

# Introduction to GACRC Teaching Cluster

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Georgia Advanced Computing Resource Center (GACRC)

EITS/University of Georgia

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# Outline

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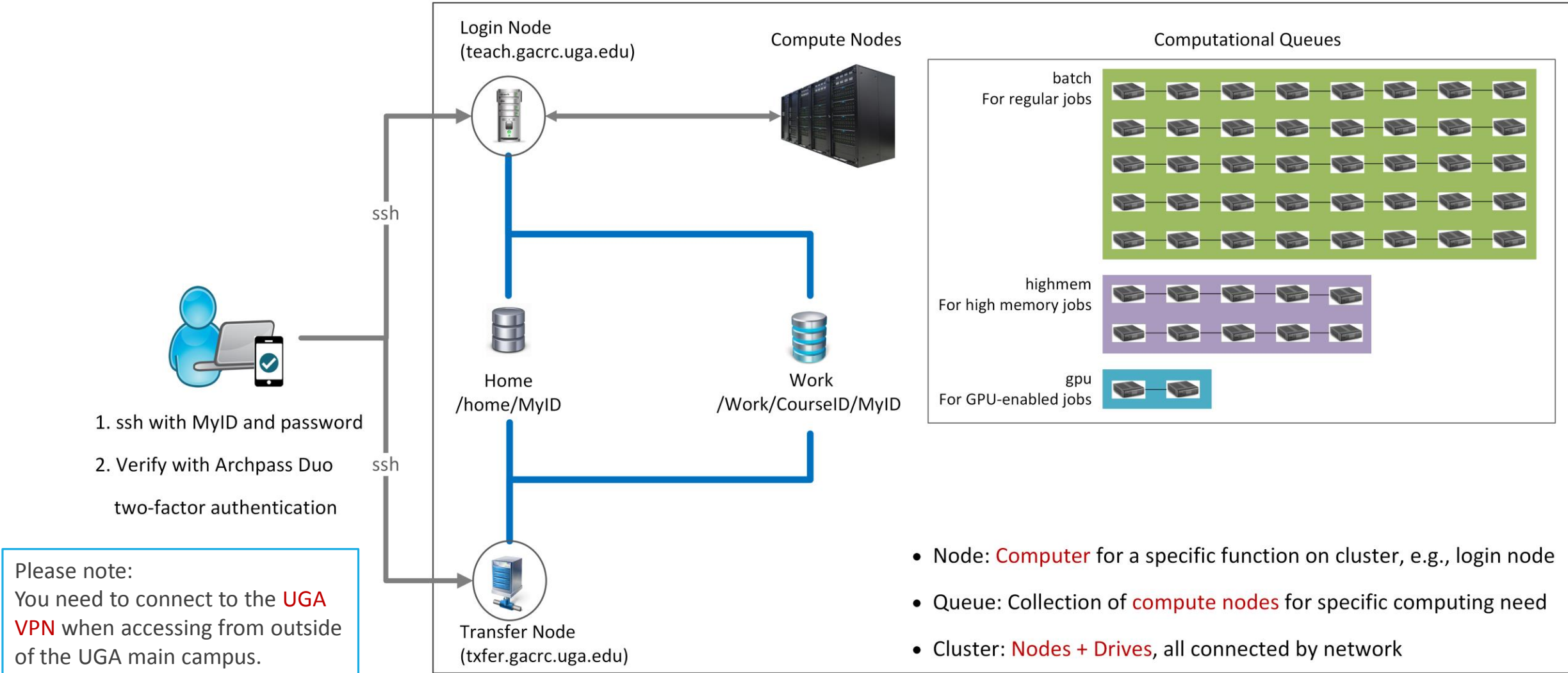
- GACRC
- Overview
- Computing Resources
  - Three Folders
  - Three Computational Queues
  - Software
- Submit Batch Job
- GACRC Wiki and Support

# GACRC

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- 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](https://wiki.gacrc.uga.edu/wiki/Getting_Help) (GACRC Support)
- <http://gacrc.uga.edu> (GACRC Web)

# Teaching Cluster



- 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

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- 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.)

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## ➤ 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

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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

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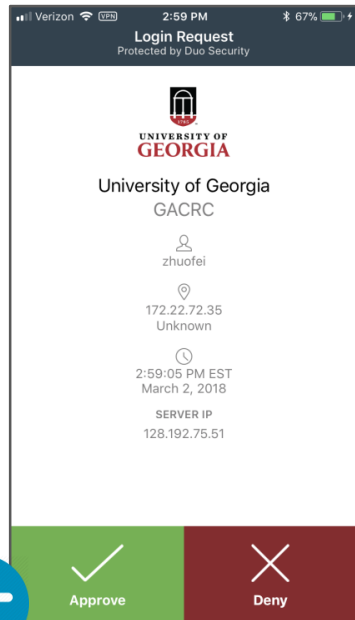
1. Open **Terminal** utility
2. Type command line: `ssh MyID@teach.gacrc.uga.edu`
3. You will be prompted for your **MyID password**
4. Teaching cluster access requires ID verification using two-factor authentication with Archpass Duo. If you are not enrolled in Archpass Duo, please refer to [https://eits.uga.edu/access\\_and\\_security/infosec/tools/archpass\\_duo/](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](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...](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:

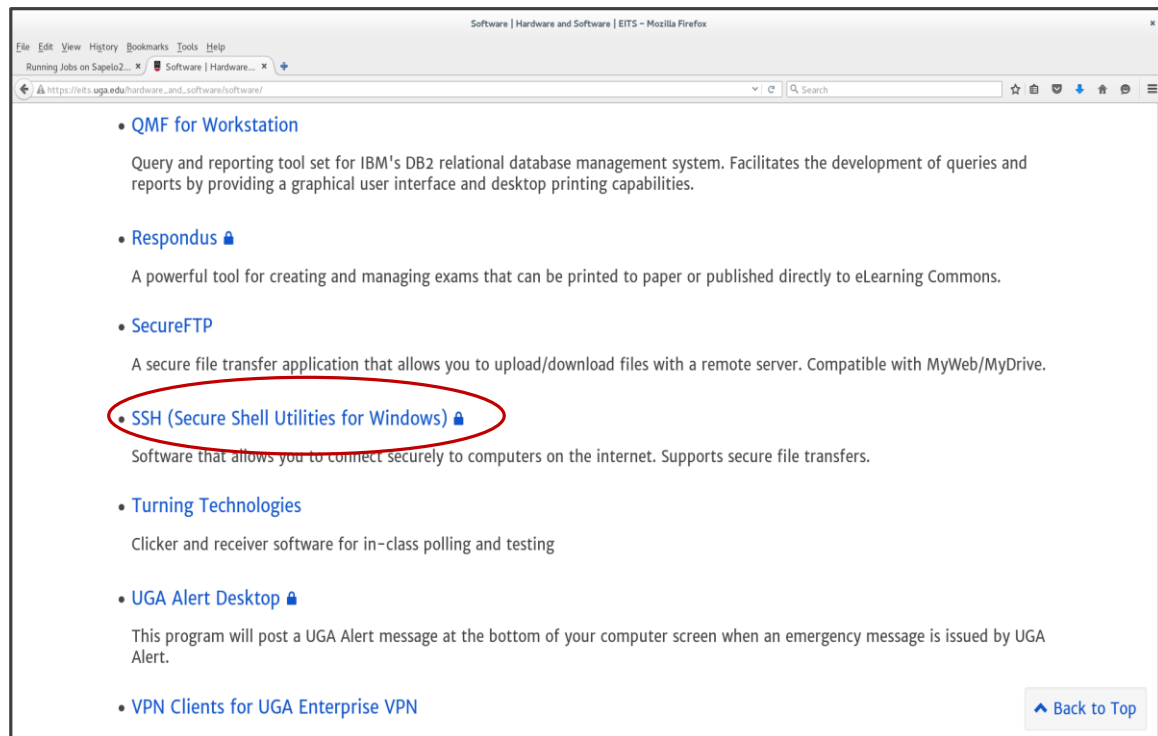
1. Duo Push to XXX-XXX-5758
2. Phone call to XXX-XXX-5758
3. Phone call to XXX-XXX-1925
- 4 5. SMS passcodes to XXX-XXX-5758 (next code starts with: 1)

