Introduction to GACRC Teaching Cluster

Georgia Advanced Computing Resource Center (GACRC)

EITS/University of Georgia

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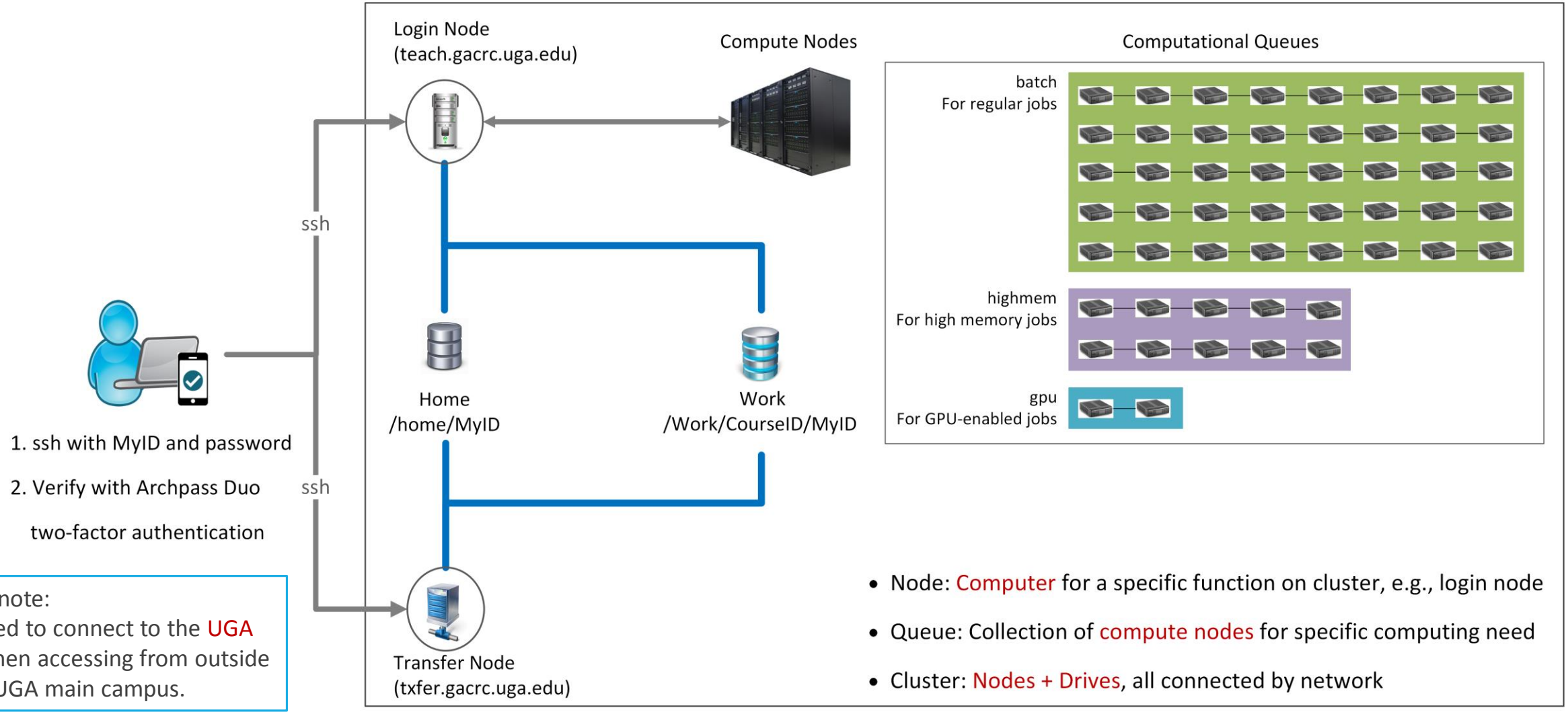
Outline

- 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/CourseID/MyID: data parking for individual user in the class (e.g., /work/binf8940/MyID)
  3. /work/CourseID/instructor_data: data shared with class by the instructors
- Three Queues:
  1. batch: for running regular computational jobs
  2. highmem: for running high-memory jobs
  3. gpu: for running GPU jobs

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. Make a job submission script in workDir : `nano ./sub.sh`
6. Submit a job from workDir : `sbatch ./sub.sh`
7. Check job status : `squeue` or Cancel a job : `scancel JobID`

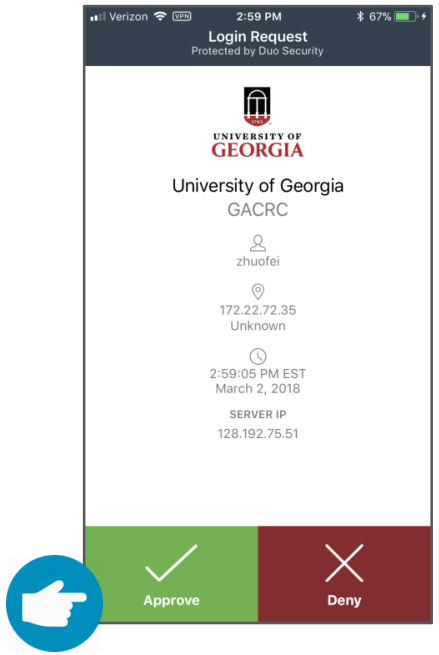
Step1: Log on to Login node - Mac/Linux using ssh

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!

