High Performance Research Computing A Resource for Research and Discovery



Introduction to Data Literacy and Data Management





TEXAS ABM UNIVERSITY School of Innovation

EARN POINTS FOR TODAY'S EVENT!

Use the **MaroonBase Student App** to earn points for attending events and using resources listed in the app. Earn points, win prizes!

Monthly drawings – 3 students win \$500 each Semester grand prizes - top 3 students earn up to \$2,000

Instructions to get started at maroonbase.tamu.edu

INNOVATION CREATIVITY LEADERSHIP ENTREPRENEURSHIP

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

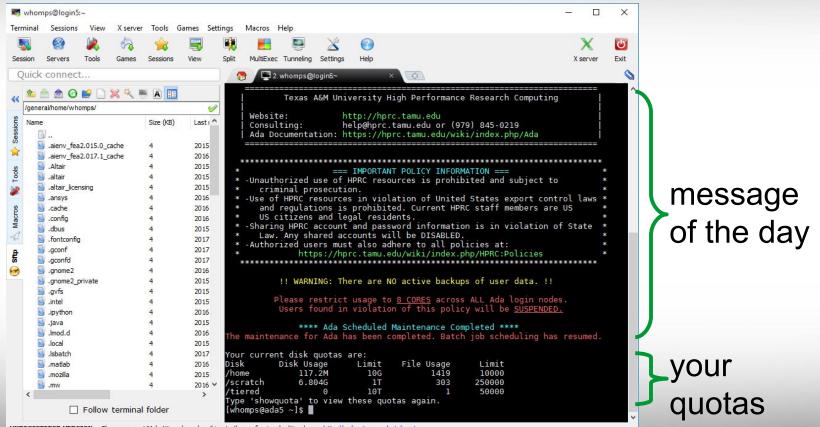
Your Login Password

- 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)



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

Texas A&M University

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

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 \rightarrow AKA quota The limits are on *Disk Space* & *File Usage*

show	wquota	View you	ur current quota w	ith this command	
Your curre Disk /home /scratch /tiered	ent disk quotas a Disk Usage 416.1M 18.64G 0	re: Limit 10G 1T 10T	File Usage 4489 122616 4	Limit 10000 250000 250000	

Data on Our Clusters: Ada

Default Limits

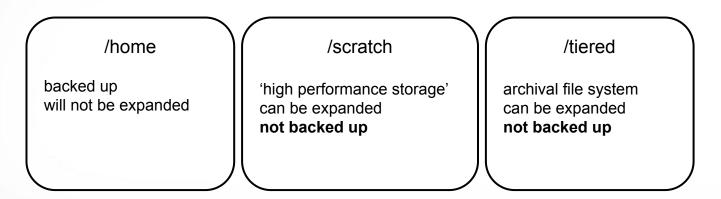
/home	10G / 10,000 files
/scratch	1T / 250,000
/tiered	10T / 250,000

Need more space? Contact help@hprc.tamu.edu

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Data on Our Clusters: Ada

What's the difference between these filesystems?



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 \rightarrow AKA quota The limits are on *Disk Space* & *File Usage*

sho	wquota	View you	ur current quota w	vith this command	
Your curre	ent disk quotas a	re:			
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

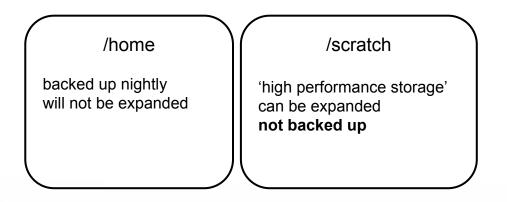
nome	10G / 10,000 files
scratch	1TB / 250,000

Need more space? Contact help@hprc.tamu.edu

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Data on Our Clusters: Terra

What's the difference between these filesystems?