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/](http://eits.uga.edu/hardware_and_software/software/)
2. You can use PuTTY as an alternative: <https://www.putty.org/>



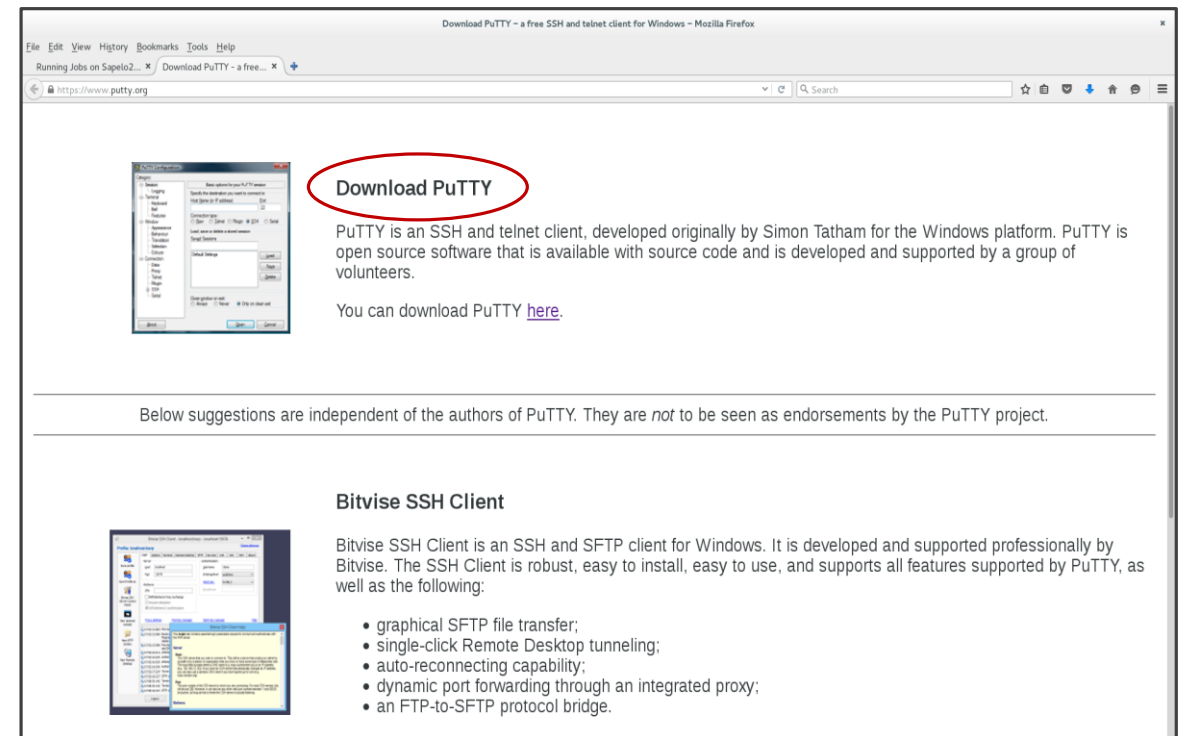
Software | Hardware and Software | EITS - Mozilla Firefox

Running Jobs on Sapelo2... x / Software | Hardware... x

[https://eits.uga.edu/hardware\\_and\\_software/software/](https://eits.uga.edu/hardware_and_software/software/)

- [QMF for Workstation](#)  
Query and reporting tool set for IBM's DB2 relational database management system. Facilitates the development of queries and reports by providing a graphical user interface and desktop printing capabilities.
- [Respondus](#)  
A powerful tool for creating and managing exams that can be printed to paper or published directly to eLearning Commons.
- [SecureFTP](#)  
A secure file transfer application that allows you to upload/download files with a remote server. Compatible with MyWeb/MyDrive.
- [SSH \(Secure Shell Utilities for Windows\)](#)  
Software that allows you to connect securely to computers on the internet. Supports secure file transfers.
- [Turning Technologies](#)  
Clicker and receiver software for in-class polling and testing
- [UGA Alert Desktop](#)  
This program will post a UGA Alert message at the bottom of your computer screen when an emergency message is issued by UGA Alert.
- [VPN Clients for UGA Enterprise VPN](#)

[Back to Top](#)



Download PuTTY - a free SSH and telnet client for Windows - Mozilla Firefox

Running Jobs on Sapelo2... x / Download PuTTY - a free... x

<https://www.putty.org/>

**Download PuTTY**

PuTTY is an SSH and telnet client, developed originally by Simon Tatham for the Windows platform. PuTTY is open source software that is available with source code and is developed and supported by a group of volunteers.

You can download PuTTY [here](#).

