

▲▲▲

Data Management in the HPC

February 23-24, 2022

Derrick Zwickl

HPC Consultant, Research Computing –
zwickl@arizona.edu

Chris Reidy

Research Facilitation Manager, Research Computing –
chrisreidy@arizona.edu



What you will learn

What: understand how to transfer, organize, and use data on the HPC.

Why: Nice data makes things easier: collaboration, reproducibility => better research

Assume

- Basic understanding of how to use the Unix shell

How

- Overview of storage options on the HPC
- Methods of transferring data in and out
- Basic HPC data management /good enough practices
- Moving data around

Basic Pipeline

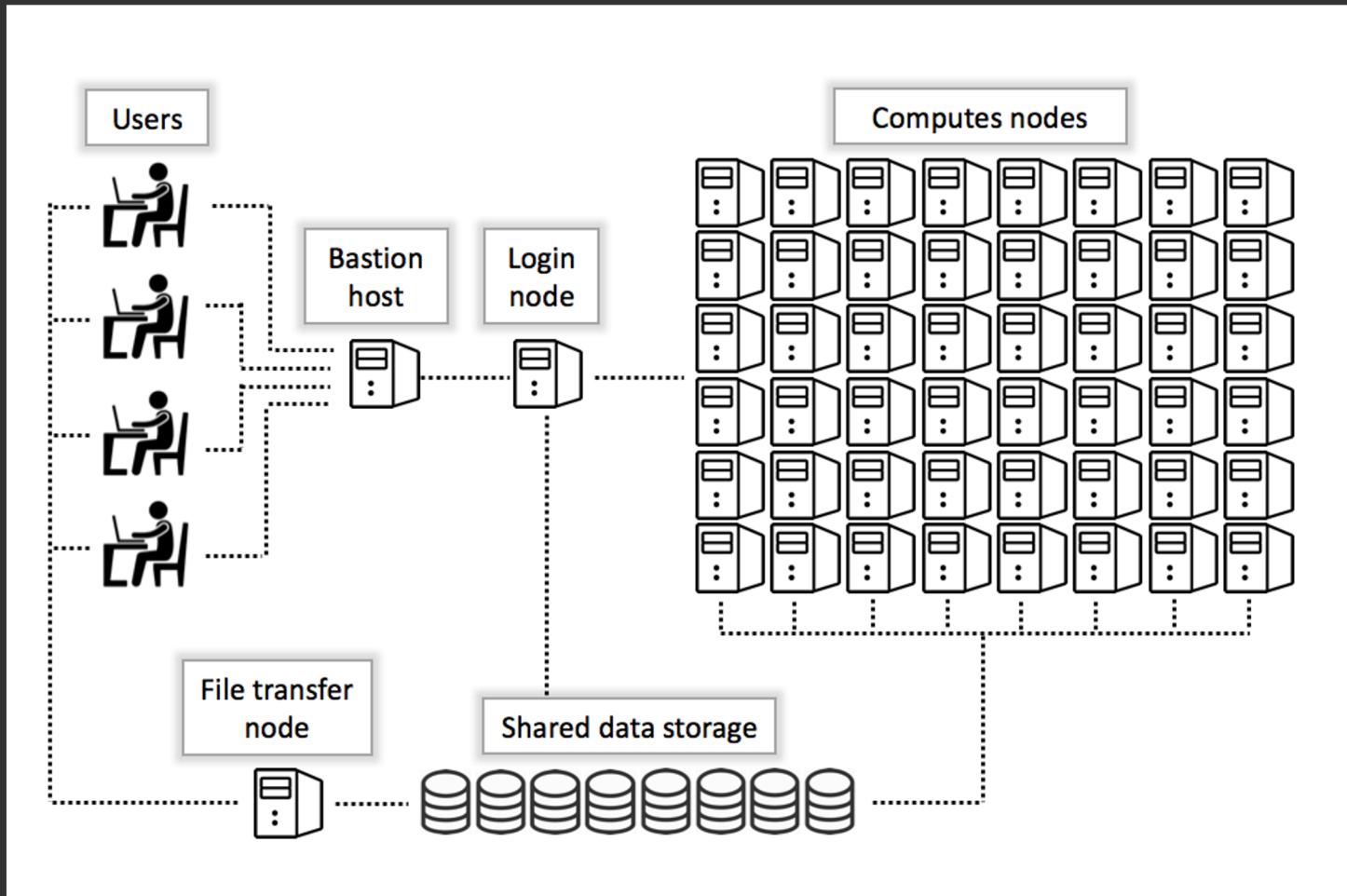
- Data input, processing, collaboration, sharing



