

High Performance Research Computing

A Resource for Research and Discovery



TEXAS A&M
UNIVERSITY.

Introduction to Data Literacy and Data Management



DIVISION OF RESEARCH
TEXAS A & M UNIVERSITY



Texas A&M University

High Performance Research Computing – <https://hprc.tamu.edu>

Contact the HPRC Helpdesk

Website: hprc.tamu.edu

Email: help@hprc.tamu.edu

Telephone: (979) 845-0219

Visit us in person: Henderson Hall, Room 114A

Help us, help you -- we need more info

- Which Cluster
- UserID/NetID
- Job id(s) if any
- Location of your jobfile, input/output files
- Application used if any
- Module(s) loaded if any
- Error messages
- Steps you have taken, so we can reproduce the problem

Logging in to the system

- SSH (secure shell)
 - The only program allowed for remote access; encrypted communication; freely available for Linux/Unix and Mac OS X hosts;
- For Microsoft Windows PCs, use *MobaXterm*
 - <https://hprc.tamu.edu/wiki/HPRC:MobaXterm>
 - You are able to view images and use GUI applications with MobaXterm
 - or *PuTTY*
 - https://hprc.tamu.edu/wiki/HPRC:Access#Using_PuTTY
 - You can not view images or use GUI applications with PuTTY

Your Login Password

- Both state of Texas law and TAMU regulations prohibit the sharing and/or illegal use of computer passwords and accounts
- Don't write down passwords
- Don't choose easy to guess/crack passwords
- Change passwords frequently

Course Topics

1. Data on our Clusters
2. Good data practices
3. Data management tools (command line)
4. Data management tools (GUI clients)

Using SSH - MobaXterm (on Windows)

The screenshot shows the MobaXterm interface. On the left is a file explorer showing the local file system. The main terminal window displays the following text:

```
whomps@login5:~
Terminal Sessions View X server Tools Games Settings Macros Help
Session Servers Tools Games Sessions View Split MultiExec Tunneling Settings Help X server Exit
Quick connect...
/general/home/whomps/
Name Size (KB) Last
..
.aienv_fea2.015.0_cache 4 2015
.aienv_fea2.017.1_cache 4 2016
.Altair 4 2015
.altair 4 2015
.altair_licensing 4 2015
.ansys 4 2016
.cache 4 2016
.config 4 2016
.dbus 4 2015
.fontconfig 4 2017
.gconf 4 2017
.gconfd 4 2017
.gnome2 4 2016
.gnome2_private 4 2015
.gvfs 4 2015
.intel 4 2015
.ipython 4 2016
.java 4 2015
.lmod.d 4 2016
.local 4 2015
.lsbatch 4 2017
.matlab 4 2016
.mozilla 4 2015
.mw 4 2016
Follow terminal folder
UNREGISTERED VERSION - Please support MobaXterm by subscribing to the professional edition here: http://mobaxterm.mobatek.net
```

```
=====
Texas A&M University High Performance Research Computing
Website: http://hprc.tamu.edu
Consulting: help@hprc.tamu.edu or (979) 845-0219
Ada Documentation: https://hprc.tamu.edu/wiki/index.php/Ada
=====
*****
== IMPORTANT POLICY INFORMATION ==
* -Unauthorized use of HPRC resources is prohibited and subject to
* criminal prosecution.
* -Use of HPRC resources in violation of United States export control laws
* and regulations is prohibited. Current HPRC staff members are US
* US citizens and legal residents.
* -Sharing HPRC account and password information is in violation of State
* Law. Any shared accounts will be DISABLED.
* -Authorized users must also adhere to all policies at:
* https://hprc.tamu.edu/wiki/index.php/HPRC:Policies
*****
!! WARNING: There are NO active backups of user data. !!

Please restrict usage to 8 CORES across ALL Ada login nodes.
Users found in violation of this policy will be SUSPENDED.

**** Ada Scheduled Maintenance Completed ****
The maintenance for Ada has been completed. Batch job scheduling has resumed.

Your current disk quotas are:
Disk Disk Usage Limit File Usage Limit
/home 117.2M 10G 1419 10000
/scratch 6.804G 1T 303 250000
/tiered 0 10T 1 50000
Type 'showquota' to view these quotas again.
[whomps@ada5 ~]$
```

message
of the day

your
quotas



Using SSH (on a Linux/Unix Client)