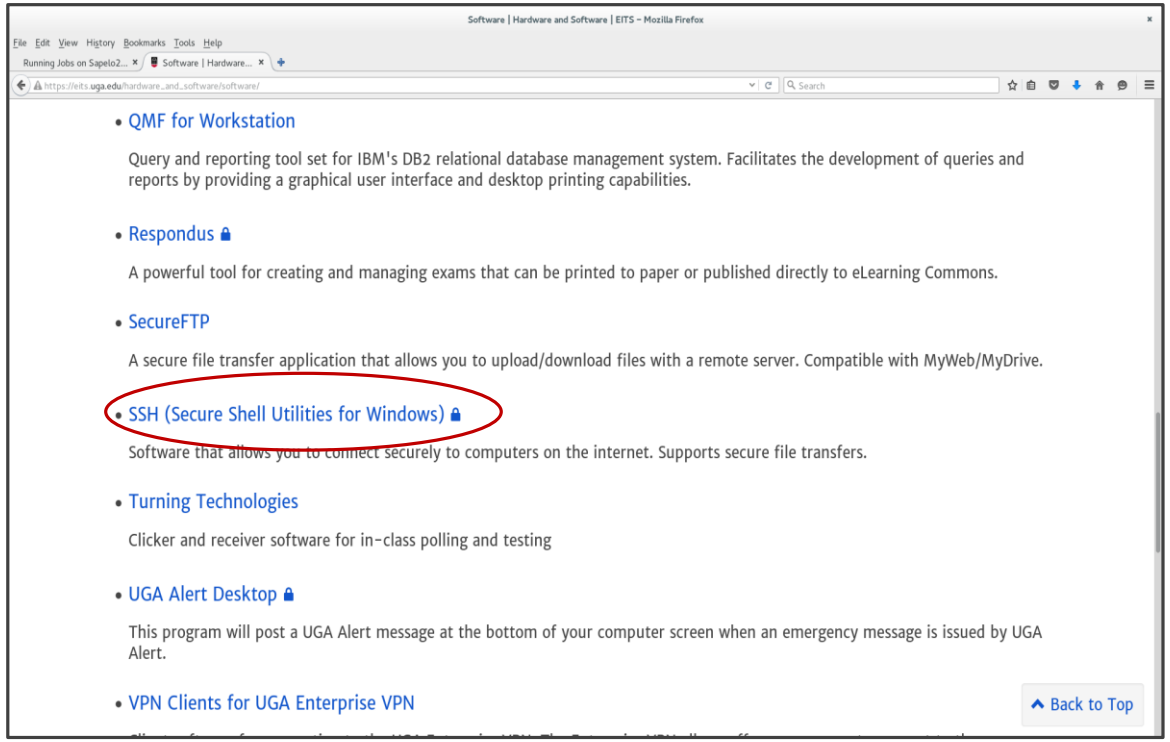


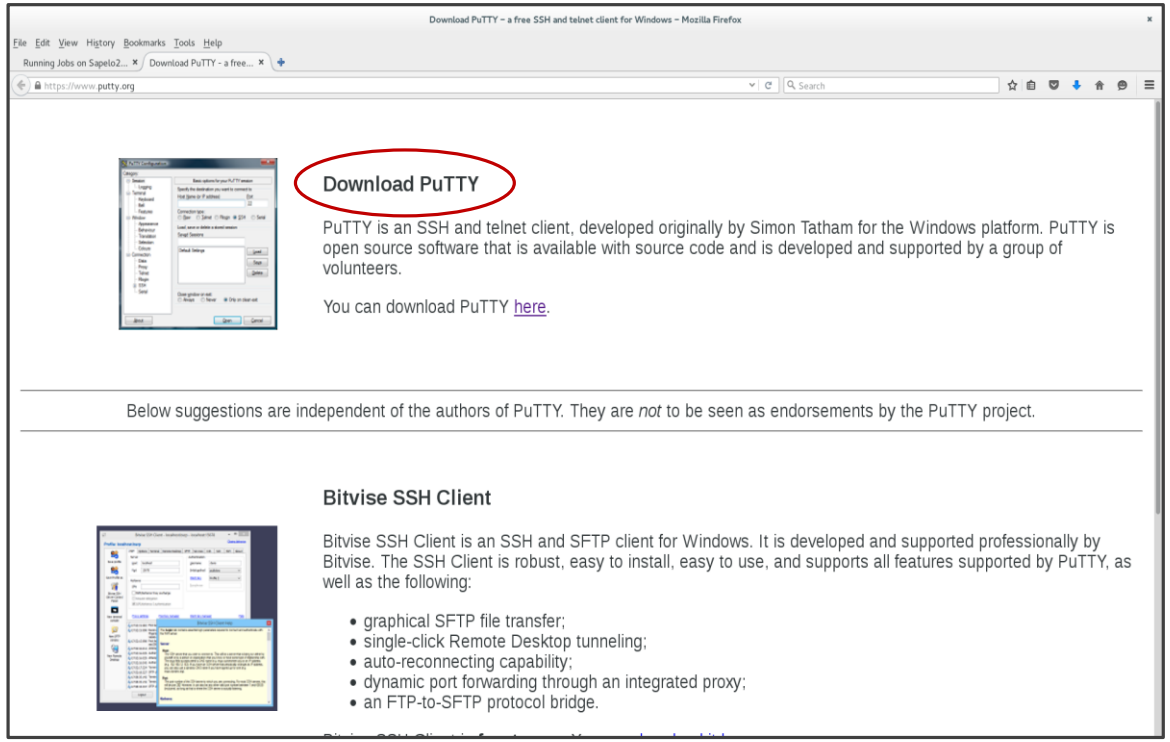
4. Verify login using Duo

```
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!
```