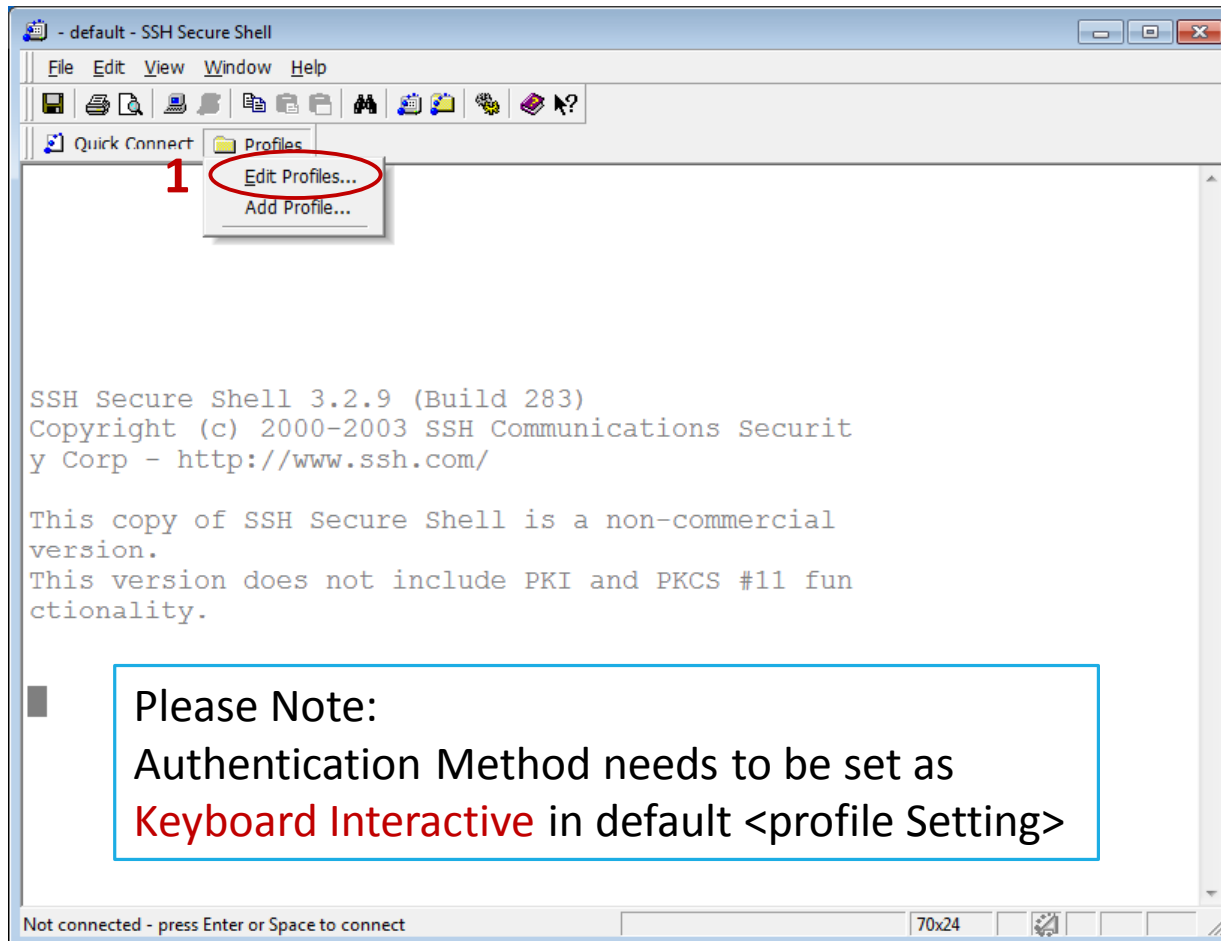
Below suggestions are independent of the authors of PuTTY. They are *not* to be seen as endorsements by the PuTTY project.

**Bitvise SSH Client**

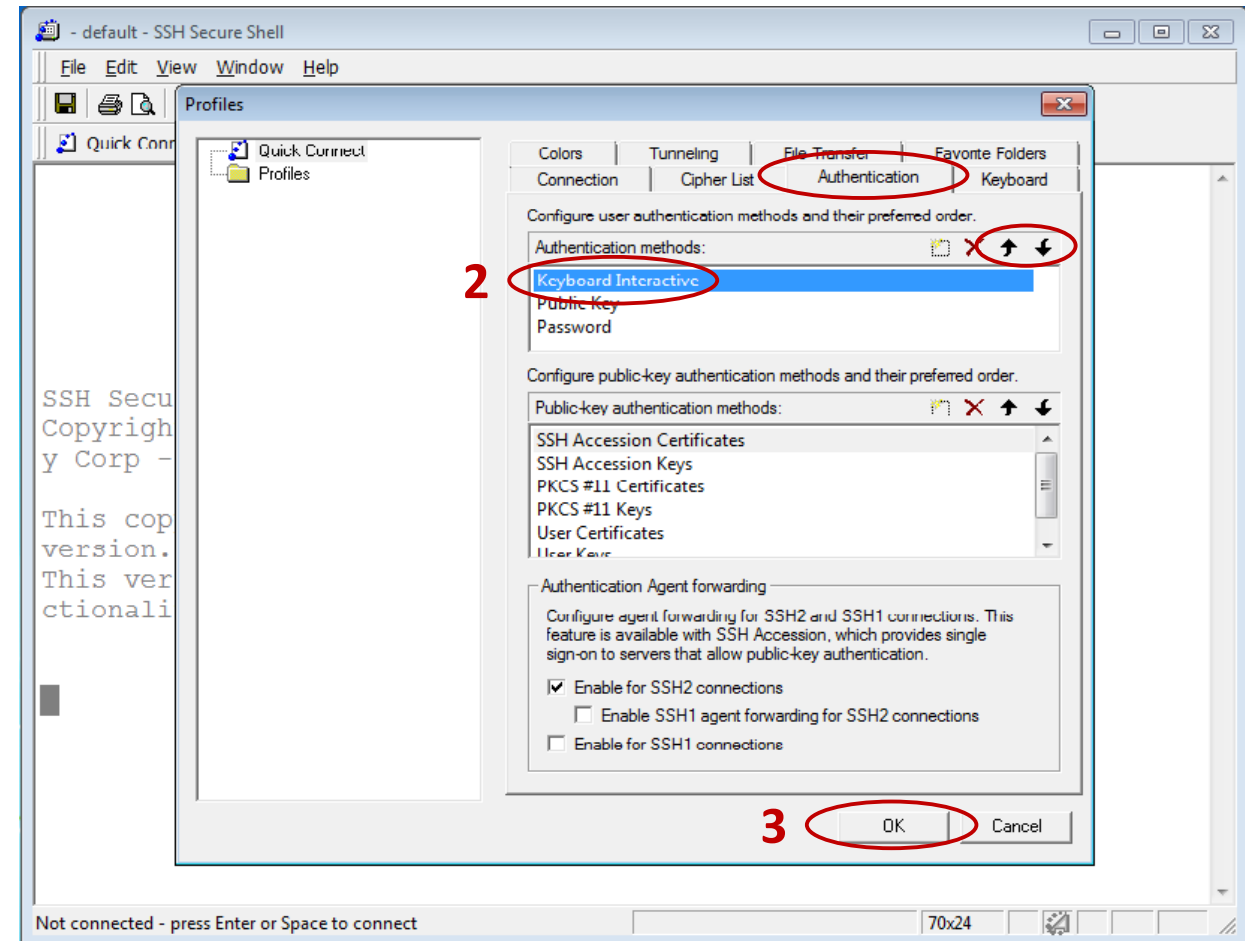
Bitvise SSH Client is an SSH and SFTP client for Windows. It is developed and supported professionally by Bitvise. The SSH Client is robust, easy to install, easy to use, and supports all features supported by PuTTY, as well as the following:

- graphical SFTP file transfer;
- single-click Remote Desktop tunneling;
- auto-reconnecting capability;
- dynamic port forwarding through an integrated proxy;
- an FTP-to-SFTP protocol bridge.