<https://hprc.tamu.edu/wiki/Ada:Access>

```
ssh user_NetID@ada.tamu.edu
```

You may see something like the following the first time you connect to the remote machine from your local machine:

```
Host key not found from the list of known hosts.  
Are you sure you want to continue connecting (yes/no)?
```

Type yes, hit enter and you will then see the following:

```
Host 'ada.tamu.edu' added to the list of known hosts.  
user_NetID@ada.tamu.edu's password:
```

Data on Our Clusters: Ada

There are limits on data on our clusters → AKA quota
The limits are on *Disk Space & File Usage*

showquota

View your current quota with this command

Your current disk quotas are:

Disk	Disk Usage	Limit	File Usage	Limit
/home	416.1M	10G	4489	10000
/scratch	18.64G	1T	122616	250000
/tiered	0	10T	4	250000

Data on Our Clusters: Ada

Default Limits

/home	10G / 10,000 files
/scratch	1TB / 250,000
/tiered	10T / 250,000

Need more space?

Contact help@hprc.tamu.edu

Data on Our Clusters: Ada

What's the difference between these filesystems?

/home

backed up nightly
will not be expanded

/scratch

'high performance storage'
can be expanded
not backed up

/tiered

archival file system
can be expanded
not backed up

Need more space?

Contact help@hprc.tamu.edu

Data on Our Clusters: Ada's Fast Transfer Nodes

Ada has 2 nodes dedicated to fast file transfers:

ada-ftn1@ada.tamu.edu

ada-ftn2@ada.tamu.edu

Access the node via ssh:

```
ssh netID@ada-ftn1@ada.tamu.edu
```

Both nodes have 40 gigabit capability

No programming environment installed → these are for transfers only!

These nodes have access to all of Ada's filesystem

/home

/scratch

/tiered

Data on Our Clusters: Terra

There are limits on data on our clusters → AKA quota
The limits are on *Disk Space & File Usage*

showquota

View your current quota with this command

Your current disk quotas are:

Disk	Disk Usage	Limit	File Usage	Limit
/home	416.1M	10G	4489	10000
/scratch	18.64G	1T	122616	250000

Data on Our Clusters: Terra

Default Limits

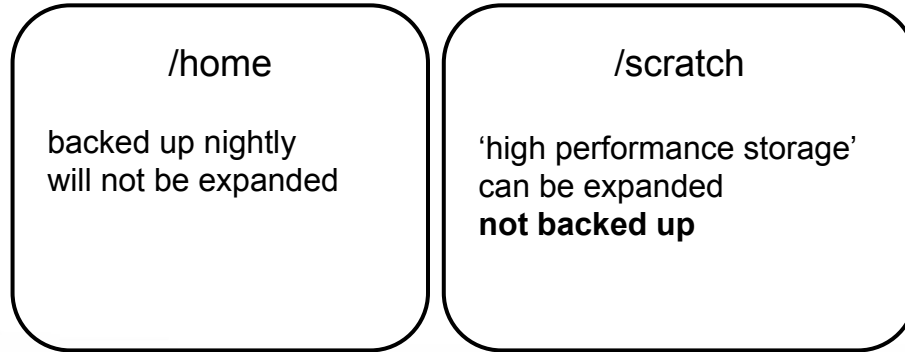
/home	10G / 10,000 files
/scratch	1TB / 250,000

Need more space?

Contact help@hprc.tamu.edu

Data on Our Clusters: Terra

What's the difference between these filesystems?



Need more space?

Contact help@hprc.tamu.edu

Good Data Practices

Rule of thumb:

1 is none

2 is one



Keep multiple copies of important data!

Having just one copy is not enough

Backup Backup Backup

Command Line Tools

1. `cp` -- copy
2. `rm` -- remove
3. `scp` -- secure copy (remote copy)
4. `sftp` -- secure file transfer
5. `tar` -- archiving

Command Line Tools: cp

Copy

Makes a copy of a file

```
cp source_file new_fileName
```

Easy solution for copying a file onto the *same machine*

How about moving data between machines?