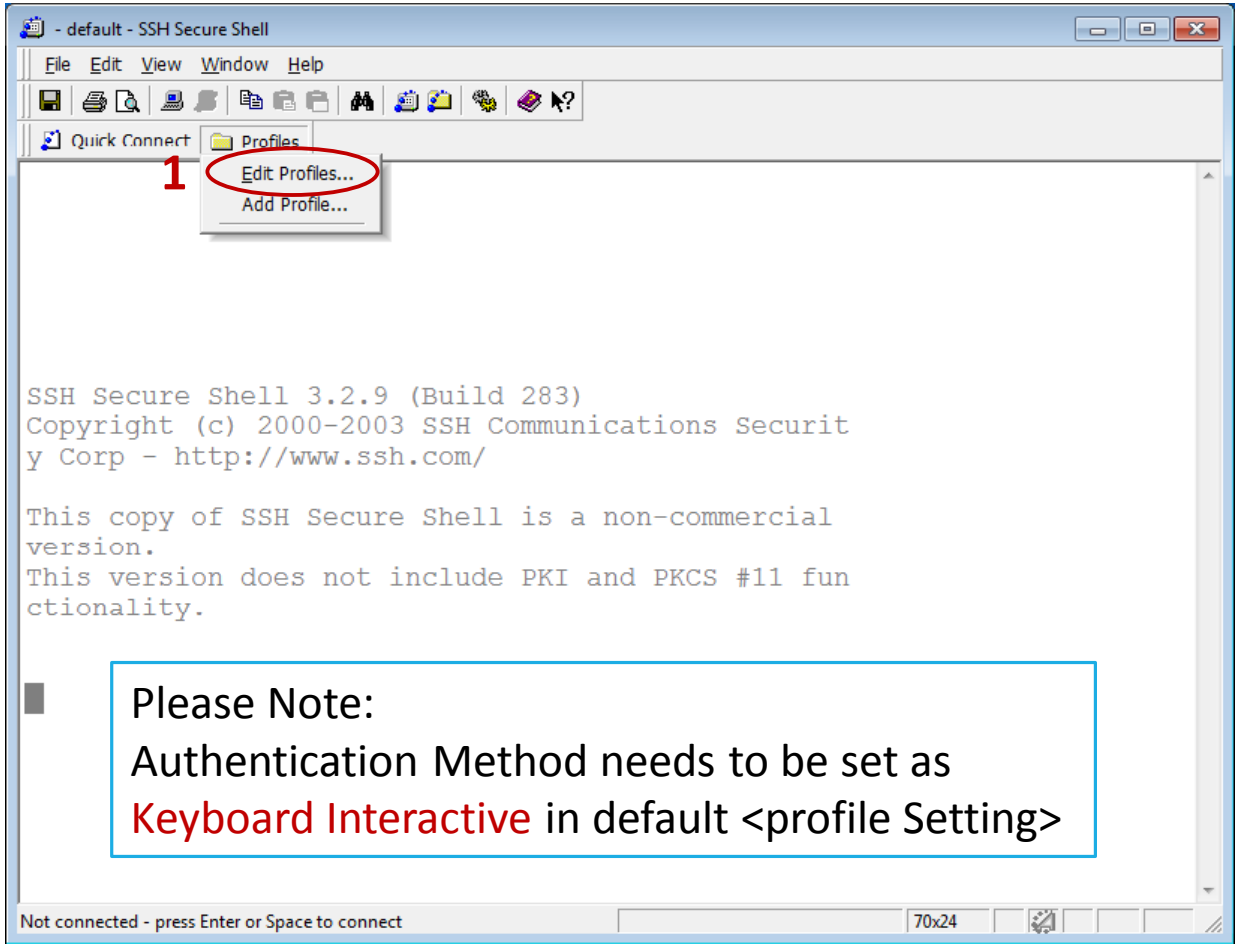
Step1 (Cont.) - Windows

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/

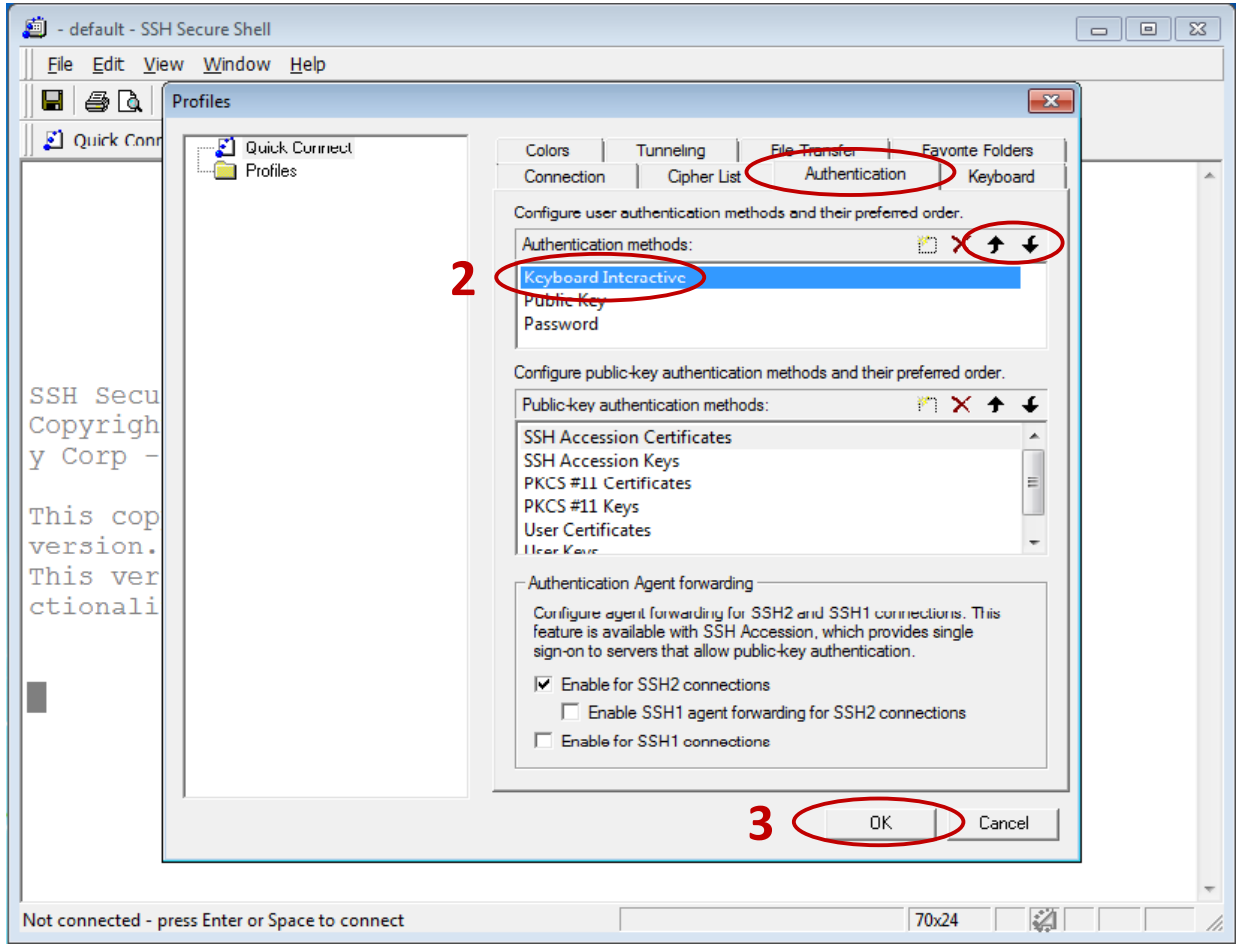




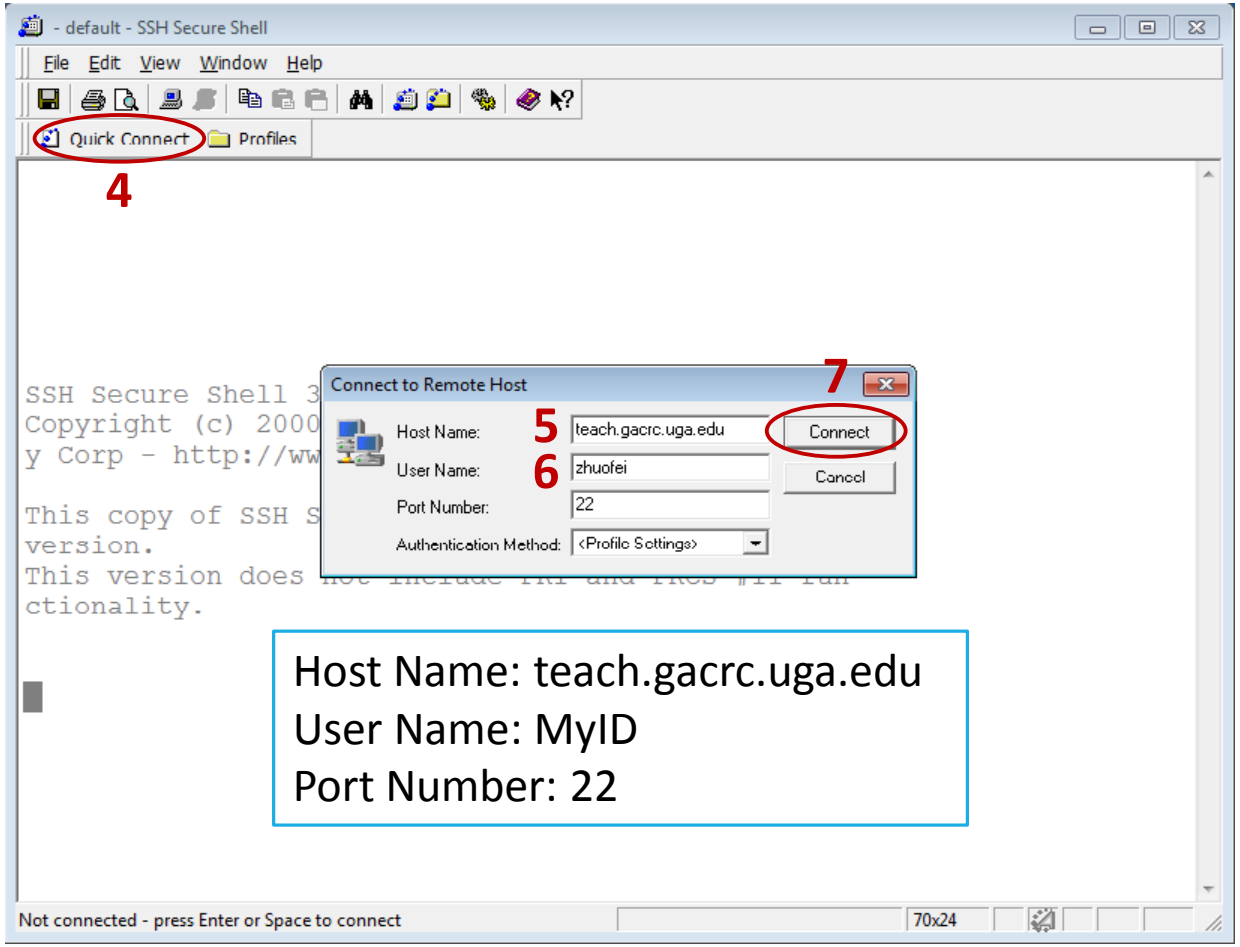
Step1 (Cont.) - Windows using SSH Secure Utilities



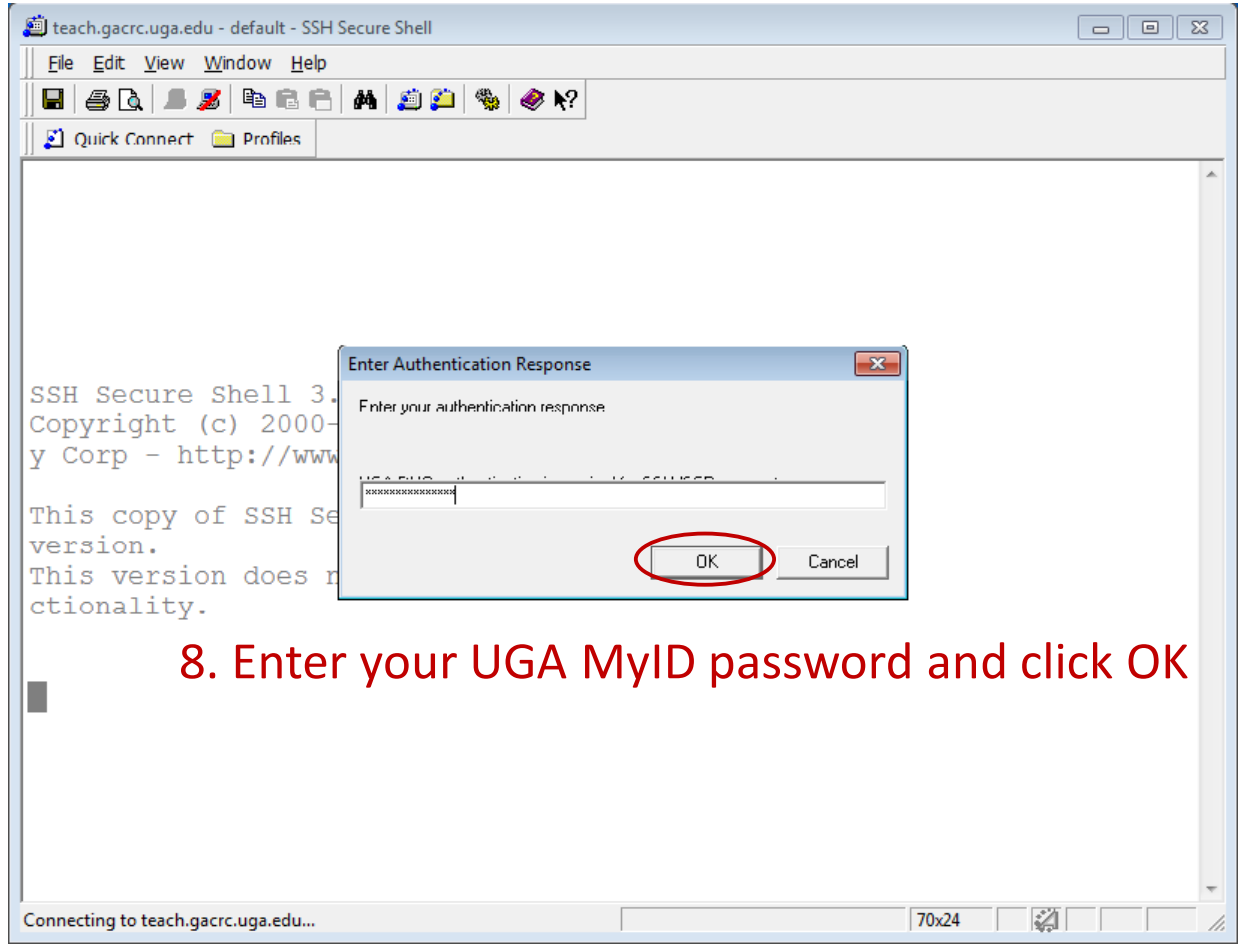
Please Note:
Authentication Method needs to be set as
Keyboard Interactive in default <profile Setting>