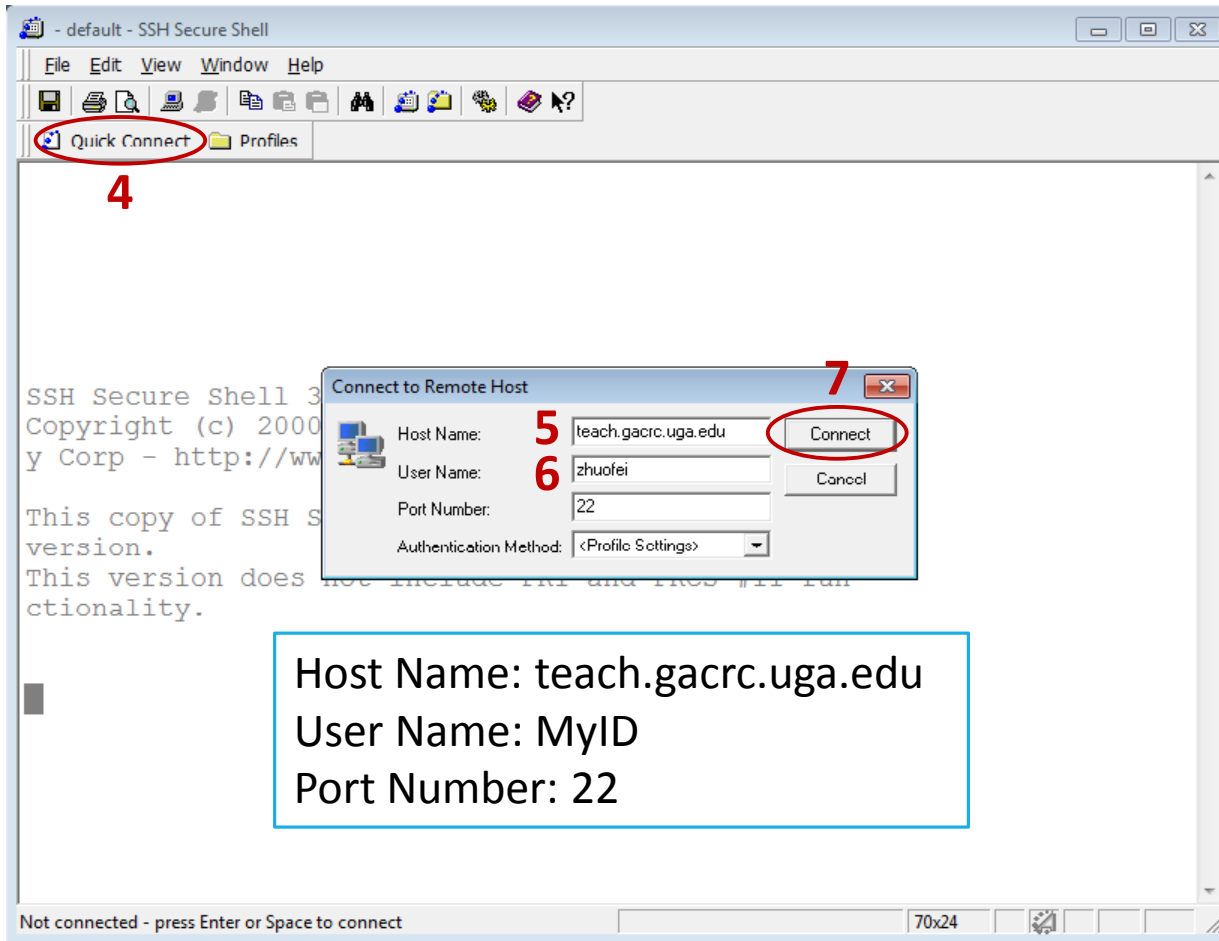
# Step1 (Cont.) - Windows using SSH Secure Utilities



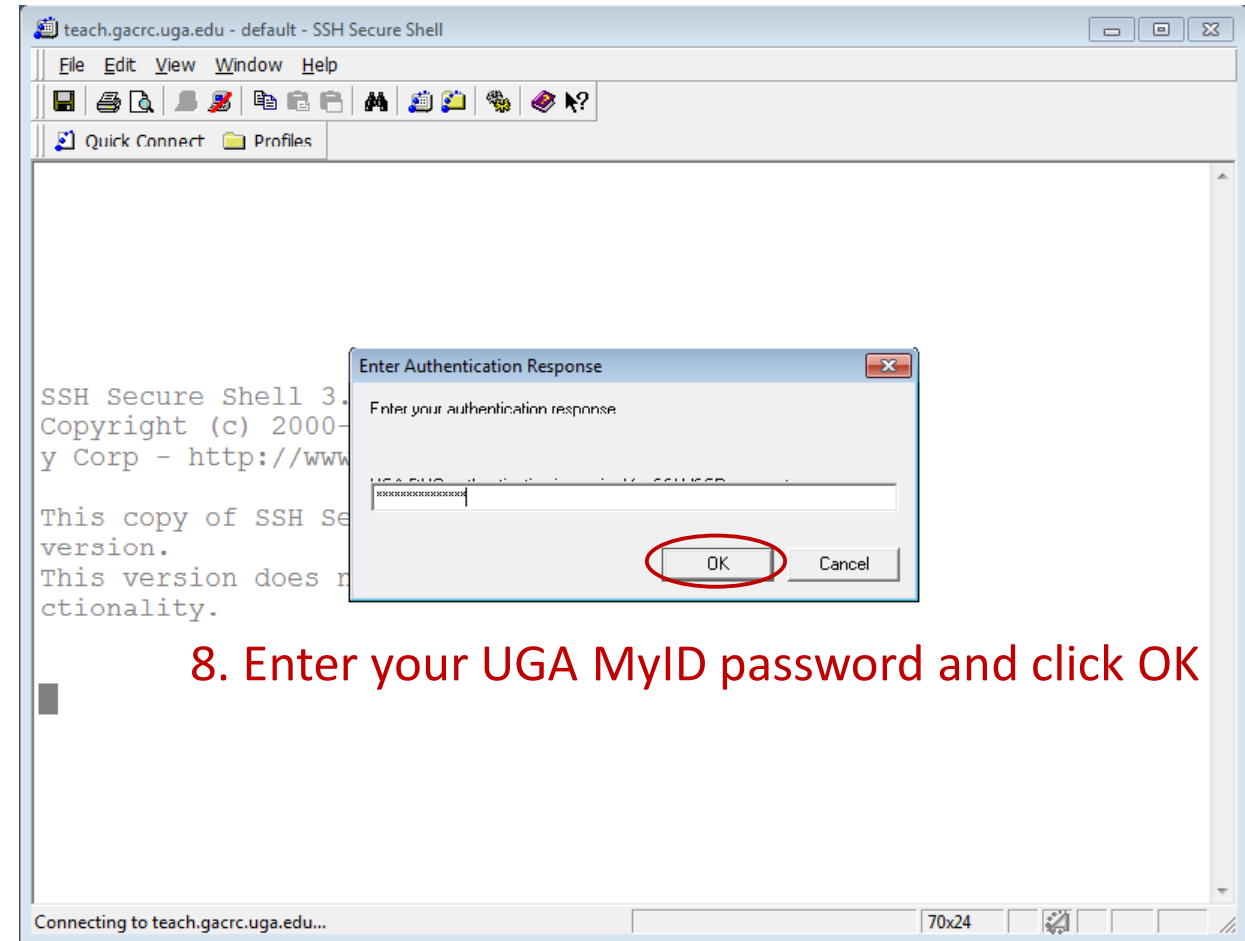
Please Note:  
Authentication Method needs to be set as **Keyboard Interactive** in default <profile Setting>



