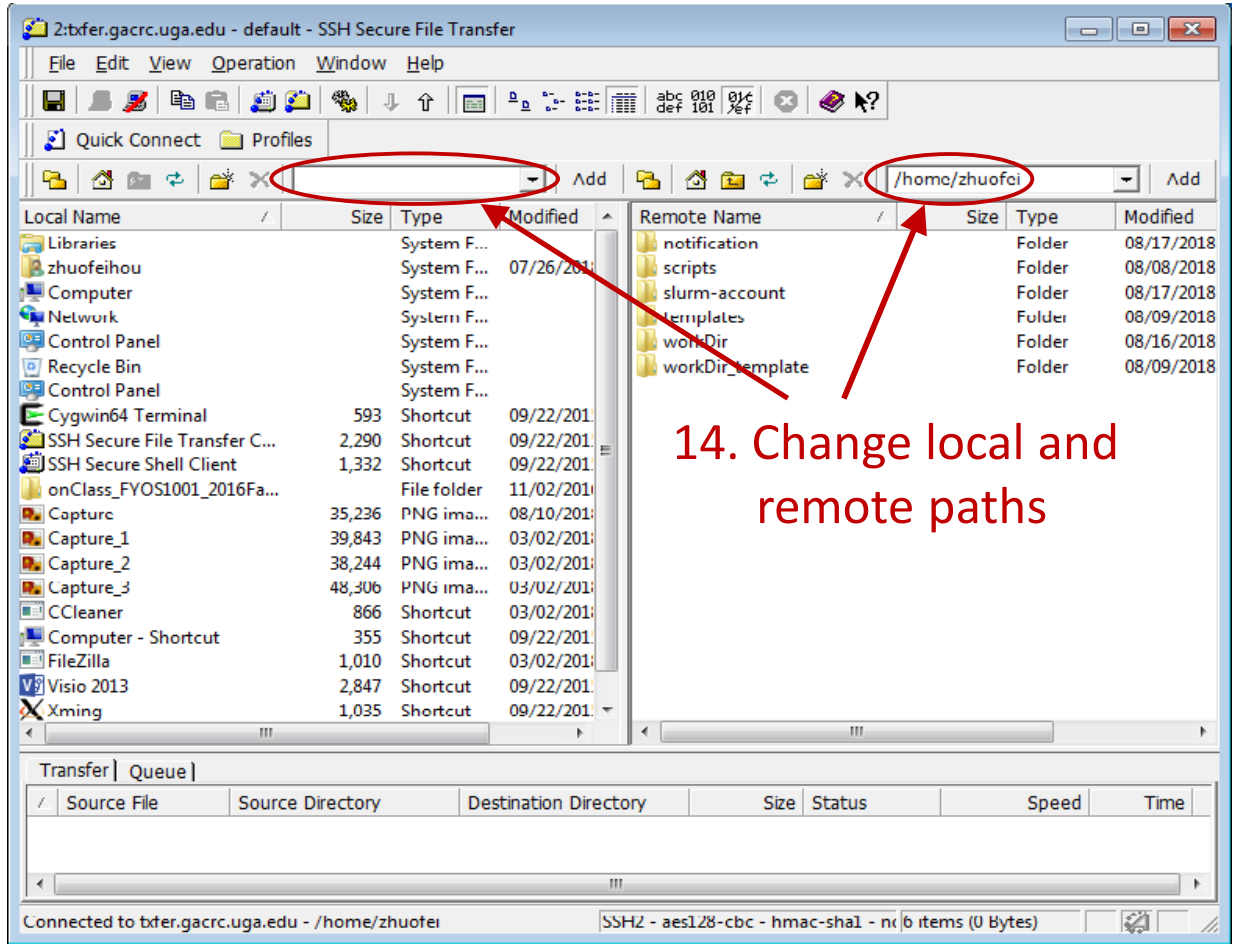


8. Enter your UGA MyID password and click OK

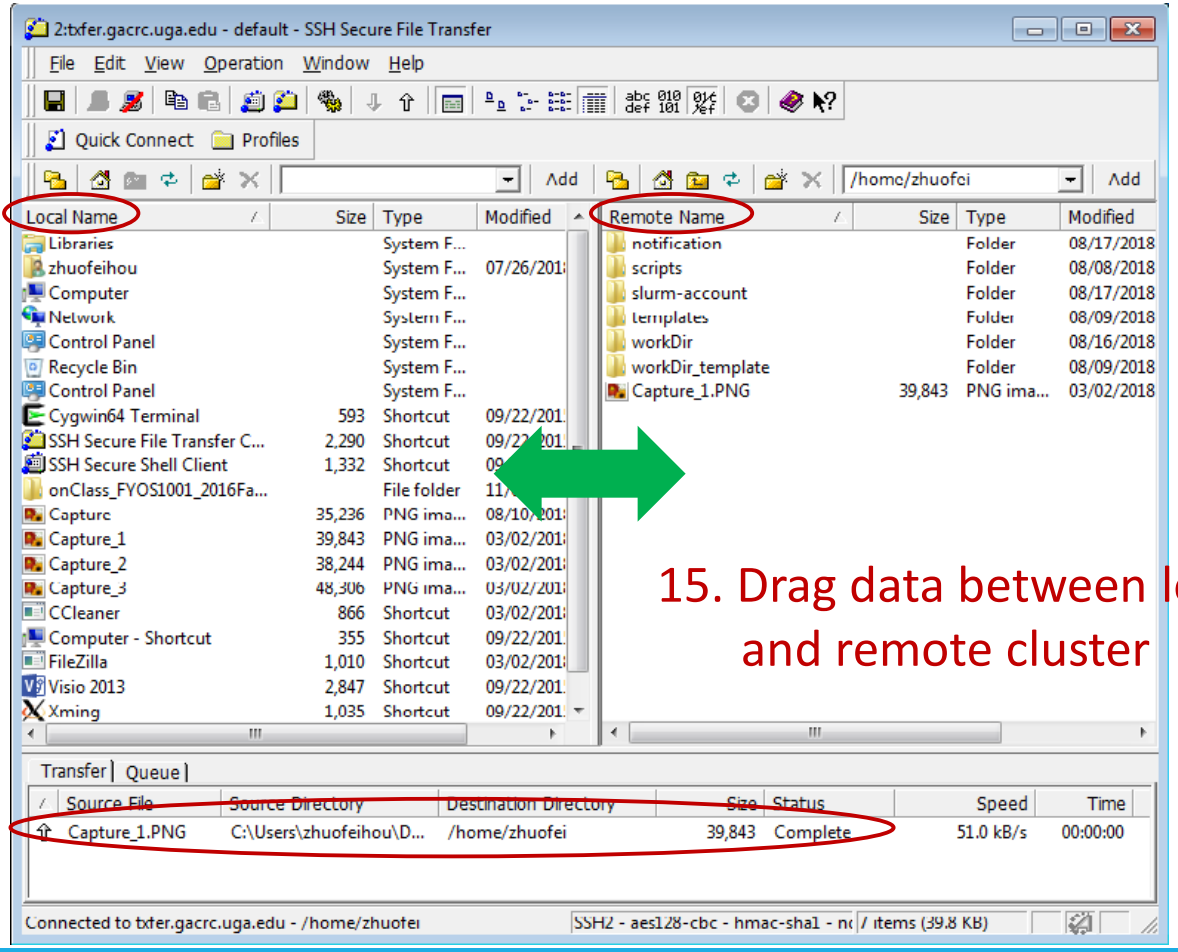
Steps 9 - 11 are the same as listed on page 13 - 14!

Step4 (Cont.) - Windows using SSH Secure Utilities





Step4 (Cont.) - Windows using SSH Secure Utilities



Step4 (Cont.): Transfer data on cluster to workDir

- Log on to Transfer node (MyID@txfer.gacrc.uga.edu)
  - ✓ Mac/Linux: ssh MyID@txfer.gacrc.uga.edu (page 8-9)
  - ✓ Windows: use SSH Secure Client app (page 14-16)
- Directories you can access on txfer:
  1. /home/MyID (Landing home)
  2. /work/phys8602/MyID
  3. /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
```

Step5: Compile your Fortran program *phys8602_mult.c* into binary