Step1 (Cont.) - Windows using SSH Secure Utilities

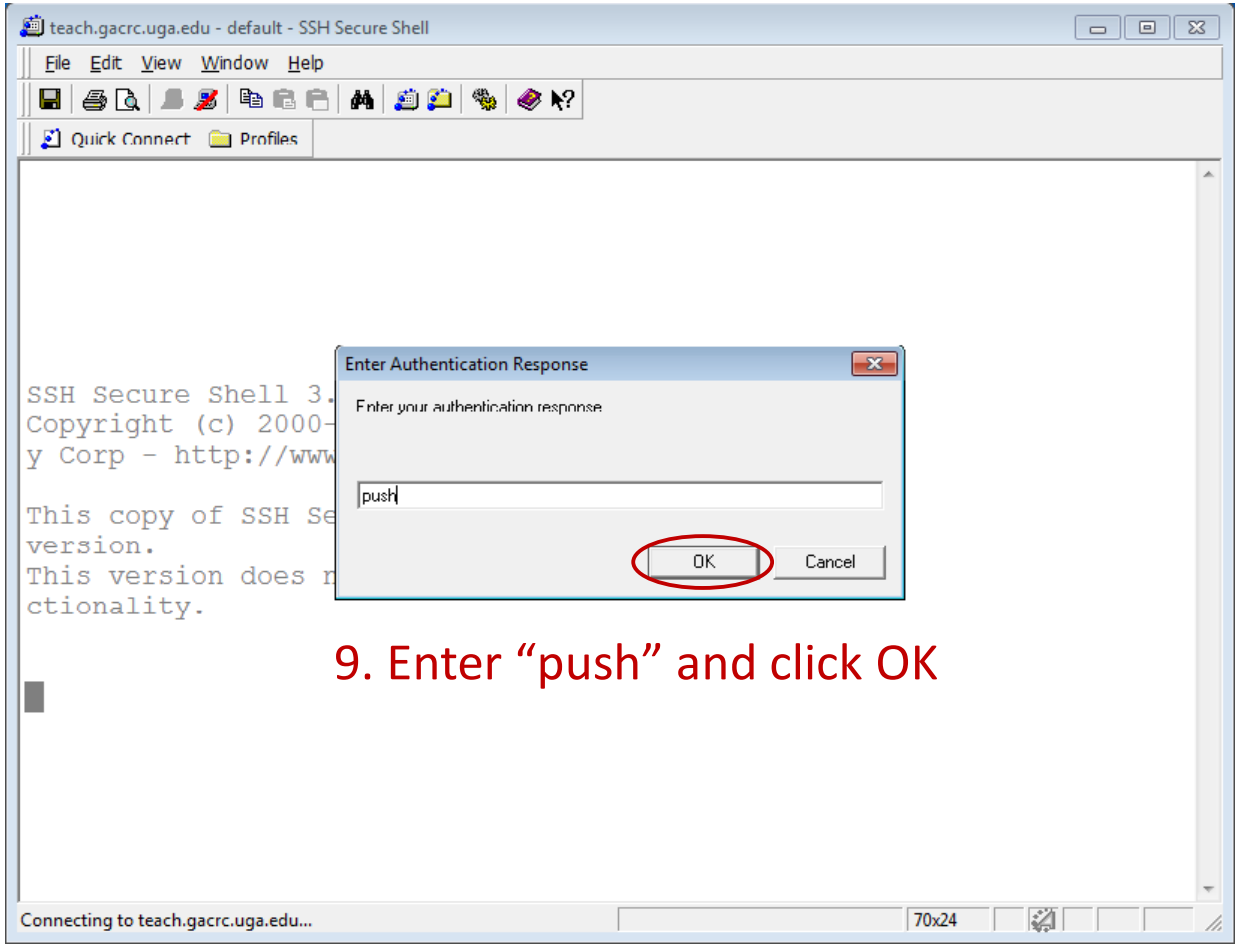


Host Name: teach.gacrc.uga.edu
User Name: MyID
Port Number: 22

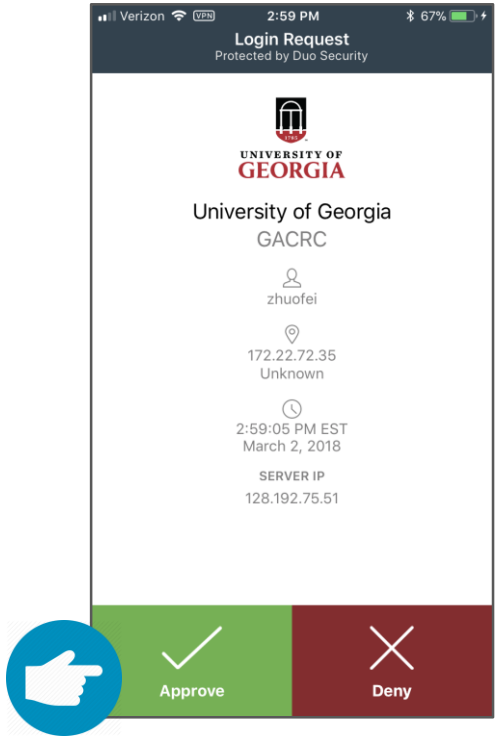


8. Enter your UGA MyID password and click OK

Step1 (Cont.) - Windows using SSH Secure Utilities