# Step1 (Cont.) - Windows using SSH Secure Utilities

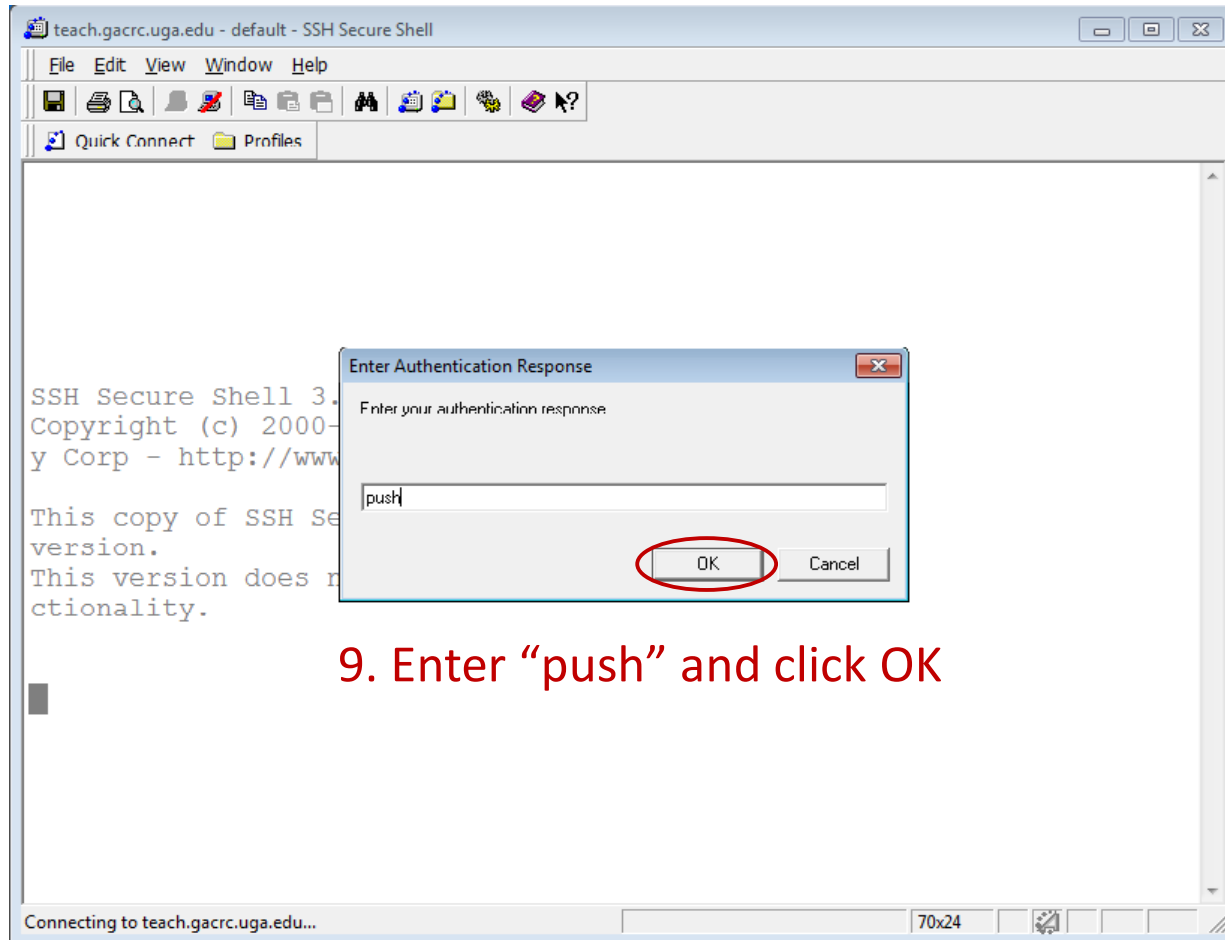


Host Name: teach.gacrc.uga.edu  
User Name: MyID  
Port Number: 22

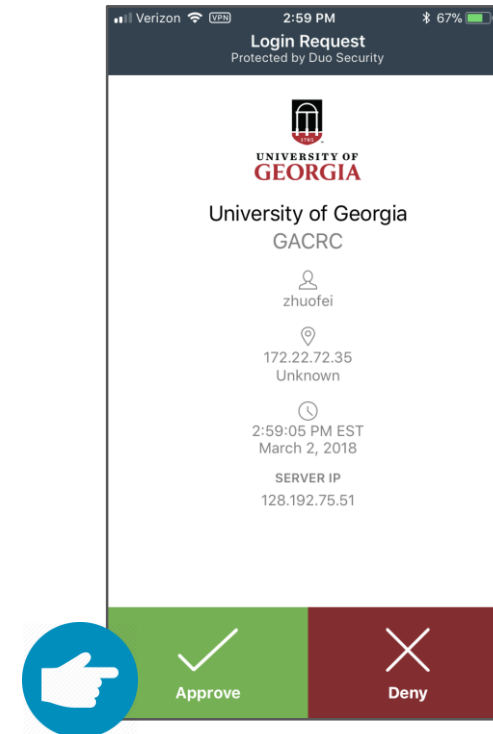