Command Line Tools: rm

Remove

Deletes a file

```
rm some_file
```

Completely deletes a file

There is no "trash bin" on the command line
add the -i flag to be prompted prior to file deletion

```
rm -i some_file
```

Command Line Tools: scp

Secure copy

Copies files between hosts on a network -- uses ssh for data transfer (hence "Secure")

```
scp source_file netId@ada.tamu.edu:/home/netID
```

Can be used to copy:

- from local to remote
- from remote to local
- between 2 remote systems from local system

Command Line Tools: sftp

Secure file transfer program

interactive file transfer program -- uses ssh (again so hence “secure”)

```
sftp netID@ada.tamu.edu
```

Connects and logs into specified host, enters command mode

- cd - change directory
- get - download file
- put - upload file
- bye - quit sftp

Command Line Tools: tar

Archiving files

saves many files together into a single file (archive)

```
tar -cvf archive.tar source
```

create a compressed archive

```
tar -czvf archive.tar.gz source
```

extract an archive

```
tar -xvf archive.tar
```

Useful for consolidating (and compressing) files prior to transfer

Important flags

-cf	create archive
-xf	extract archive
-v	verbose
-z	compress with gzip

GUI Clients

There are many GUI solutions for file transfer:

1. MobaXterm
2. WinSCP
3. FileZilla

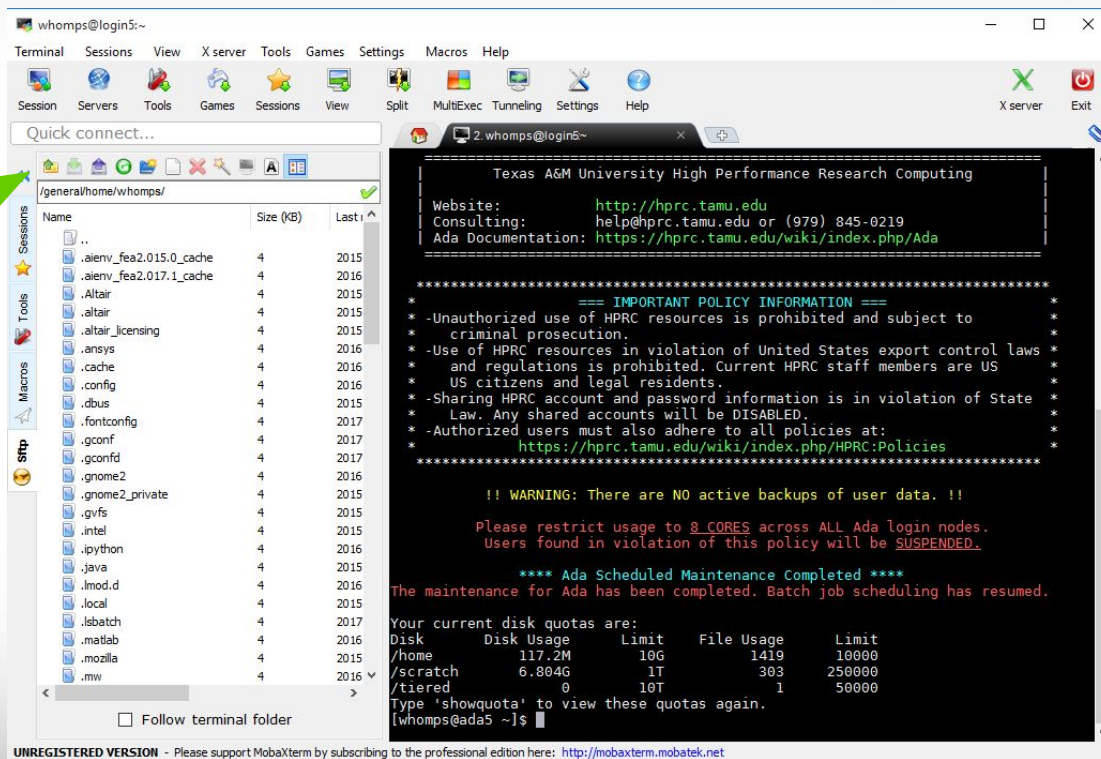
Globus

GUI Clients: MobaxTerm

Available on Windows machines

SFTP side panel in
MobaxTerm

Can download, upload
files with a few clicks
from the CLI



UNREGISTERED VERSION - Please support MobaXterm by subscribing to the professional edition here: <http://mobaxterm.mobatek.net>