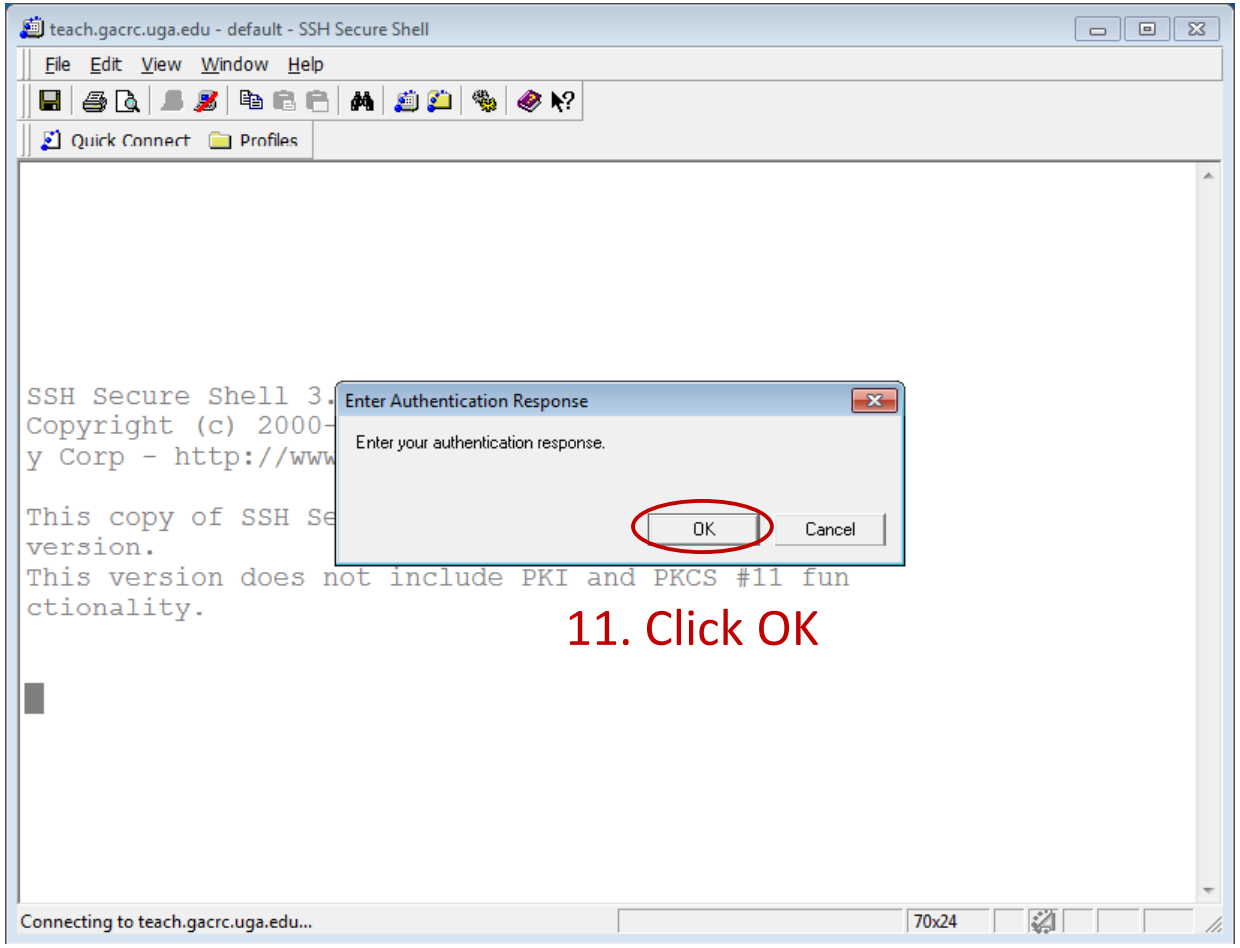


9. Enter “push” and click OK

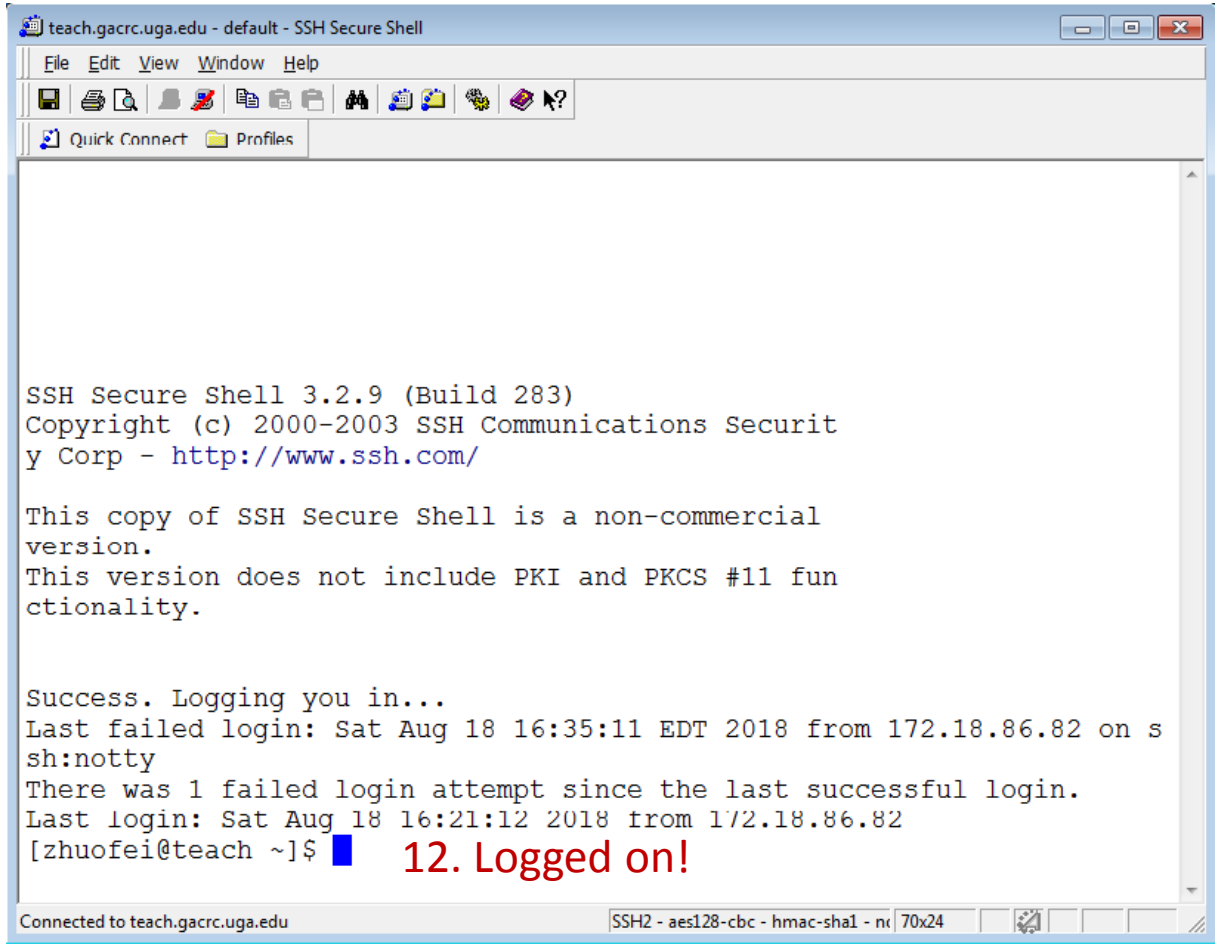


10. Verify login using Duo

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
```

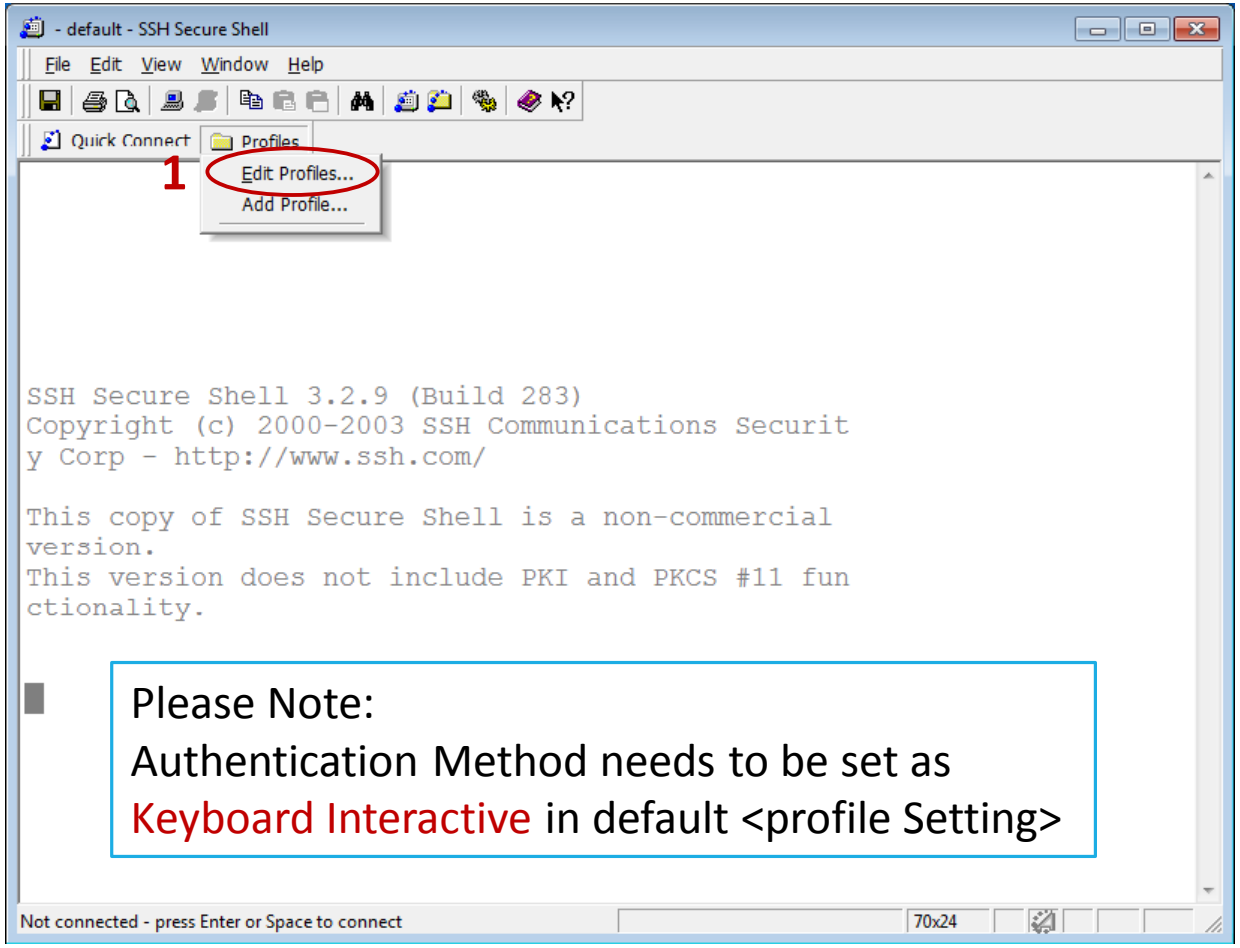
E.g. 2: use scp on local computer, from workDir on cluster ➔ Local