8. Enter your UGA MyID password and click OK

# Step1 (Cont.) - Windows using SSH Secure Utilities

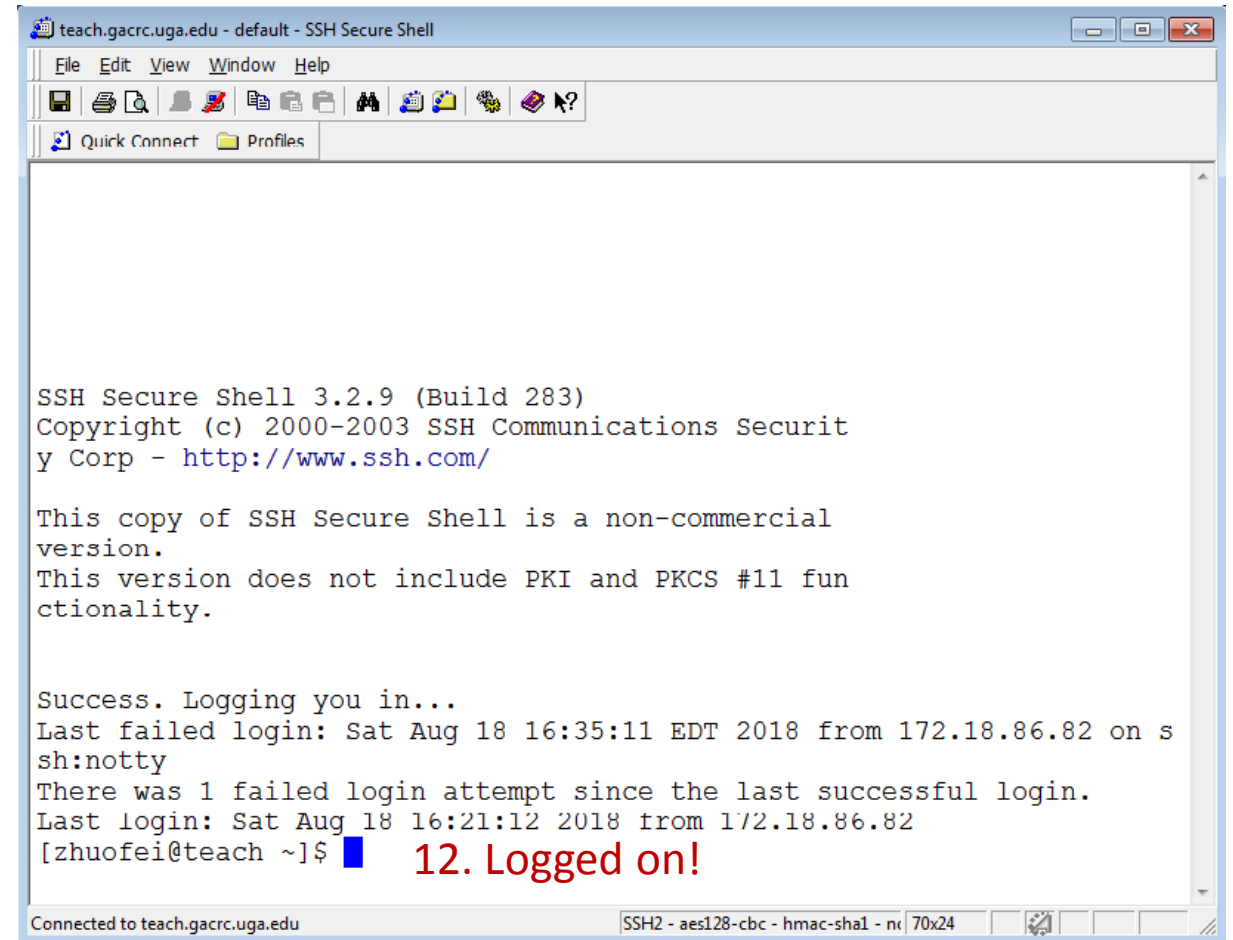
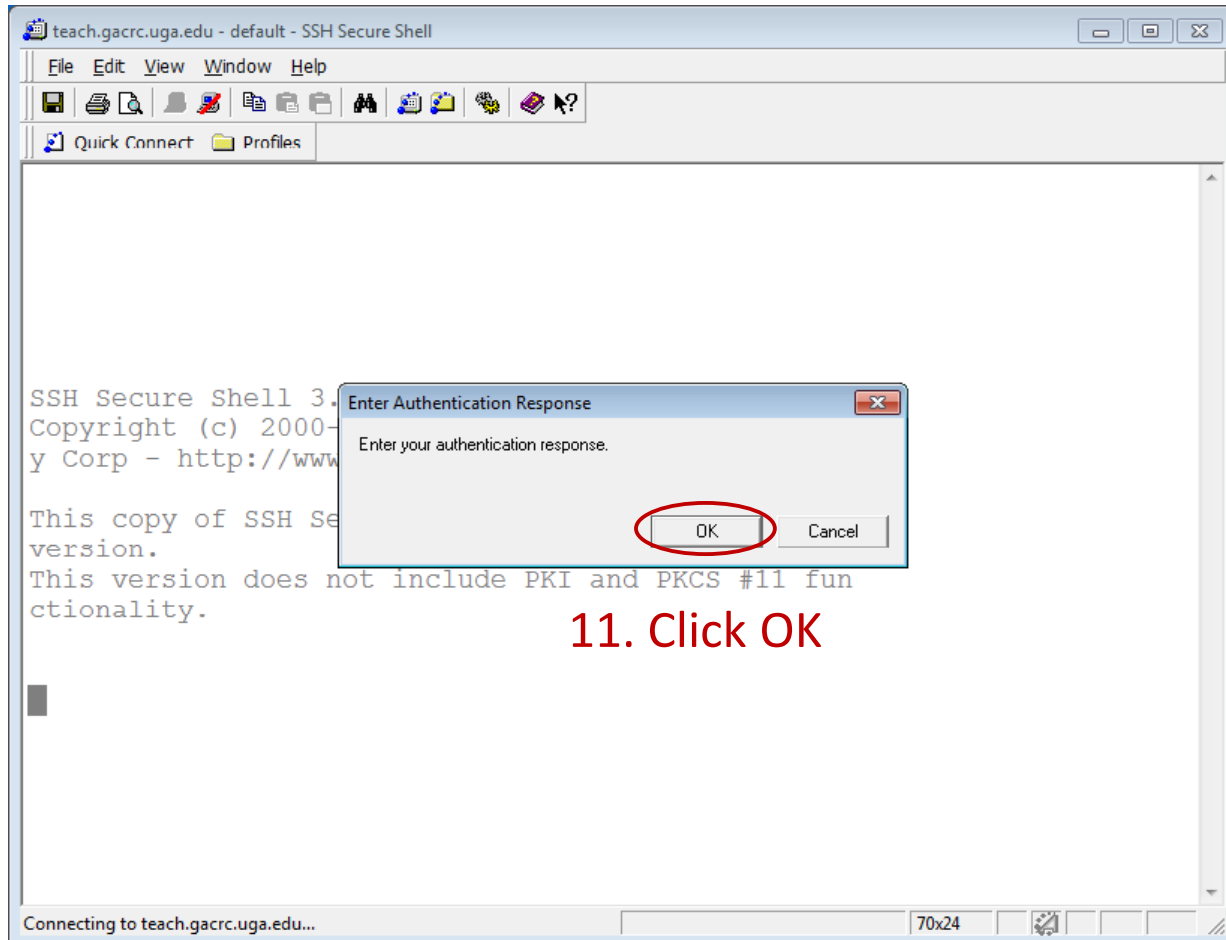