```
[zhuofei@teach ~]$ cat phys8602_mult.c
/* 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@teach ~]$ module  load  PGI/17.9                    ➔ load PGI compilers
[zhuofei@teach ~]$ pgcc  phys8602_mult.c  -o  phys8602_mult.x   ➔ compile into binary
[zhuofei@teach ~]$ ./phys8602_mult.x                         ➔ run binary
```

Note:
phys8602_mult.c is put in /usr/local/training/phys
You can copy it into your working directory for use

Step6: Make a job submission script *phys8602_sub.sh*

```
$nano phys8602_sub.sh
```

Note:
phys8602_sub.sh is put in /usr/local/training/phys
You can copy it into your working directory for use

```
#!/bin/bash
#SBATCH --job-name=testJob                  # Job name
#SBATCH --partition=fsr8602                 # Partition (queue) for PHYS8602
#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; 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=END,FAIL                # Mail events (BEGIN, END, FAIL, ALL)

cd $SLURM_SUBMIT_DIR
time ./phys8602_mult.x                      # run binary compiled in step 5
```

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

Step7: Submit a job from workDir using sbatch

```
$ sbatch phys8602_sub.sh
Submitted batch job 139
```

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 your compiled binary

Step8: Check job status using squeue

```
$ squeue -l
Wed Aug  8 13:40:02 2018
JOBID PARTITION     NAME     USER      STATE       TIME  TIME_LIMI  NODES NODELIST
162      fsr8602   testJob   zhuofei   PENDING     0:00    00:10:00      1 (None)
160      fsr8602   testJob   zhuofei   RUNNING     0:02    00:10:00      1 c2-11
161      fsr8602   testJob   zhuofei   RUNNING     0:02    00:10:00      1 c2-11

$ squeue
JOBID PARTITION     NAME     USER    ST       TIME  NODES NODELIST
162      fsr8602   testJob   zhuofei PD       0:15      1 (None)
160      fsr8602   testJob   zhuofei  R       0:17      1 c2-11
161      fsr8602   testJob   zhuofei  R       0:17      1 c2-11
```

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.

Step8 (Cont.): Cancel job using scancel

```
$ squeue -l
Wed Aug  8 14:03:47 2018
JOBID PARTITION   NAME     USER    STATE   TIME   TIME_LIMI  NODES NODELIST
169   fsr8602  testJob   zhuofei  RUNNING   0:07   00:10:00      1 c1-38
168   fsr8602  testJob   zhuofei  RUNNING   0:10   00:10:00      1 c1-39

$ scancel 169

[zhuofei@teach workDir]$ squeue -l
Wed Aug  8 14:03:47 2018
JOBID PARTITION   NAME     USER    STATE   TIME   TIME_LIMI  NODES NODELIST
169   fsr8602  testJob   zhuofei COMPLETI   0:15   00:10:00      1 c1-39
168   fsr8602  testJob   zhuofei  RUNNING   0:18   00:10:00      1 c1-38

$ squeue -l
Wed Aug  8 14:04:08 2018
JOBID PARTITION   NAME     USER    STATE   TIME   TIME_LIMI  NODES NODELIST
168   fsr8602  testJob   zhuofei  RUNNING  0:35   00:10:00      1 c1-38
```

Step8 (Cont.): Check job details using scontrol show job

```
$ scontrol show job 174

JobId=174 JobName=testJob
   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=00:00:28 TimeLimit=00:10:00 TimeMin=N/A
   SubmitTime=2018-08-08T14:28:44 EligibleTime=2018-08-08T14:28:44
   StartTime=2018-08-08T14:28:44 EndTime=2018-08-08T16:28:44 Deadline=N/A
   ...
   Partition=fsr8602 AllocNode:Sid=teach:30986
   NodeList=c1-38
   NumNodes=1 NumCPUs=1 NumTasks=1 CPUs/Task=1 ReqB:S:C:T=0:0:*:*
   ...
   Command=/home/zhuofei/workDir/phys8602_sub.sh
   WorkDir=/home/zhuofei/workDir
   StdErr=/home/zhuofei/workDir/log.174
   StdOut=/home/zhuofei/workDir/log.174
```

Step8 (Cont.): Check node info using sinfo