```
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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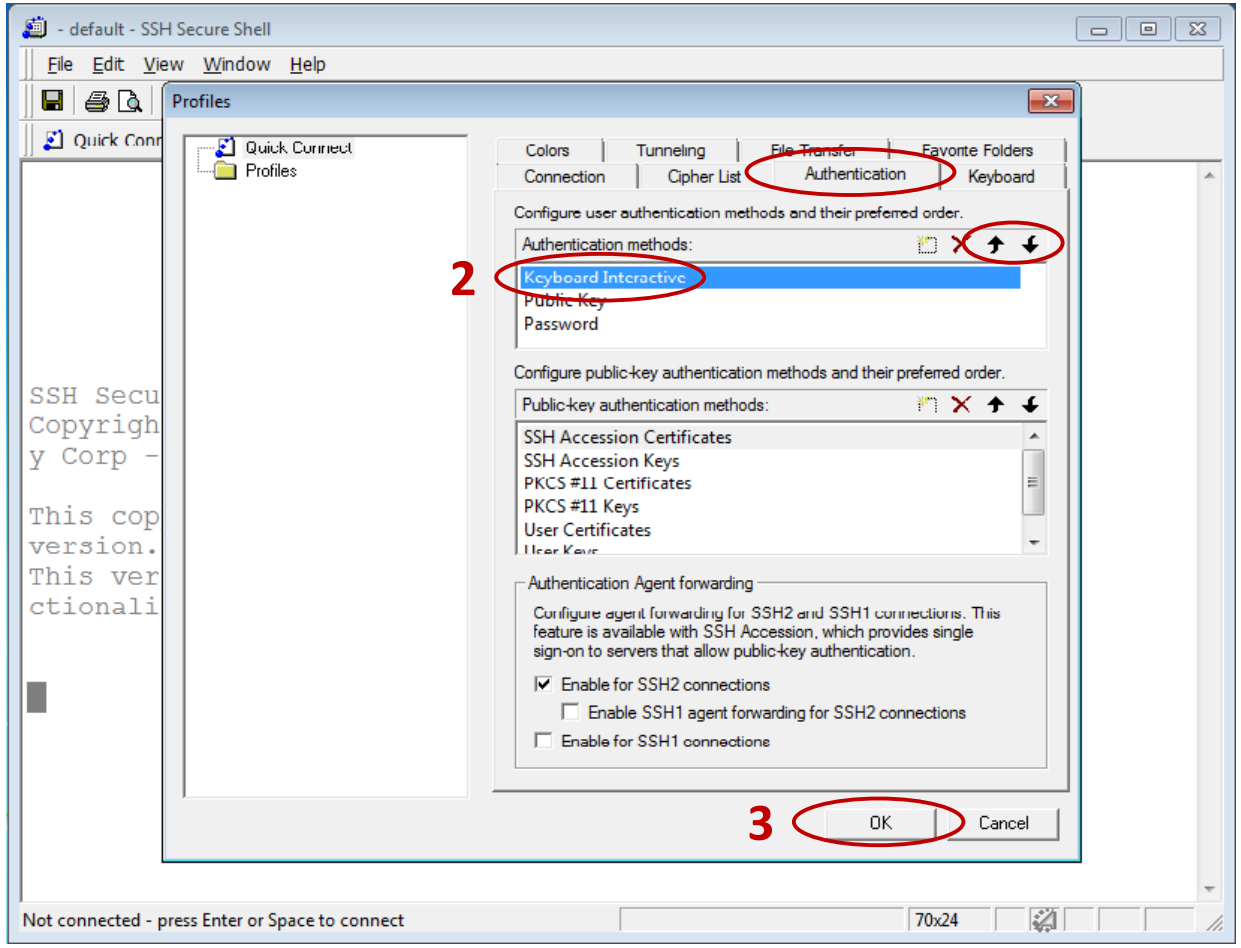
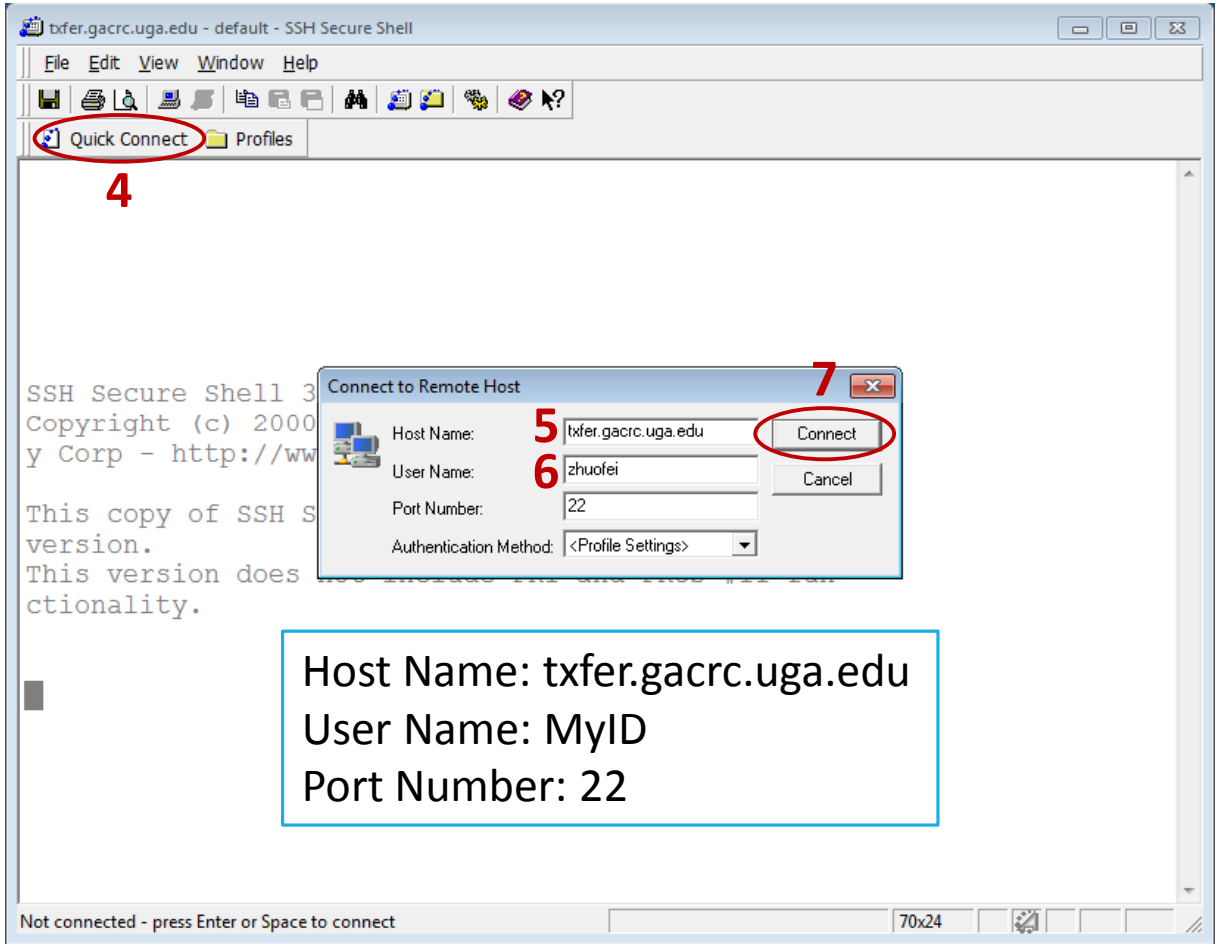
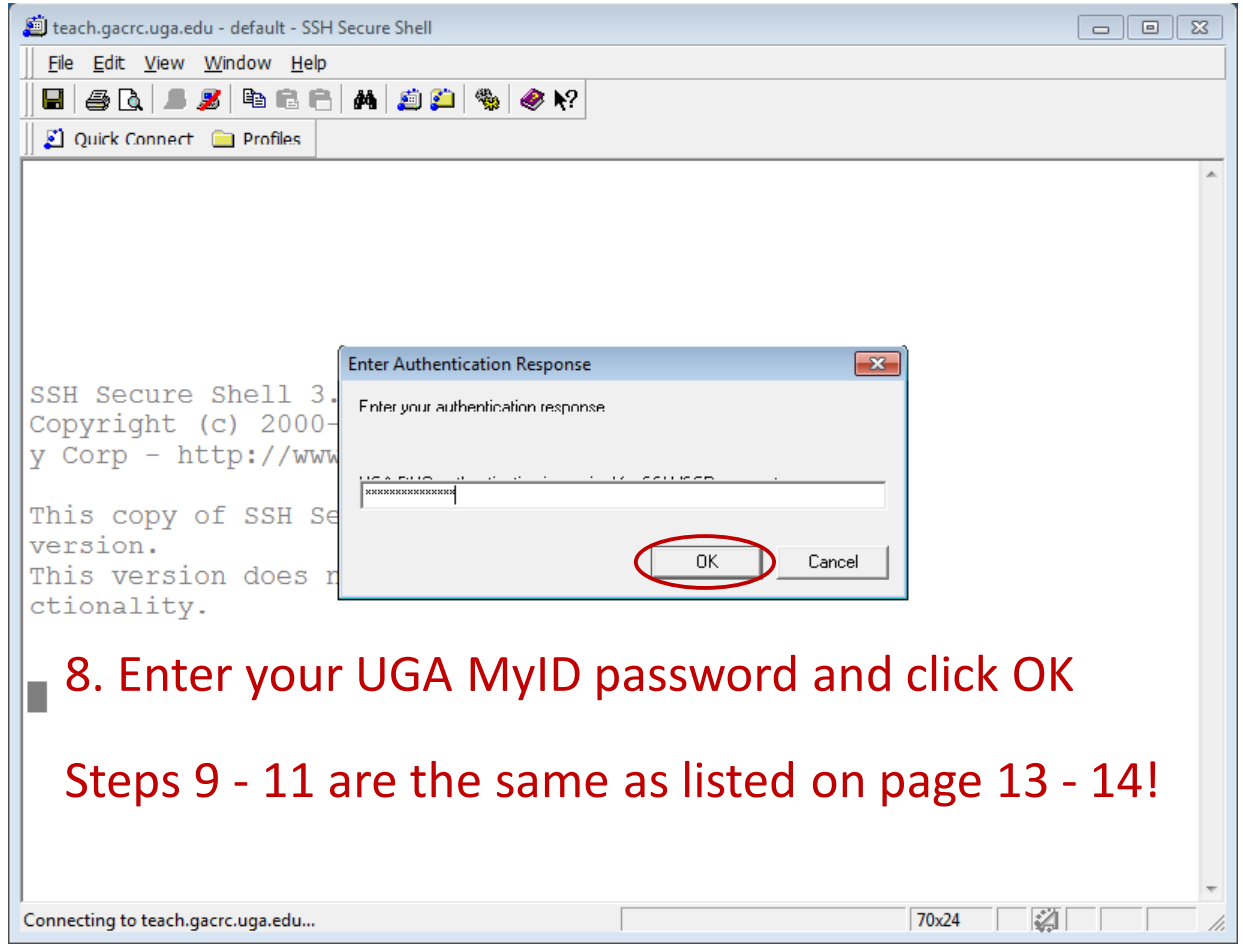