9. Enter "push" and click OK



10. Verify login using Duo

# Step1 (Cont.) - Windows using SSH Secure Utilities



## 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

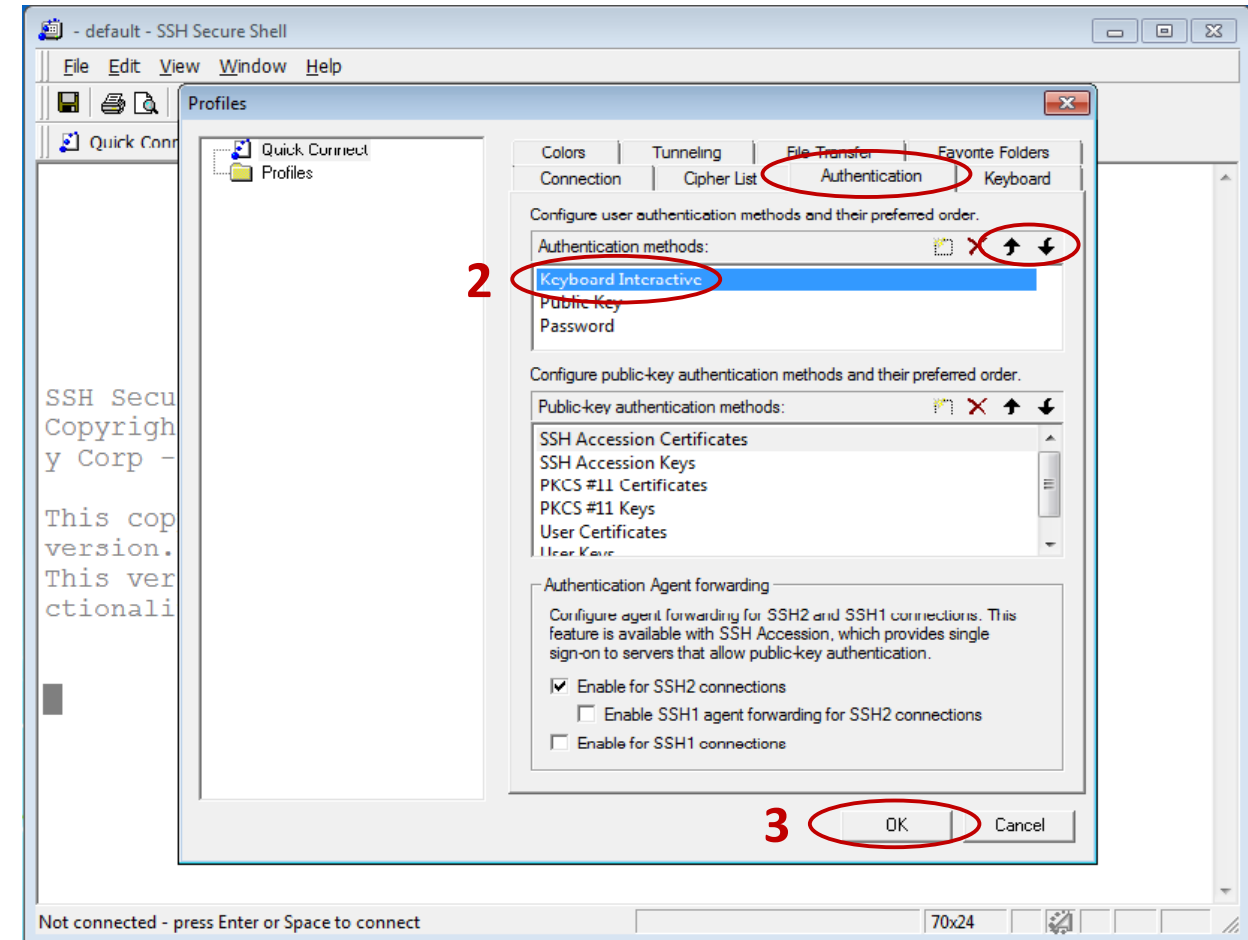
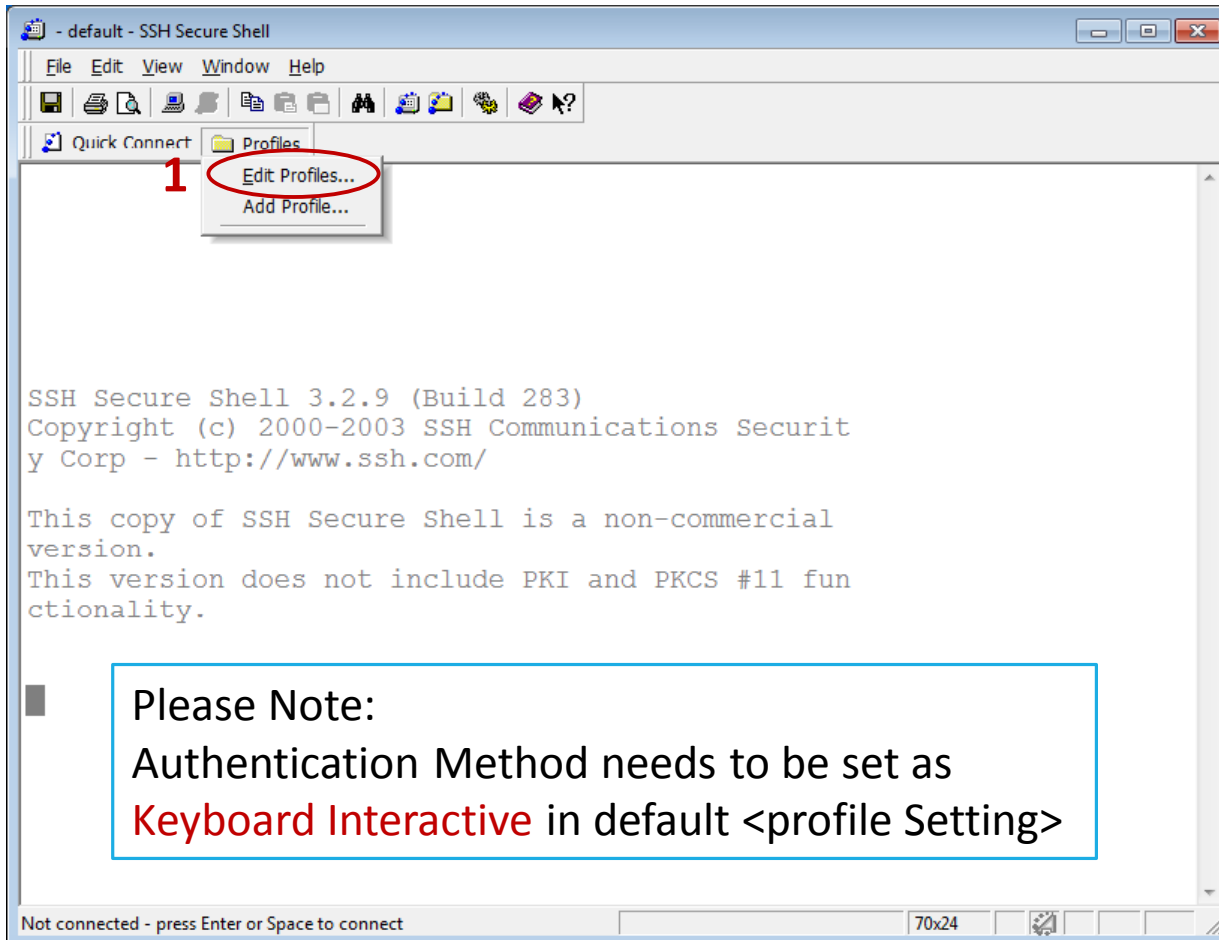
```
scp zhuofei@txfer.gacrc.uga.edu:/home/zhuofei/workDir/file .
```

```
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](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



# Step4 (Cont.) - Windows using SSH Secure Utilities

SSH Secure Shell 3.0  
Copyright (c) 2000  
by Corp - http://www.ssh.com

This copy of SSH Secure Shell is a version.  
This version does not have all the functionality.

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

Not connected - press Enter or Space to connect

SSH Secure Shell 3.0  
Copyright (c) 2000  
by Corp - http://www.ssh.com

This copy of SSH Secure Shell is a version.  
This version does not have all the functionality.

Enter Authentication Response  
Enter your authentication response

Connecting to teach.gacrc.uga.edu...

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

txfer.gacrc.uga.edu - default - SSH Secure Shell

File Edit View Window Help

Quick Connect Profiles

**13. Click yellow button**

```
SSH Secure Shell 3.2.9 (Build 283)
Copyright (c) 2000-2003 SSH Communications Security Corp - http://www.ssh.com/

This copy of SSH Secure Shell is a non-commercial version.
This version does not include PKI and PKCS #11 functionality.