```
$ sinfo
PARTITION AVAIL  TIMELIMIT  NODES    STATE  NODELIST
highmem      up 7-00:00:00      5   idle c1-[36-37,40],c2-[9-10]
gpu          up 1-00:00:00      1  down* c2-2
interq       up 1-00:00:00      3   idle c2-[4-6]
batch        up 7-00:00:00     39   idle c1-[1-35,38-39],c2-[11-12]
fsr8602      up       10:00     39   idle c1-[1-35,38-39],c2-[11-12]
fsr4601      up        1:00     39   idle c1-[1-35,38-39],c2-[11-12]
```

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

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

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

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

Transfer File:

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

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

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

GACRC Support

https://uga.teamdynamix.com/TDClient/Requests/ServiceCatalog?CategoryID=11593

➢ 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 queue 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 >

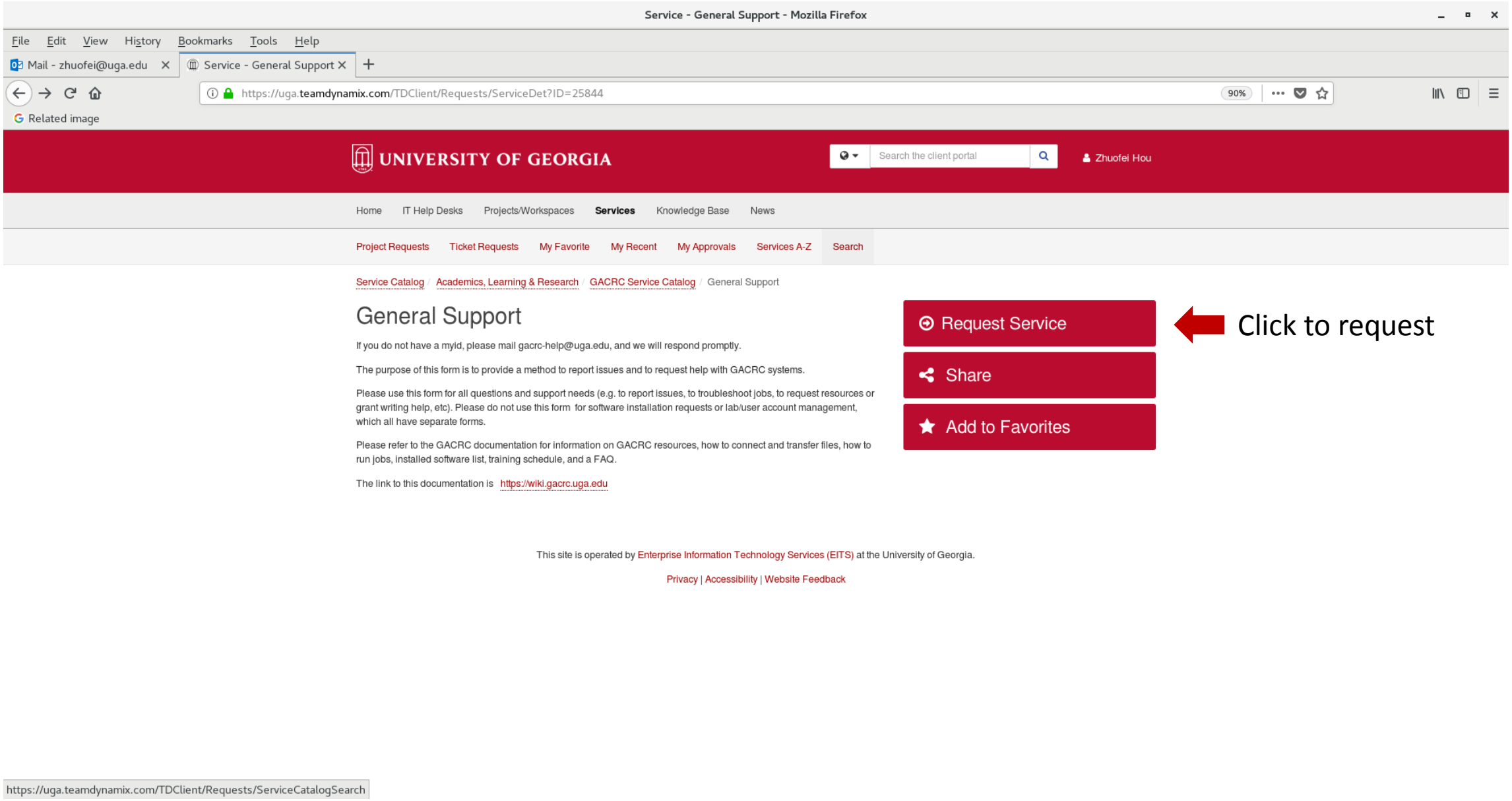
Popular Services

- 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
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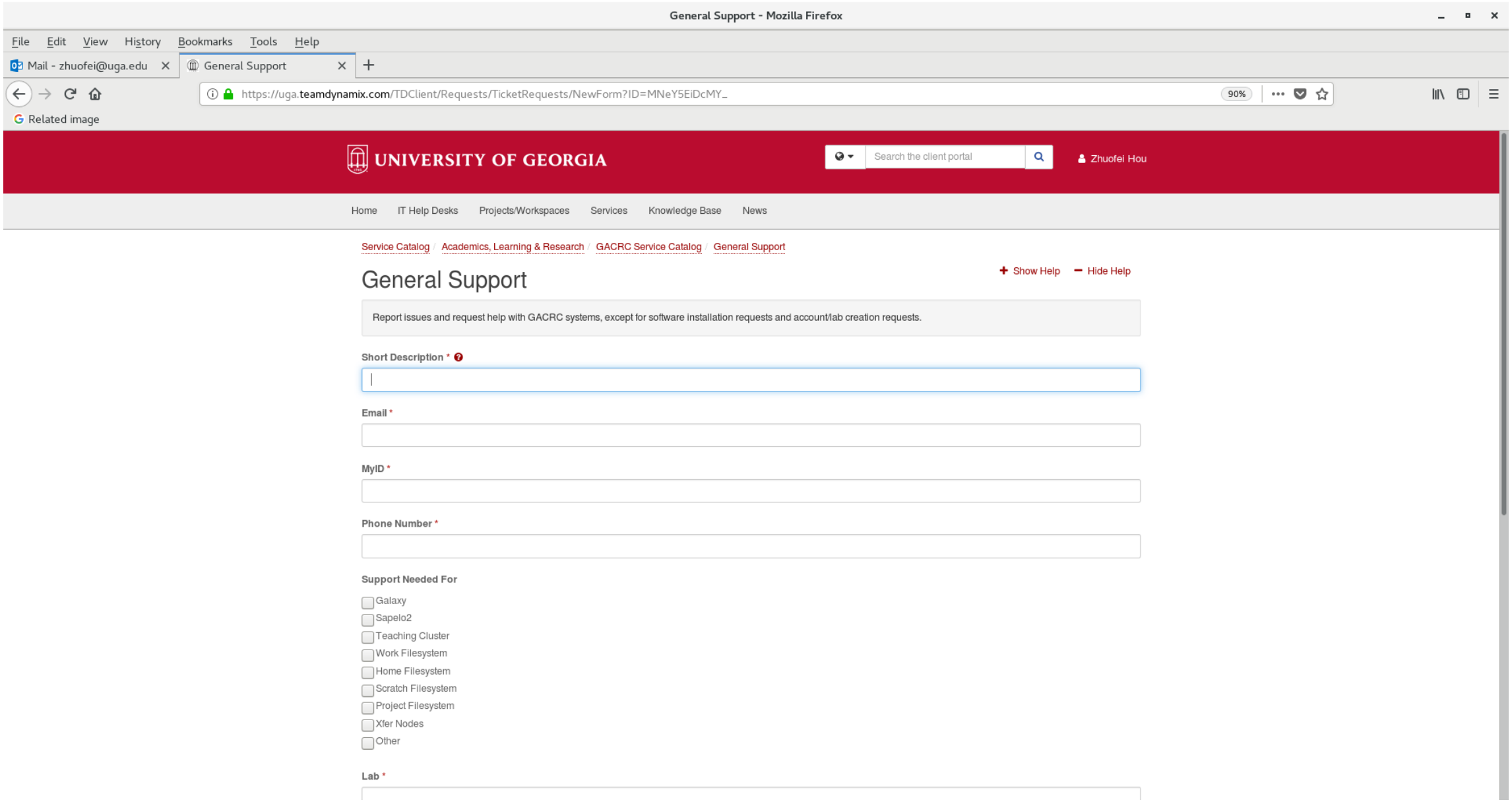
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Report issues and request help with GACRC systems, except for software installation requests and account/lab creation requests.
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Teaching Cluster
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Thank You!