Step4 (Cont.) - Windows using SSH Secure Utilities



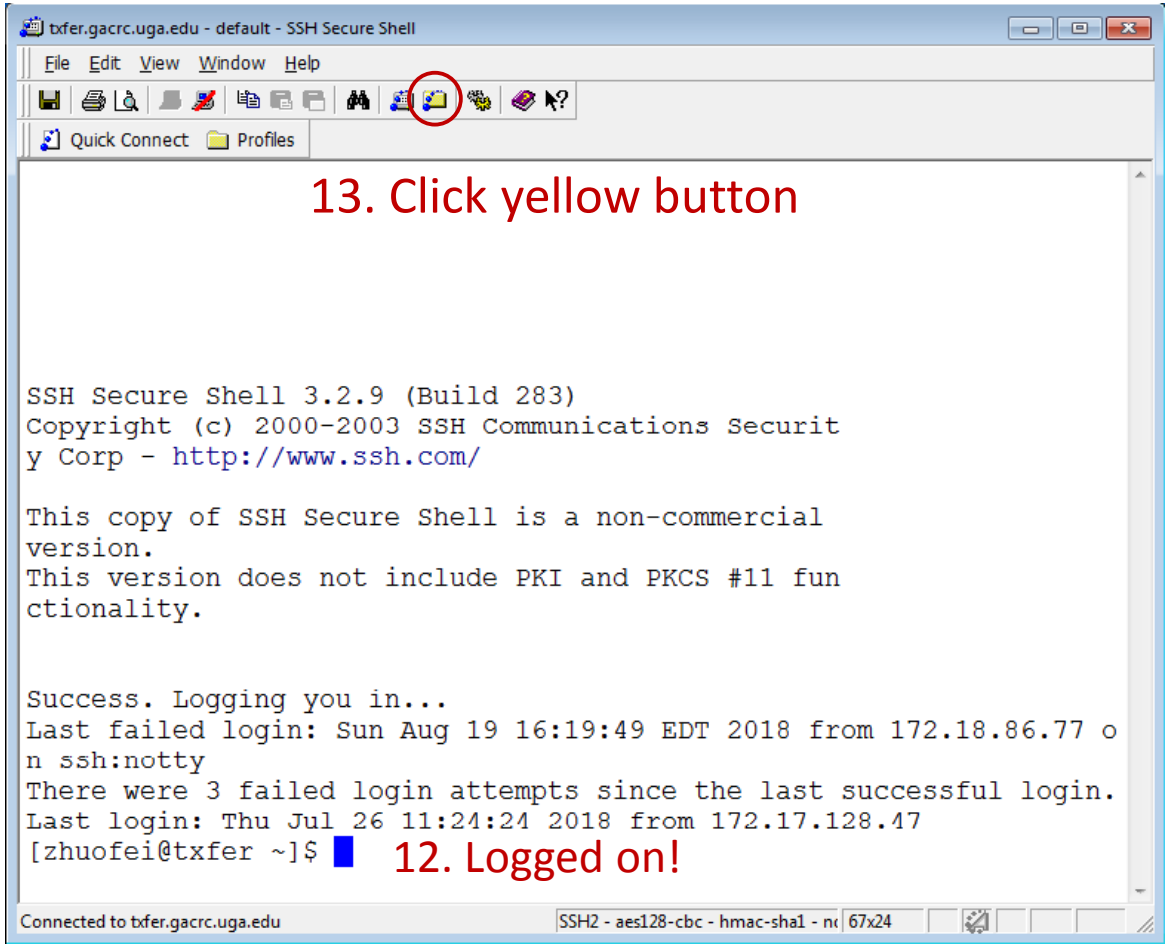
Host Name: txfer.gacrc.uga.edu
User Name: MyID
Port Number: 22

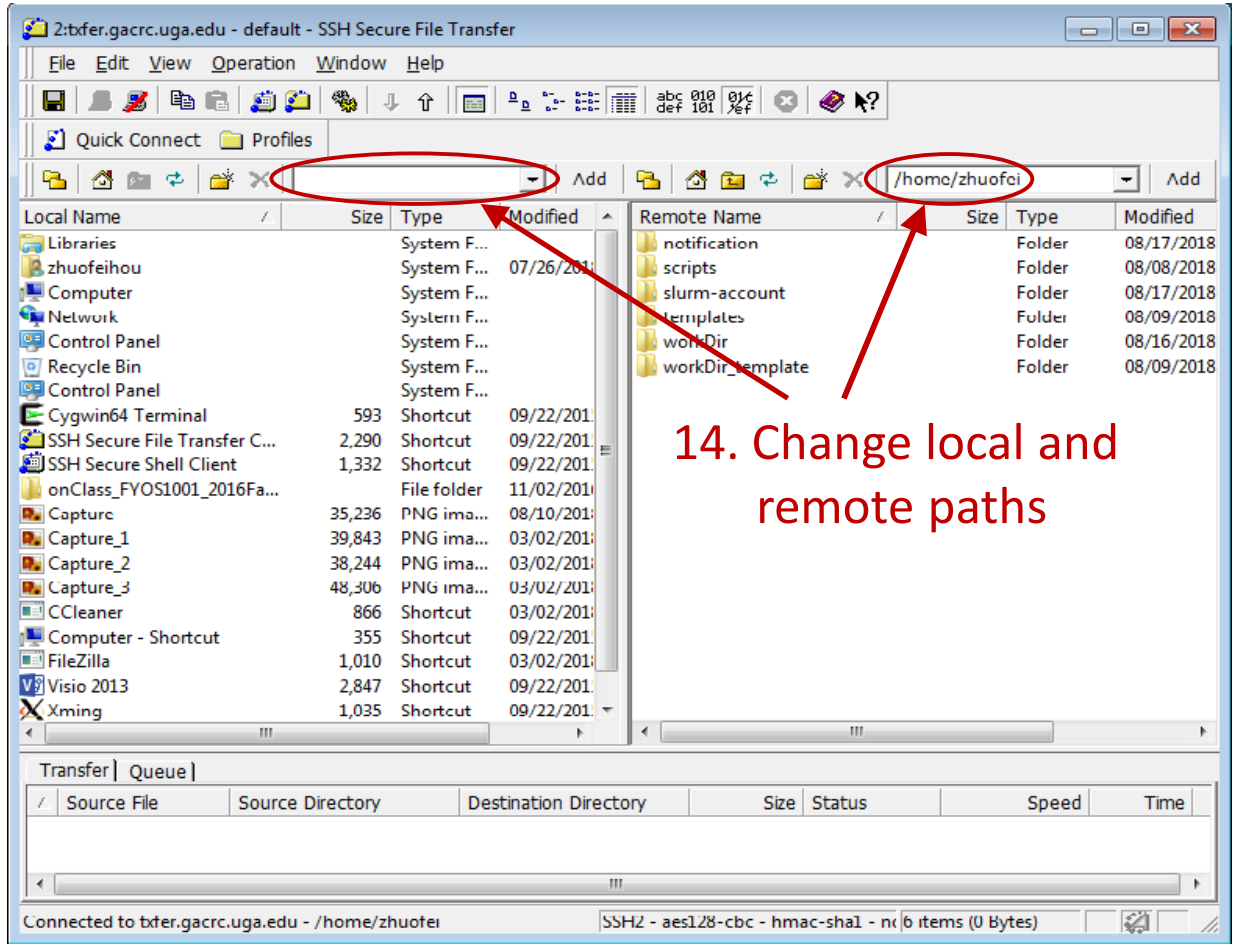


8. Enter your UGA MyID password and click OK

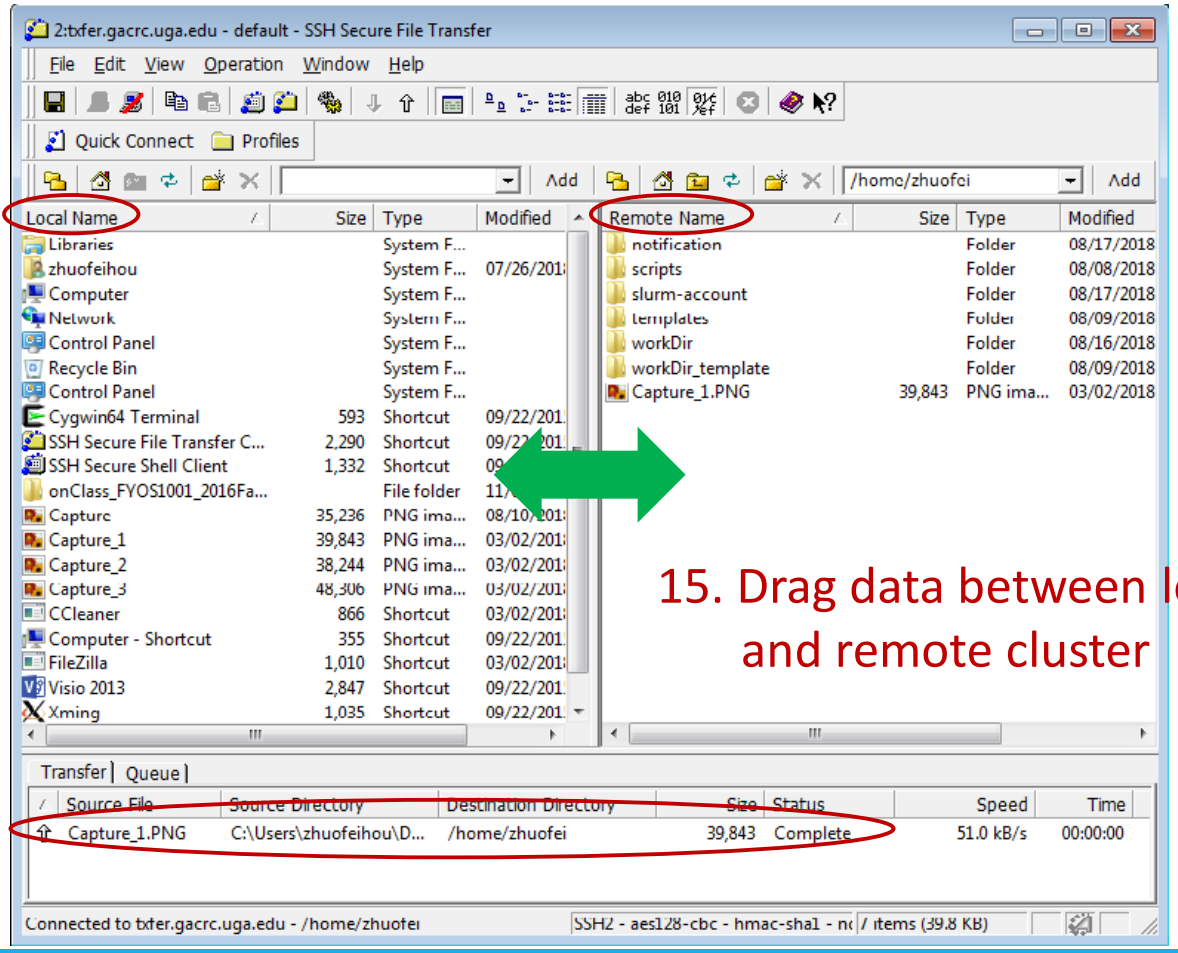
Steps 9 - 11 are the same as listed on page 13 - 14!