Success. Logging you in...
Last failed login: Sun Aug 19 16:19:49 EDT 2018 from 172.18.86.77 on ssh:notty
There were 3 failed login attempts since the last successful login.
Last login: Thu Jul 26 11:24:24 2018 from 172.17.128.47
[zhuofei@txfer ~]$
```

Connected to txfer.gacrc.uga.edu

2:txfer.gacrc.uga.edu - default - SSH Secure File Transfer

File Edit View Operation Window Help

Quick Connect Profiles

Local Name Size Type Modified Remote Name Size Type Modified

Local Name	Size	Type	Modified	Remote Name	Size	Type	Modified
Libraries		System F...		notification		Folder	08/17/2018
zhuofeihou		System F...	07/26/2018	scripts		Folder	08/08/2018
Computer		System F...		slurm-account		Folder	08/17/2018
Network		System F...		templates		Folder	08/09/2018
Control Panel		System F...		workDir		Folder	08/16/2018
Recycle Bin		System F...		workDir_template		Folder	08/09/2018
Control Panel		System F...					
Cygwin64 Terminal	593	Shortcut	09/22/2018				
SSH Secure File Transfer C...	2,290	Shortcut	09/22/2018				
SSH Secure Shell Client	1,332	Shortcut	09/22/2018				
onClass_FYOS1001_2016Fa...		File folder	11/02/2018				
Capture	35,236	PNG ima...	08/10/2018				
Capture_1	39,843	PNG ima...	03/02/2018				
Capture_2	38,244	PNG ima...	03/02/2018				
Capture_3	48,306	PNG ima...	03/02/2018				
CCleaner	866	Shortcut	03/02/2018				
Computer - Shortcut	355	Shortcut	09/22/2018				
FileZilla	1,010	Shortcut	03/02/2018				
Visio 2013	2,847	Shortcut	09/22/2018				
Xming	1,035	Shortcut	09/22/2018				

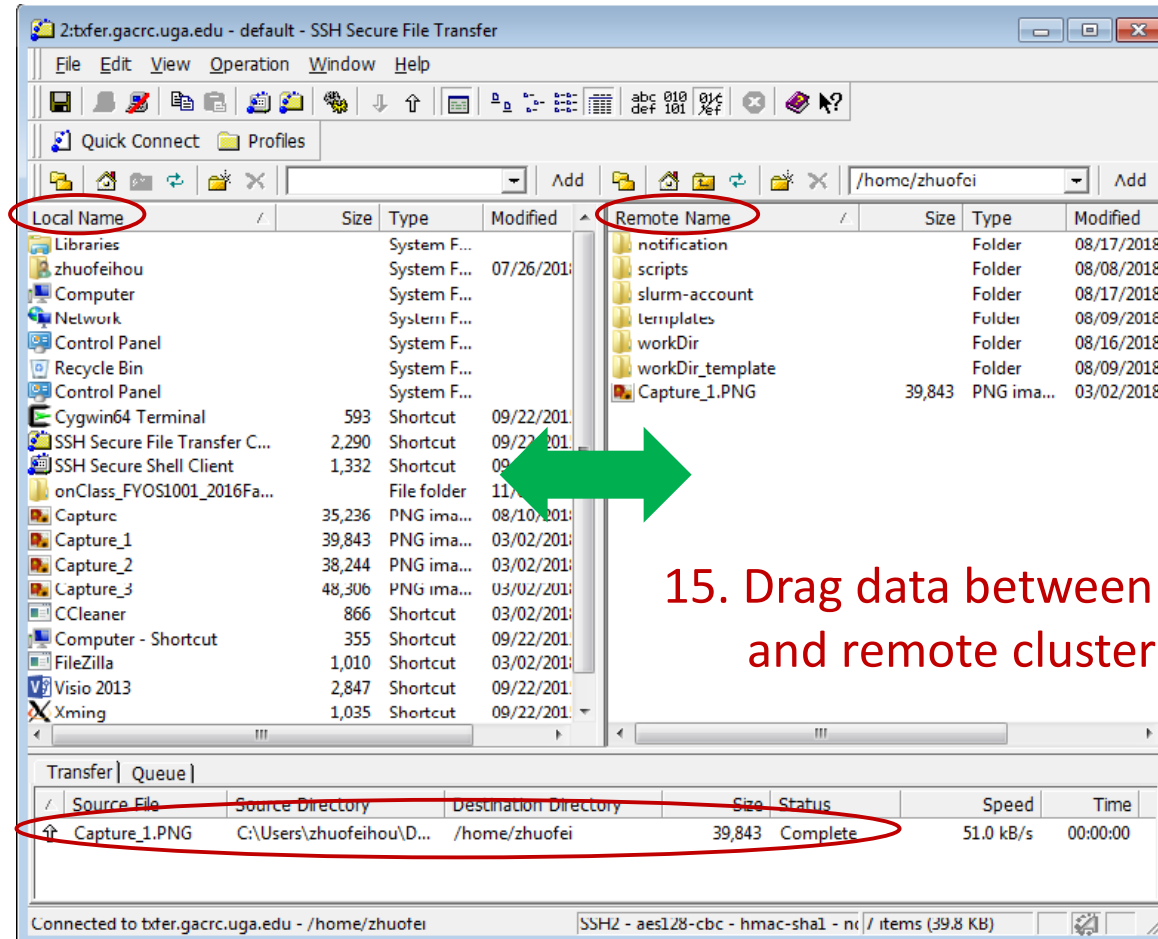
Transfer Queue

Source File	Source Directory	Destination Directory	Size	Status	Speed	Time

Connected to txfer.gacrc.uga.edu - /home/zhuofei

**14. Change local and remote paths**

# Step4 (Cont.) - Windows using SSH Secure Utilities



15. Drag data between local computer and remote cluster

## 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



```
zhuofei@n124:/lustre1/zhuofei/workDir
GNU nano 2.0.9 File: sub.sh Modified
hello nano! I am Zhuofei!
^G Get Help      ^O WriteOut      ^R Read File     [ New File ]
^X Exit          ^J Justify       ^W Where Is     ^Y Prev Page
^_               ^K Cut Text      ^U UnCut Text   ^V Next Page
^C Cur Pos      ^T To Spell
```

## 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](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>

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Running Jobs: [https://wiki.gacrc.uga.edu/wiki/Running\\_Jobs\\_on\\_the\\_teaching\\_cluster](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](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](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](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!



## Request Support

\* indicates Required fields.

**Your Name \***

**MyID \***

**E-mail \***

**Phone Number**

**Brief Description**

**Request Details \***

**Cluster**  sapelo2  sapelo  teach  other

- \* 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!