Need more space? Contact help@hprc.tamu.edu

Good Data Practice

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

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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

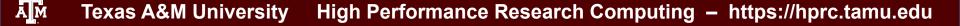
Deletes a file

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
- 4. Cyberduck

Globus Connect







GUI Clients: MobaxTerm

whomps@login5:~ X Available on Windows machines Terminal Sessions View X server Tools Games Settings Macros Help Ċ 2 X Solit MultiExec Tunneling Settings Help Exit Session Servers Tools Games Sessions View X server Ouick connect... / 📮 2. whomps@login5:~ 0 🚖 🖸 💕 🗋 💥 🥄 💻 🗛 🛅 Texas A&M University High Performance Research Computing /general/home/whomps/ s/ Website: http://hprc.tamu.edu Size (KB) Last 1 ^ Name Consulting: help@hprc.tamu.edu or (979) 845-0219 Ada Documentation: https://hprc.tamu.edu/wiki/index.php/Ada aienv fea2.015.0 cache 2015 SFTP side panel in aieny fea2.017.1 cache 2016 Altair 2015 === IMPORTANT POLICY INFORMATION === MobaxTerm .altair 2015 * -Unauthorized use of HPRC resources is prohibited and subject to .altair_licensing 2015 criminal prosecution. * -Use of HPRC resources in violation of United States export control laws 2016 .ansys and regulations is prohibited. Current HPRC staff members are US .cache 2016 US citizens and legal residents. .config 2016 * -Sharing HPRC account and password information is in violation of State .dbus 2015 Law. Any shared accounts will be DISABLED. 2017 .fontconfig * -Authorized users must also adhere to all policies at: Can download, upload 2017 .aconf /wiki/index.php/HPRC:Policies 2017 .aconfd files with a few clicks .anome2 2016 .gnome2 private 2015 !! WARNING: There are NO active backups of user data. !! .gvfs 2015 from the CLI Please restrict usage to <u>8 CORES</u> across ALL Ada login nodes. .intel 2015 Users found in violation of this policy will be SUSPENDED. .ipython 2016 📓 .java 2015 **** Ada Scheduled Maintenance Completed **** Imod.d 2016 he maintenance for Ada has been completed. Batch job scheduling has resumed. Iocal 2015 Isbatch 2017 Your current disk quotas are: matlab 2016 Disk Disk Usage Limit File Usage Limit 117.2M 10G 1419 10000 /home .mozilla 2015 /scratch 6 804G 303 250000 2016 \ .mw 10T 50000 /tiered ype 'showquota' to view these quotas again. Follow terminal folder [whomps@ada5 ~]\$

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

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Yew Site My Workspace	Session Eile protocol:			
Private Cloud backup	SFTP V			
My server	Host name:	Port number:		
University	example.com	22 🚔		
	User name: Pas	sword:		
Secondary	martin			
	<u>S</u> ave ▼	A <u>d</u> vanced ▼		

GUI Clients: FileZilla

Open source - available on all platforms

2 Factor Authentication makes FileZilla hard to use

Connects to host directly with SFTP

Allows for transfers through the GUI

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Host: sftp://ada.tamu.ed		lan Password:	•••••	Port: Quickconn	ect		
Status: Connecting to ada. Status: Connected to ada. Status: Retrieving director Status: Listing directory /g Status: Directory listing of	amu.edu / listing	successful					
Local site: /Users/dylan/				Remote site: /general/home/d	ylan		
Guest Shared Shared Volumes bin cores dev			I	▼ 1? / ▼ 1? general ▼ 1? home ▶ the dylan			
Filename 🔨		Filesize Filetype	Last rr	Filename 🔨	Filesize Filetype	Last modified Permissions	Owner/Group
 Trash Jash_sessions .cache .config .cups .ipython itmstransporter jupyter .keras Jocal .matplotlib .ngrok2 .node-gyp .npm .oracle_jre_usage .putty .runelite .ssh .yim		Directory Directory	09/01, 09/12, 02/27, 05/20 04/03 06/26 06/26 06/26 06/26 02/27, 06/26 02/27, 06/26 02/27, 02/27, 02/27, 02/27, 02/27, 02/27, 02/27, 02/27, 02/27, 02/27, 02/26, 02/27, 02/26, 02/26, 02/26, 02/26, 02/26, 02/27, 02/26, 02/26, 02/26, 02/27, 02/26, 02/26, 02/27, 02/26, 02/26, 02/27, 02/26, 02/27, 02/		Directory Directory Directory Directory Directory Directory Directory Directory Directory Directory Directory Directory Directory Directory Directory Directory Directory Directory Directory Directory	04/03/2019 1 drwx 04/03/2019 1 drwxr-xr-x	dylan dylan dylan dylan
	tal size: 71,759 bytes			.nautilus 19 files and 37 directories. Total siz	Directory e: 57 345 bytes	11/01/2018 1 drwxr-xr-x	dylan dylan
	(a) 5120. 7 1,700 b) (05	e file	Size Priority				