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

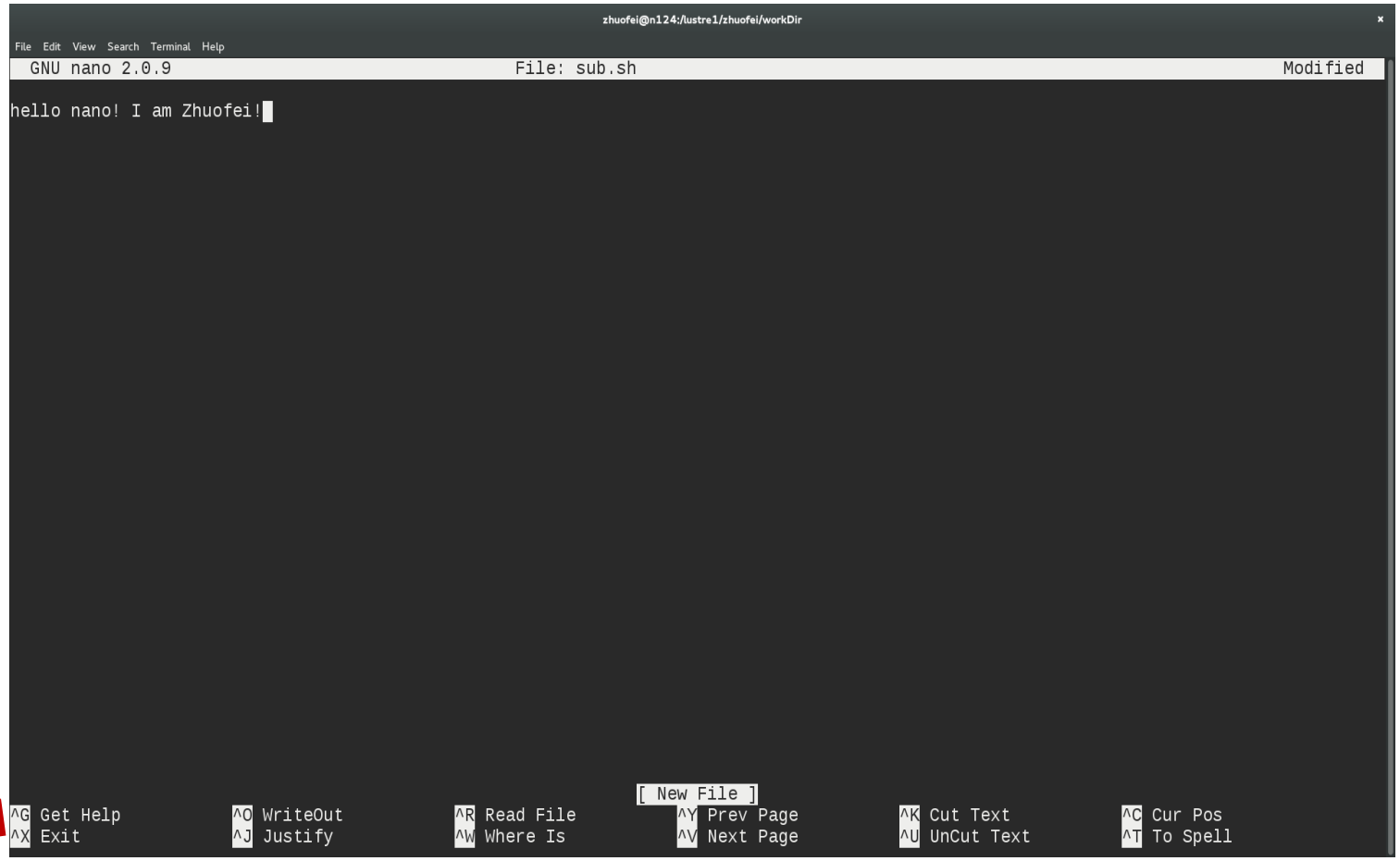
```
mv /work/pbio6550/MyID/datafile /home/MyID/workDir
```

Step5: Make a job submission script in workDir using nano

```
$ nano sub.sh
```

nano is a small and friendly text editor on Linux.

Ctrl-x to save file and quit from nano



Step5 (Cont.)

Please copy

1. sample input data
2. job submission script

to your current working folder:

cp /usr/local/training/sample.fasta .

cp /usr/local/training/sub_blast.sh .

```
#!/bin/bash
#SBATCH --job-name=testBLAST          # Job name
#SBATCH --partition=batch             # Partition (queue) name
#SBATCH --ntasks=1                    # Single task job
#SBATCH --cpus-per-task=4             # Number of cores per task
#SBATCH --mem=20gb                    # Total memory for job
#SBATCH --time=2:00:00                # Time limit hrs:min:sec
#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 $SLURM_SUBMIT_DIR
module load BLAST+/2.6.0-foss-2016b-Python-2.7.14
time blastn -num_threads 4 -query sample.fasta -db /db/ncbiblast/nrte/06222018/nt\
            -out results.${SLURM_JOB_ID} -outfmt 6 -max_target_seqs=2
```

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

Step6: Submit a job from workDir using sbatch

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

Tips: sub_blast.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 the blast commands

Step7: 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       batch   testBLAS  zhuofei   PENDING   0:00   2:00:00      1 (None)
160       batch   testBLAS  zhuofei   RUNNING   0:02   2:00:00      1 c2-11
161       batch   testBLAS  zhuofei   RUNNING   0:02   2:00:00      1 c2-11

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

Step7 (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   batch   testBLAS  zhuofei  RUNNING   2:07    2:00:00      1 c1-38
168   batch   testBLAS  zhuofei  RUNNING   3:14    2:00:00      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   batch   testBLAS  zhuofei COMPLETI   2:25    2:00:00      1 c1-39
168   batch   testBLAS  zhuofei  RUNNING   3:32    2:00:00      1 c1-38

$ squeue -l
Wed Aug  8 14:04:08 2018
JOBID PARTITION   NAME     USER    STATE   TIME   TIME_LIMI  NODES NODELIST
168   batch   testBLAS  zhuofei  RUNNING   3:35    2:00:00      1 c1-38
```

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

```
$ scontrol show job 174

JobId=174 JobName=testBLAST
   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=00:04:28 TimeLimit=02:00:00 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=batch AllocNode:Sid=teach:30986
   NodeList=c1-38
   NumNodes=1 NumCPUs=4 NumTasks=1 CPUs/Task=4 ReqB:S:C:T=0:0:*:*
   ...
   Command=/home/zhuofei/workDir/sub_blast.sh
   WorkDir=/home/zhuofei/workDir
   StdErr=/home/zhuofei/workDir/log.174
   StdOut=/home/zhuofei/workDir/log.174
```

Step7 (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    idle   c2-2
interq       up 1-00:00:00      3    idle   c2-[4-6]
batch        up 3-00:00:00      3    mix    c1-38,c2-[11-12]
batch        up 3-00:00:00      1    alloc  c1-1
batch        up 3-00:00:00     36    idle   c1-[2-35,39]
```

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://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
- ✓ Job ID
- ✓ Job submission script and command you used to submit the job
- ✓ Your working directory on cluster

➢ Software Installation:

- ✓ Specific name and version of the software
- ✓ Download website
- ✓ Supporting package information if have

Please note:

1. In general only software widely used by the GACRC computing community will be centrally installed.
2. Make sure of the correctness of datasets being used by your jobs!

GACRC's HelpDesk
The Georgia Advanced Computing Resource Center
A Collaborative Partnership between the *Vice President for Research* and the *Vice President for Information Technology*

Request Support

* indicates Required fields.

Your Name *	First & Last
MyID *	myid
E-mail *	you@example.edu
Phone Number	411-555-1212
Brief Description	
Request Details *	(less than 2,000 characters)
Cluster	☐ sapelo2 ☐ sapelo ☑ teach ☐ other

Review

* For questions on cluster or software, please include the command/script used, working path and working nodes (interactive / queue name) if applicable.
* For software installation, please specify software name, version and include link to the software if applicable.
* Please review your message on the next page and then click the Submit button.

Thank You!