◆ ◆ ◆

Logging in

The diagram of the UA HPC cluster



Login node is like an elevator

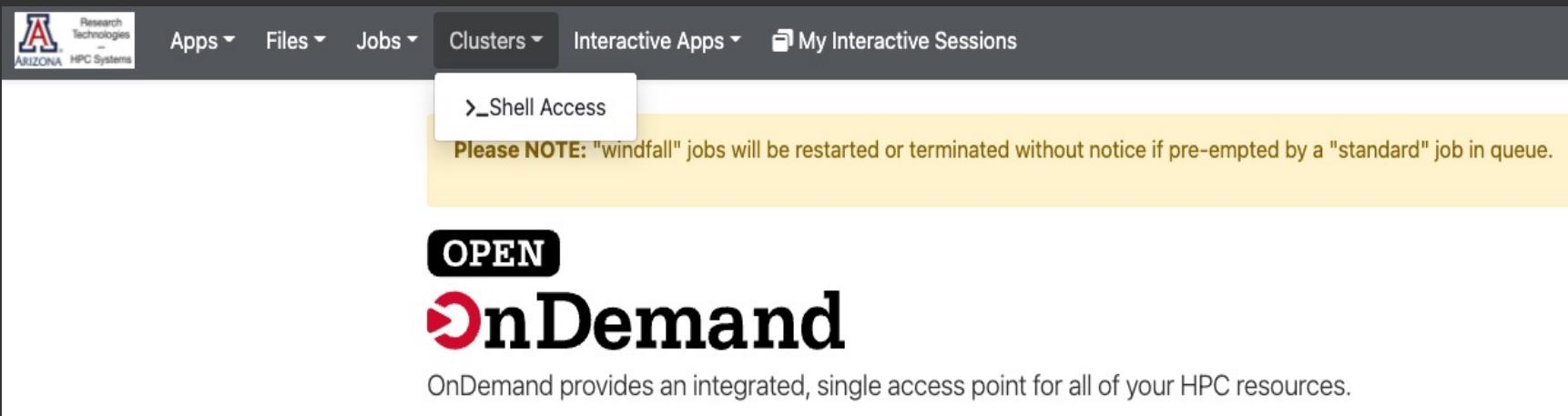


Login node is like an elevator



Cluster Login

- Open **ood.hpc.arizona.edu** in your web browser and login with your NetID and password.
- From the “Clusters” drop-down menu choose “shell access”



The screenshot shows the OnDemand web interface. At the top, there is a navigation bar with links for Apps, Files, Jobs, Clusters (which is currently selected and highlighted in blue), Interactive Apps, and My Interactive Sessions. A tooltip labeled '>_Shell Access' points to the Clusters menu item. Below the navigation bar, a yellow banner contains the text: "Please NOTE: 'windfall' jobs will be restarted or terminated without notice if pre-empted by a 'standard' job in queue." In the center, there is a large "OPEN" button with a red arrow icon and the text "OnDemand". Below this, a subtext states: "OnDemand provides an integrated, single access point for all of your HPC resources."

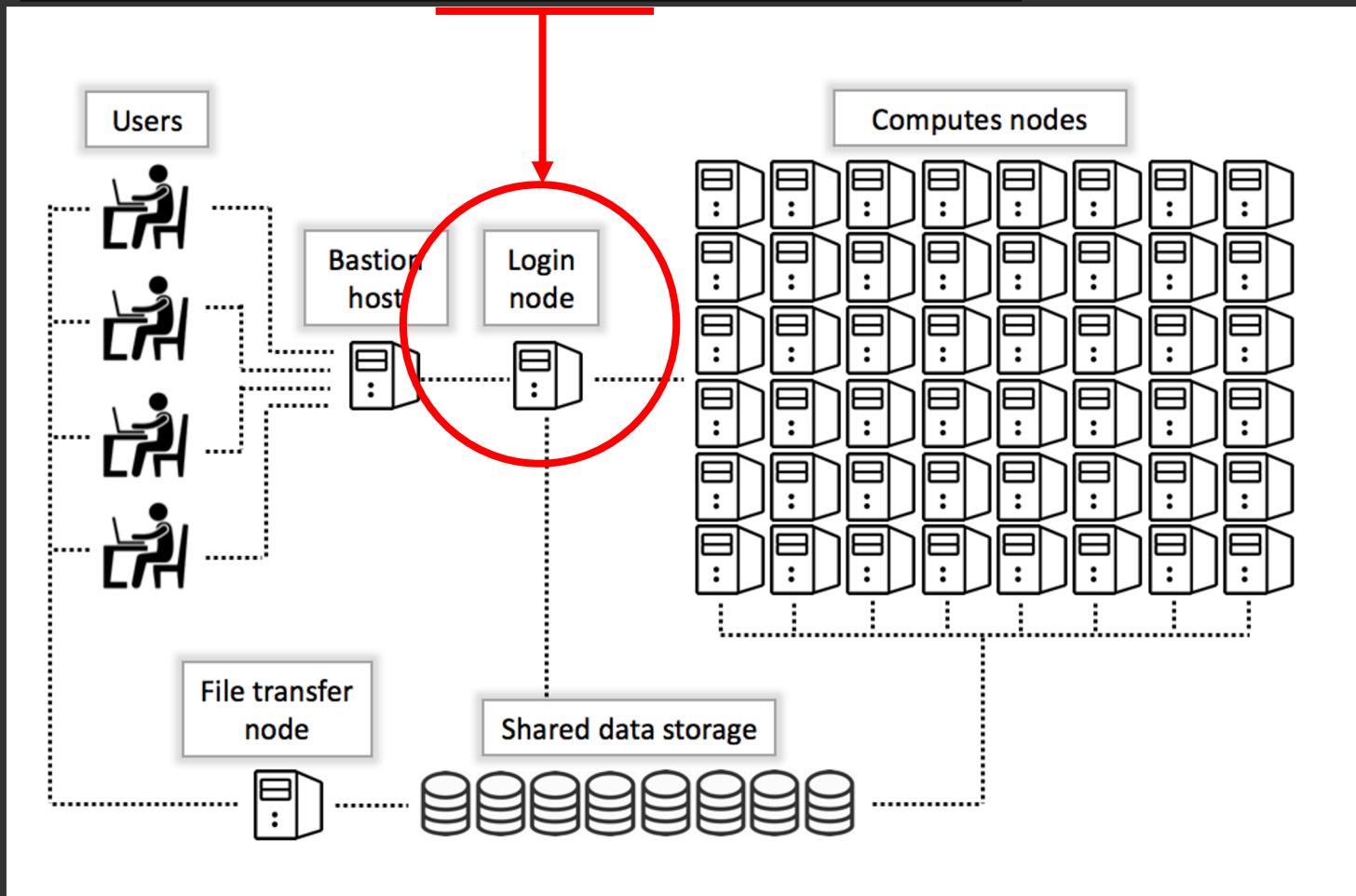
or use ssh from command line

```
~/ $ ssh zwickl@hpc.arizona.edu
Last login: Tue Feb 22 15:50:18 2022 from on-campus-10-138-68-75.vpn.arizona.edu
This is a bastion host used to access the rest of the RT/HPC environment.

Type "shell" to access the job submission hosts for all environments
-----
[zwickl@gatekeeper ~]$ shell
```