GUI Clients: CyberDuck

Available on Windows & MacOS

2 Factor Authentication makes FileZilla hard to use

Connects to host directly with SFTP

Allows for transfers through the GUI

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Open Connection Quick Connect	dylan@ada.tamu.edu – SFTP ★ ↓ C 2 Action Refresh Edit	(Unregistered)
	🔲 /general/home/dylan	🗘 🔺 Q Search
Filename	∧ Size	Modified
Р 🔜 Desklop		10/4/10, 0.20 111
Documents		10/4/18, 6:20 PM
dos_script.sh	36 B	11/5/19, 11:54 AM
🕨 🚞 Downloads		10/4/18, 6:20 PM
Example1Out.8875787	1.7 KB	9/5/19, 4:12 PM
helpdesk-scripts.tar	20.5 КВ	8/2/19, 11:55 AM
intro_to_linux		9/5/19, 2:13 PM
matlab_crash_dump.12621-1	3.8 KB	9/19/19, 5:40 PM
matlab_crash_dump.12621-2	0 B	9/19/19, 5:40 PM
🕨 🚞 PA2		1/22/20, 11:55 AM
▶ 💼 R.		8/5/19, 10:44 AM
🕨 🚞 rodriguez.dylan		10/4/18, 6:20 PM
▶ 💼 sasuser.v94		9/23/19, 9:32 AM
Scripts		1/6/20, 2:36 PM
▶ 🚞 some_dir		9/12/19, 4:36 PM
some_dir.tar.gz	2.8 KB	9/13/19, 2:17 PM
some_file	92 B	9/12/19, 4:25 PM
star-job.lsf	341 B	10/1/19, 2:30 PM
7 test.py	48 B	1/30/19, 4:21 PM
testJob.lsf	663 B	9/5/19, 4:19 PM
20 Files		<u> </u>

GUI Clients: Globus

Web based, with application you can download

Ada endpoints: ada-ftn1 ada-ftn2

Terra endpoint terra-ftn

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https://www.globus.org/

🞐 globus	≡∙	🗂 File Manager						P	anels	
File Manager		Collection TAMU ada-ftn1				Q	TAMU terra-ftn			Q
		Path /~/					/~/			
		select all 🔶 🙄 🏢			🗸 Sort	≡,	select all 👔 🕄			🗸 Sort
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✓ dylan@tamu.edu ☐→ Logout		intro_to_linux	09/05/2019 02:13pm	-	>		test.job	04/15/2019 03:12	696 B	
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		rodriguez.dylan	10/04/2018 05:20p	-	>	ی ۱				
		Scripts	08/02/2019 11:52am	-	>	0				
		some_dir	09/12/2019 04:36pm	-	>					
		some_dir.tar	09/12/2019 04:38pm	2.75 KB						
		some_file	09/12/2019 04:25pm	92 B						
		test.py	01/30/2019 04:21pm	48 B						
			Start 🕞		Transfer &	Sync O	ptions 🗸	(d) Start		

Questions?