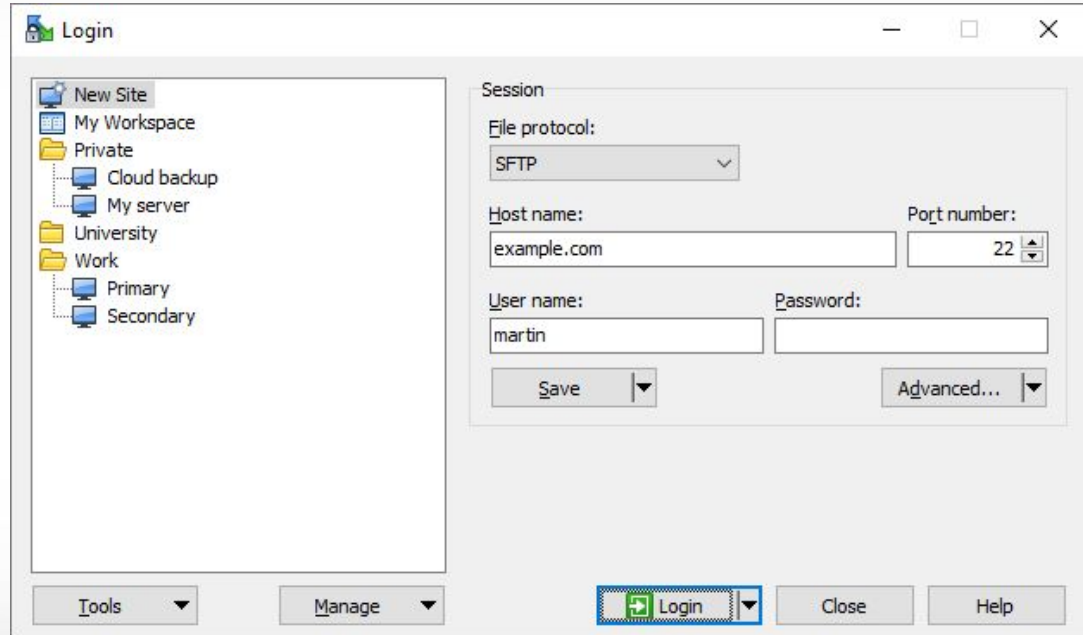


GUI Clients: WinSCP

Available on Windows machines

Connects to host directly with SFTP

Allows for transfers through the GUI

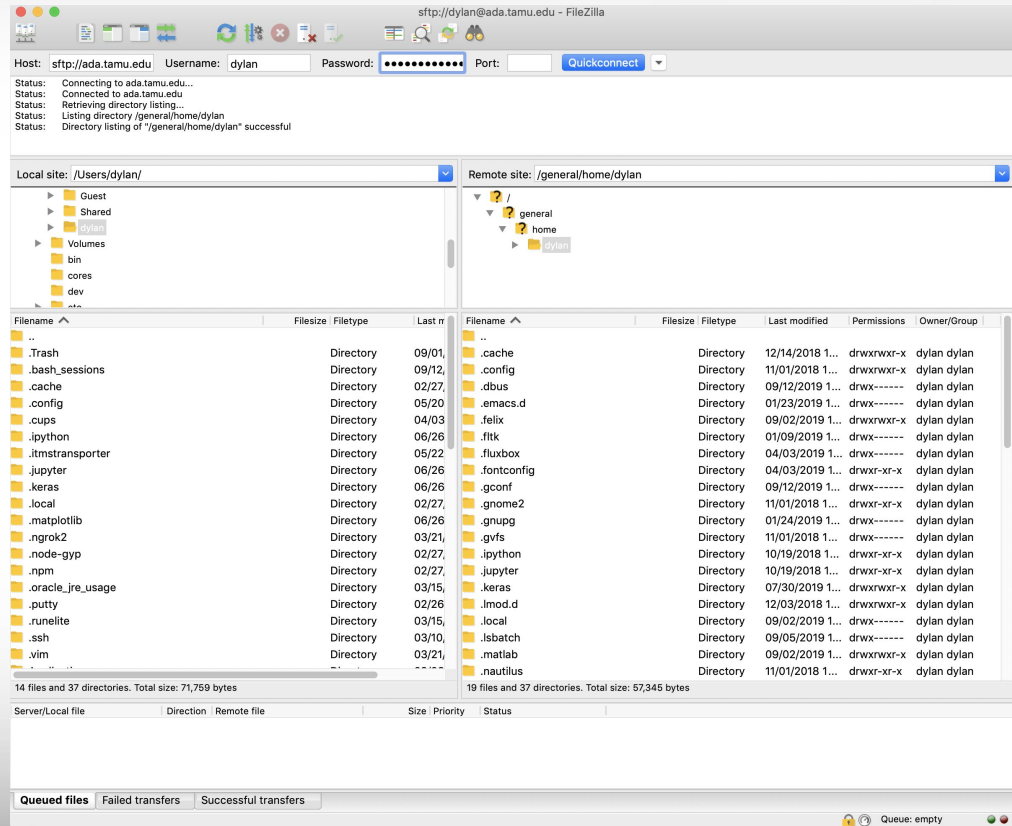


GUI Clients: FileZilla

Open source, available on all platforms