Login node

```
[dshyshlov@login2 ~]$
```

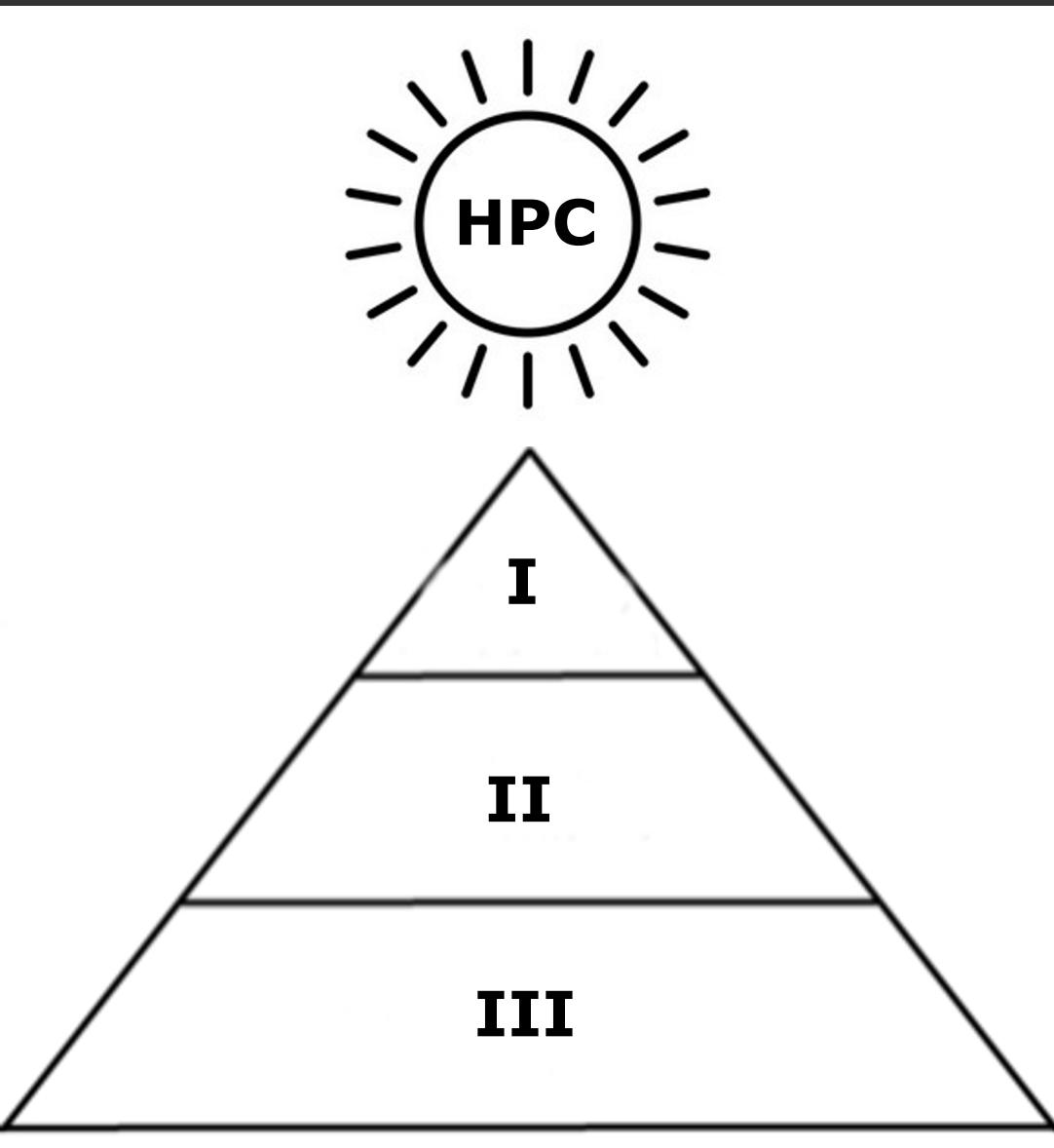


• • •

Data Storage Options



HPC Storage



- Tiered storage
- HPC storage:
Active data
- Google drive:
Non-active data
- Cloud storage:
Archived data

HPC Storage – Tier I

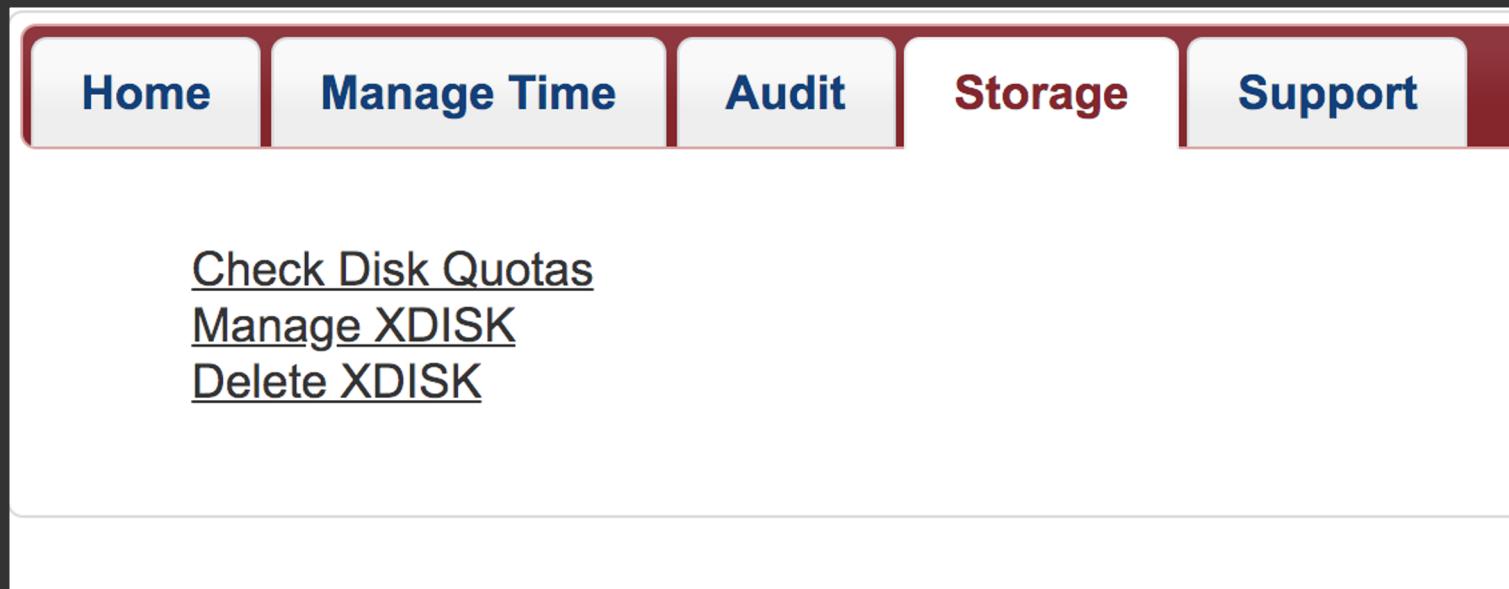
- Three storage options (all FREE):
- User level
 - /home
 - 50 GB
 - aka home directory or ~/
- Group (PI) level
 - /groups
 - 500 GB
 - /xdisk
 - temporary “scratch” storage
 - up to 20 TB for up to 150 days (plus another 150 day extension)
 - Requested and managed by PIs
- No rented storage