Connects to host directly with SFTP

Allows for transfers through the GUI



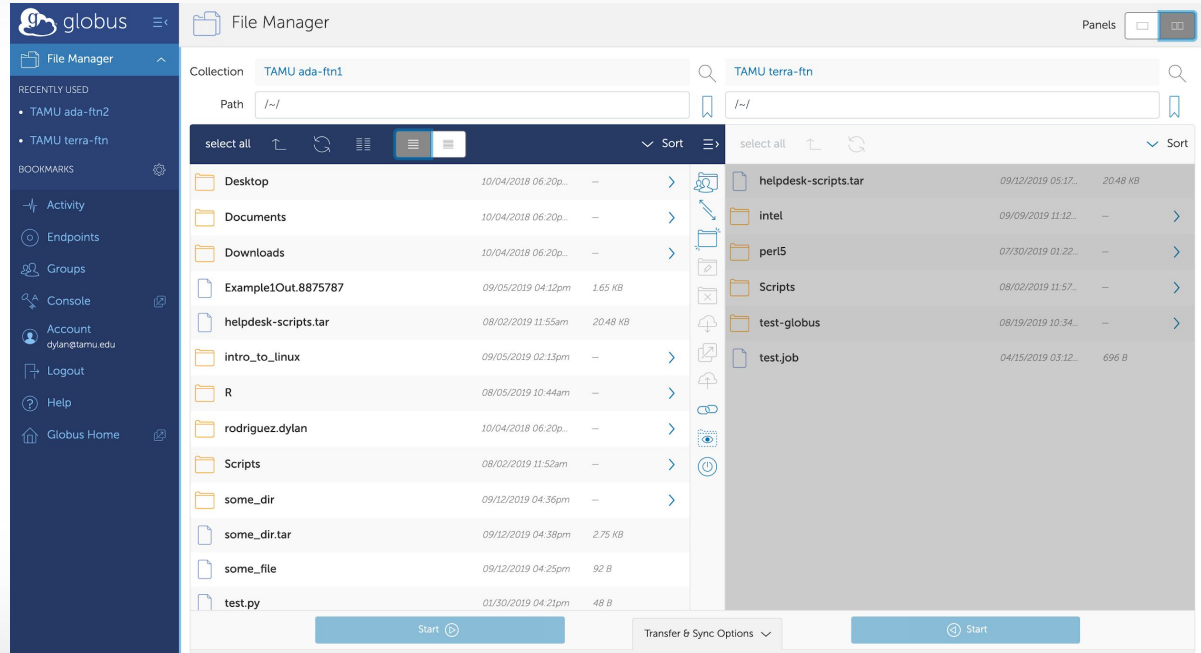
GUI Clients: Globus

Web based, with application you can download

Ada endpoints:
ada-ftn1
ada-ftn2

Terra endpoint
terra-ftn

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



Questions?