HPC Storage – Tier I



Monitoring storage

- portal.hpc.arizona.edu



Monitoring storage

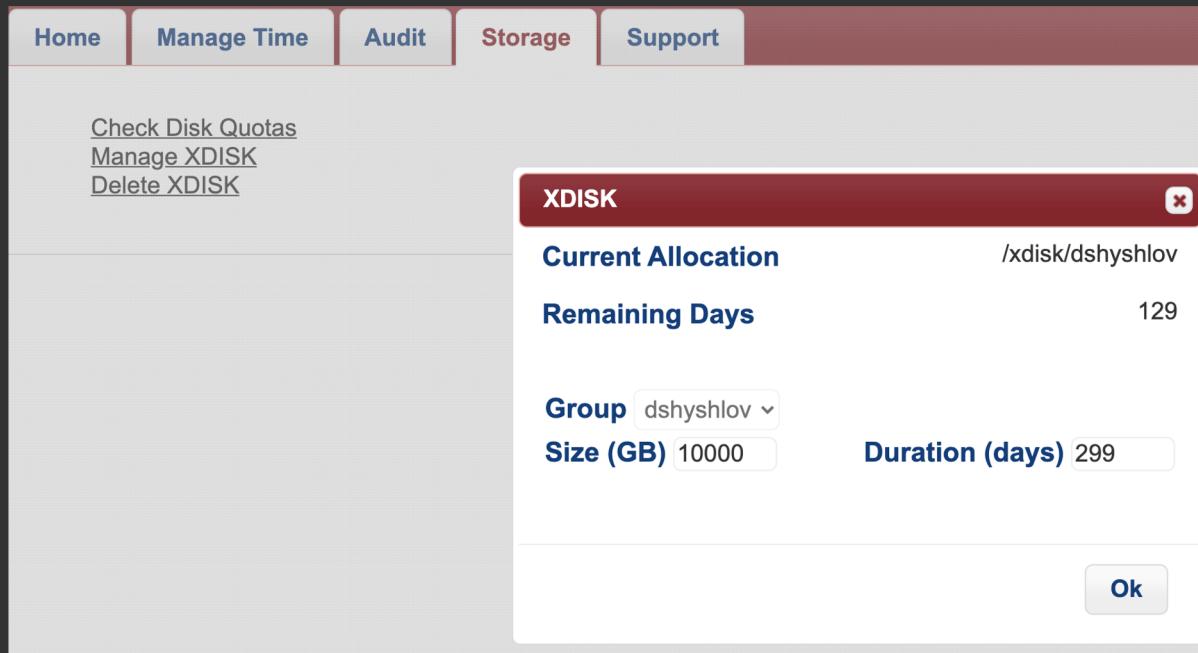
- command line - uquota

```
[dshyshlov@login3 ~]$ uquota
```

	used	soft limit	hard limit
/groups/dshyshlov	209.6G	500.0G	500.0G
/home	13.9G	50.0G	50.0G
/xdisk/dshyshlov	3.9G	9.8T	9.8T

Monitoring storage – xdisk

- Xdisk is temporary storage
- Max duration – 150 days
- One extension – another 150 days
- PI's can monitor and manage xdisk on the portal



Delegating xdisk permissions

- PI's can delegate permissions to manage xdisk.

The screenshot shows a user interface with a dark background and a white header bar. The header bar contains five buttons: "Home" (red), "Manage Time" (blue, currently selected), "Audit" (blue), "Storage" (blue), and "Support" (blue). Below the header, there is a list of links: "Access HPC Resources", "UA HPC Usage Metrics", "Batch Job Builder", "Manage Delegates", and "Switch User". A tooltip box is overlaid on the "Manage Delegates" link, containing the text: "Allow other users to manage your time and groups".

Home Manage Time Audit Storage Support

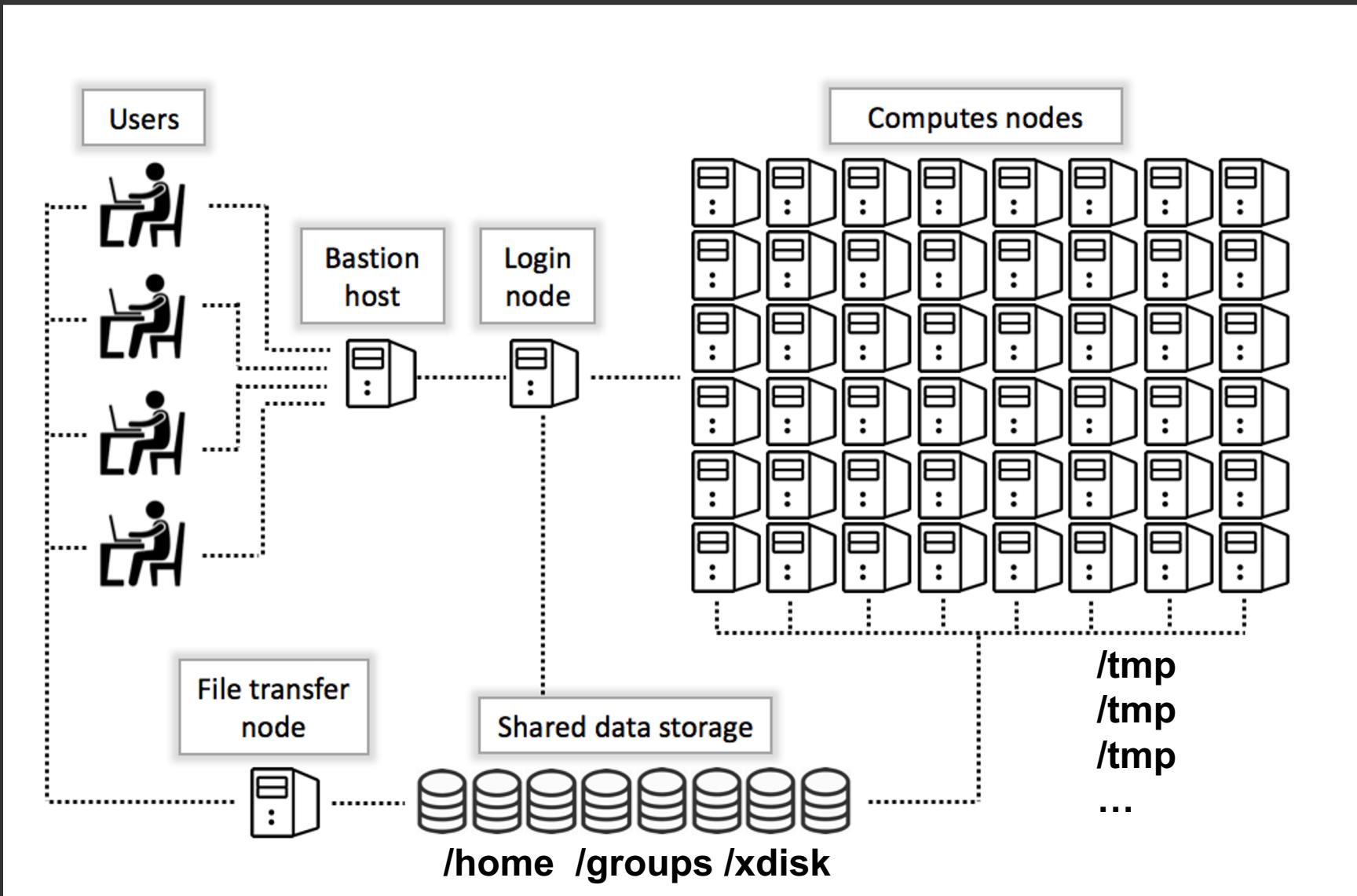
Access HPC Resources
UA HPC Usage Metrics
Batch Job Builder
Manage Delegates
Switch User

Allow other users to manage your time and groups

HPC Storage

- Compute node disk
 - /tmp
 - local disk on compute nodes
 - not connected to the main storage
 - the best performance for calculations
 - Ocelote – 800 GB is available on each node
 - Puma – 1.4 TB is available on each node
 - data is removed once the job is finished, so need to script copying input/output data to the main storage

HPC Storage

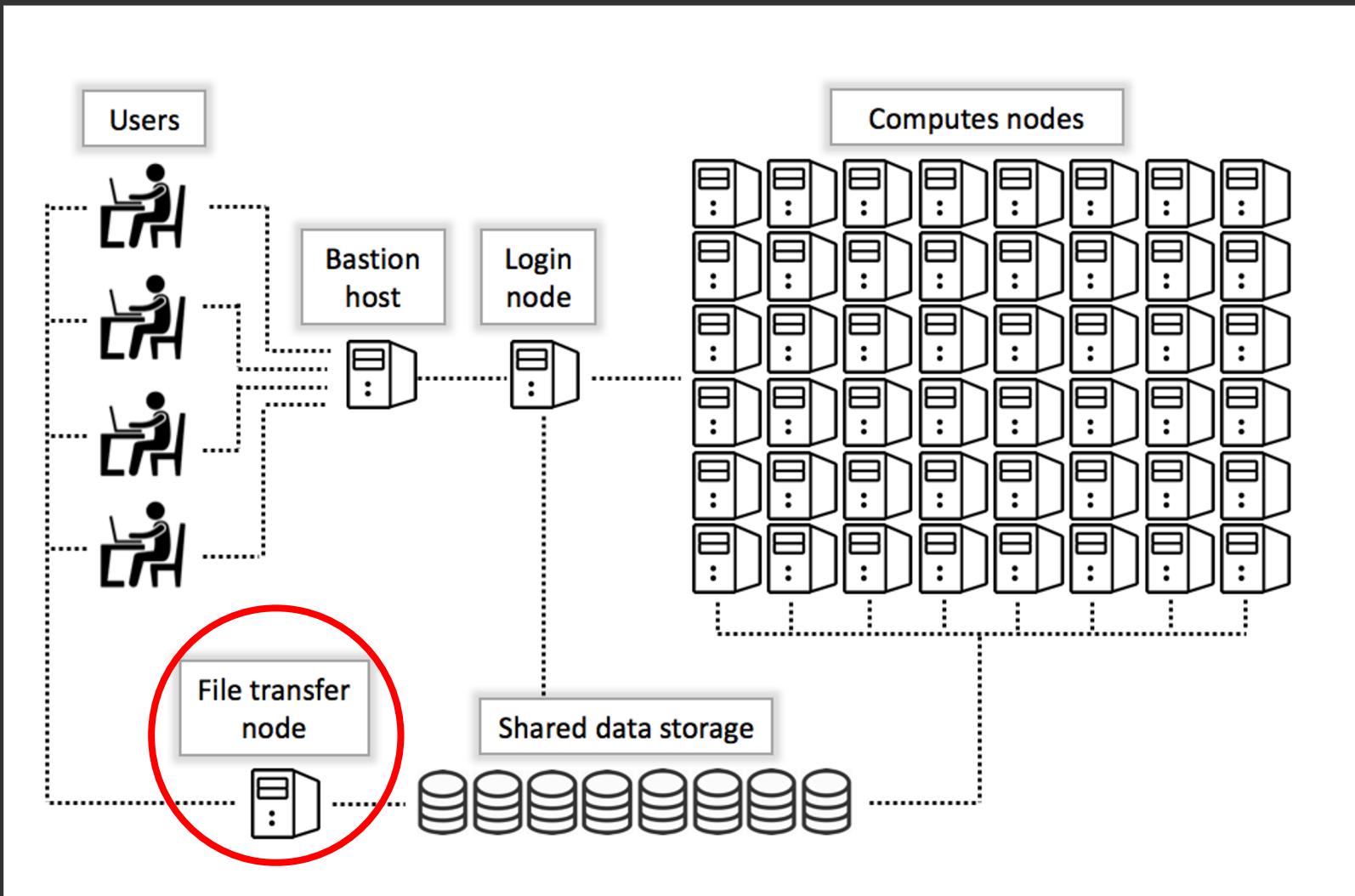


▲▲▲

Transferring Files



Transferring Files



filexfer.hpc.arizona.edu

File transfer between local computer and HPC

- GUI



- Command line

- wget
- scp
- sftp

File transfer in web browser

- Open On Demand: ood.hpc.arizona.edu

The screenshot shows the Open On Demand web interface. At the top, there is a navigation bar with links for Home, Apps, Files, Jobs, Clusters, Interactive Apps, My Interactive Sessions, Help, and Log Out. A user note "Please NOTE: 'windfall' terminated without notice if pre-empted by a 'standard' job in queue." is displayed. Below the navigation, a sidebar shows the current directory path: Home Directory, /groups, and /xdisk. The main area displays a file list with columns for Type, Name, Size, and Modified at. The file list includes:

Type	Name	Size	Modified at
Folder	bin	-	2/22/2022 2:18:45 PM
Folder	containerTest	-	2/22/2022 9:55:45 AM
Folder	DLcheckpointing	-	2/18/2022 4:50:14 PM

At the bottom right, there are buttons for Open in Terminal, New File, New Directory, Upload, Download, Copy/Move, and Delete.

Command line file transfer

- Command line transfer is easy with scp command

copy recursively,
maintaining permissions

- `scp -rp what_to_copy where_to_copy`

remote cluster location
default target is home directory

```
~/Desktop/ $ scp -rp data_dir zwickl@filexfer.hpc.arizona.edu:
```

```
~/Desktop/ $ scp -rp data_dir zwickl@filexfer.hpc.arizona.edu:/groups/chrisreidy/
```

```
~/Desktop/ $ scp -rp zwickl@filexfer.hpc.arizona.edu:data_dir .
```

To download, use the remote
location as the first argument

•••

Managing Files

Sharing data between HPC users

- You can share data with another HPC user without moving the data
- Open file permissions
- Create symbolic links

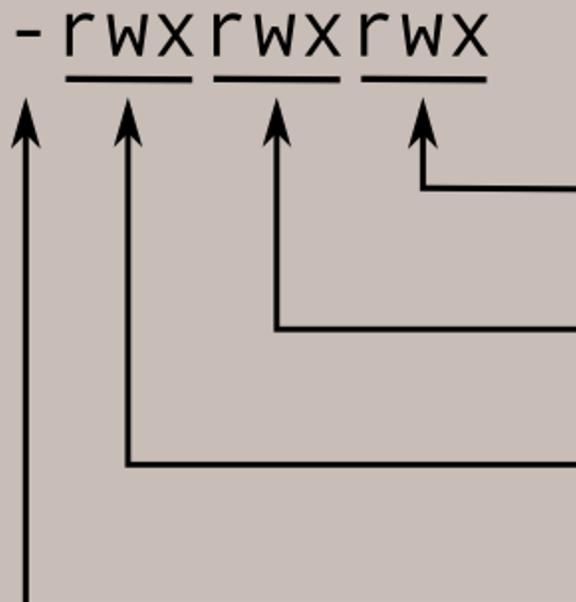
File permissions

- Check file permissions – `ls -l`

```
-rw-r--r-- 1 dshyshlov rc 639 Oct 10 15:58 script.pbs
```

Owner

Group



Read, write, and execute
permissions for all other users.

Read, write, and execute
permissions for the group owner
of the file.

Read, write, and execute
permissions for the file owner.

File type:
- indicates regular file
d indicates directory

File permissions

- View file permissions in OOD

Please NOTE: "windfall" jobs will be restarted or terminated without notice if pre-empted by a "standard" job in queue.

Open in Terminal + New File New Directory Upload Download Copy/Move Delete

Home Directory /home/u2/zwickl Change directory Copy path

Check this box → Show Owner/Mode Show Dotfiles Filter: _____

Showing 15 of 47 rows - 0 rows selected

Type	Name	Size	Modified at	Owner	Mode
□	bin	-	2/22/2022 2:18:45 PM	zwickl	755
□	containerTest	-	2/22/2022 9:55:45 AM	zwickl	755
□	DLcheckpointing	-	2/18/2022 4:50:14 PM	zwickl	755

Permissions ↑

Numerical file permissions

Octal Value	File Permissions Set	Permissions Description
0	---	No permissions
1	--x	Execute permission only
2	-w-	Write permission only
3	-wx	Write and execute permissions
4	r--	Read permission only
5	r-x	Read and execute permissions
6	rw-	Read and write permissions
7	rwx	Read, write, and execute permissions

Numerical file permissions

- Permissions can be summarized with the digits 1-7
- One number appears for each of the user, group and all permission categories
- So, 777 = rwxrwxrwx
755 = rwxr-xr-x

Change file permissions

- Command to change permissions – chmod
 - `chmod +x filename` - make file executable for everyone
 - `chmod g+rwx filename` - open all permissions for your group
 - `chmod 777 filename` - open all permissions for everyone
 - `chmod -R 777 filename` - same as above but recursively (for all the subdirectories and files)

Symbolic links

- Create a soft link to a file or directory
 - `ln -s path/to/the/destination link_name`
 - perfect for situations when you need to share read only data
 - requires permissions to link directory of another user
- Examples:
- Create a shortcut to your /groups in your /home
 - `ln -s /groups/PInetID ~/my_groups`
- Share data on xdisk (permissions!)
 - `ln -s /xdisk/PInetID/project ~/project_data`

File & Space Management Tools

- Show disk usage command - du

```
$ du scripts/  
24 scripts/slurm_testing  
8 scripts/puma/test  
380 scripts/puma  
12 scripts/elgato  
3304 scripts/ocelote  
36 scripts/chaining  
7264 scripts/
```

- Useful flags:
 - -h – human readable format
 - -s – display only the total
 - --max-depth=N – limit depth of subdirectories to N

```
$ du -sh scripts/  
7.1M scripts/
```

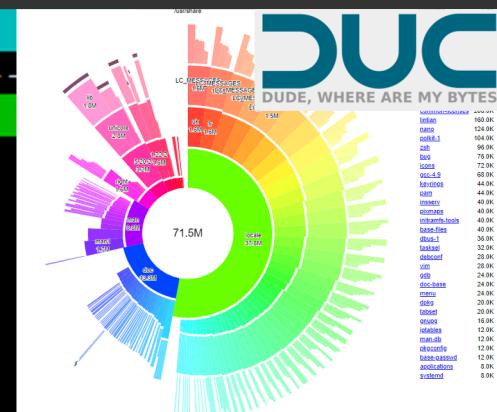
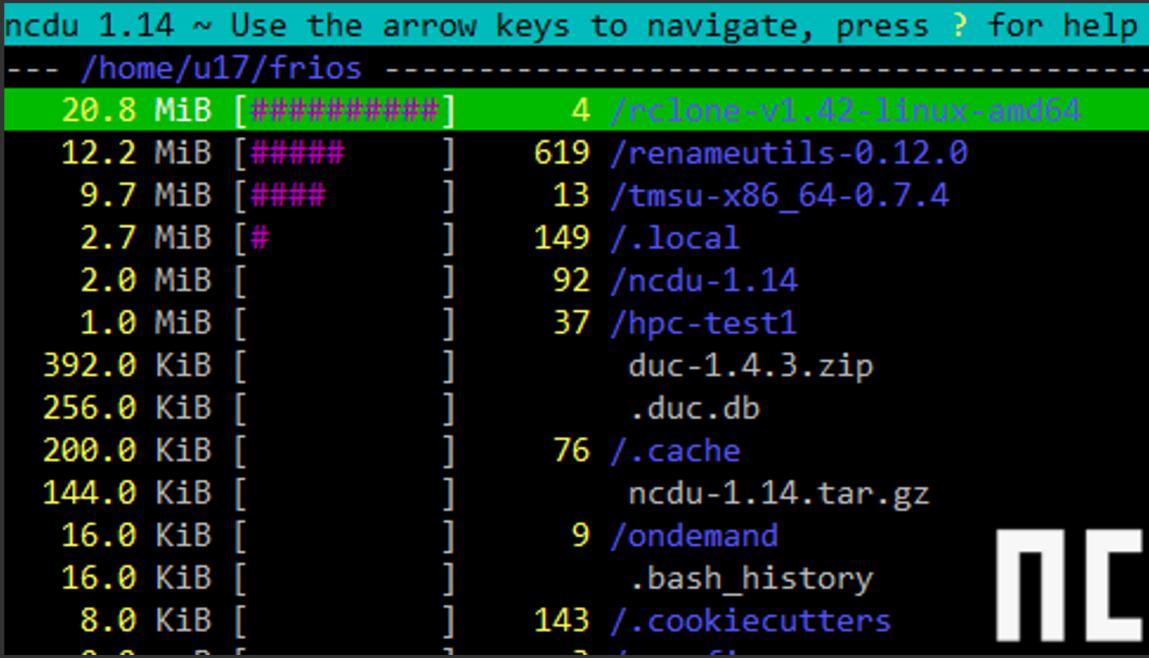
File & Space Management Tools

- Checking your space & file limit: uquota

```
frios@login2 ~$ uquota
```

	used	soft limit	hard limit	files/limit
frios home & PBS	46.84M	14G	15G	1044
/extra/frios	56.72G	200G	200G	2/120000

- Checking folder usage and count: NCDU



NCdu

Operate on Data

- Things that can “break” the system:
 - heavy use of the login node
 - too many jobs
 - too many files
 - heavy I/O jobs
 - copying GB of data

Preview for Part 2

- File and folder tidiness
- Scriptable methods of transferring data into/out of the HPC
- Additional tools for managing files and projects
- Data archiving