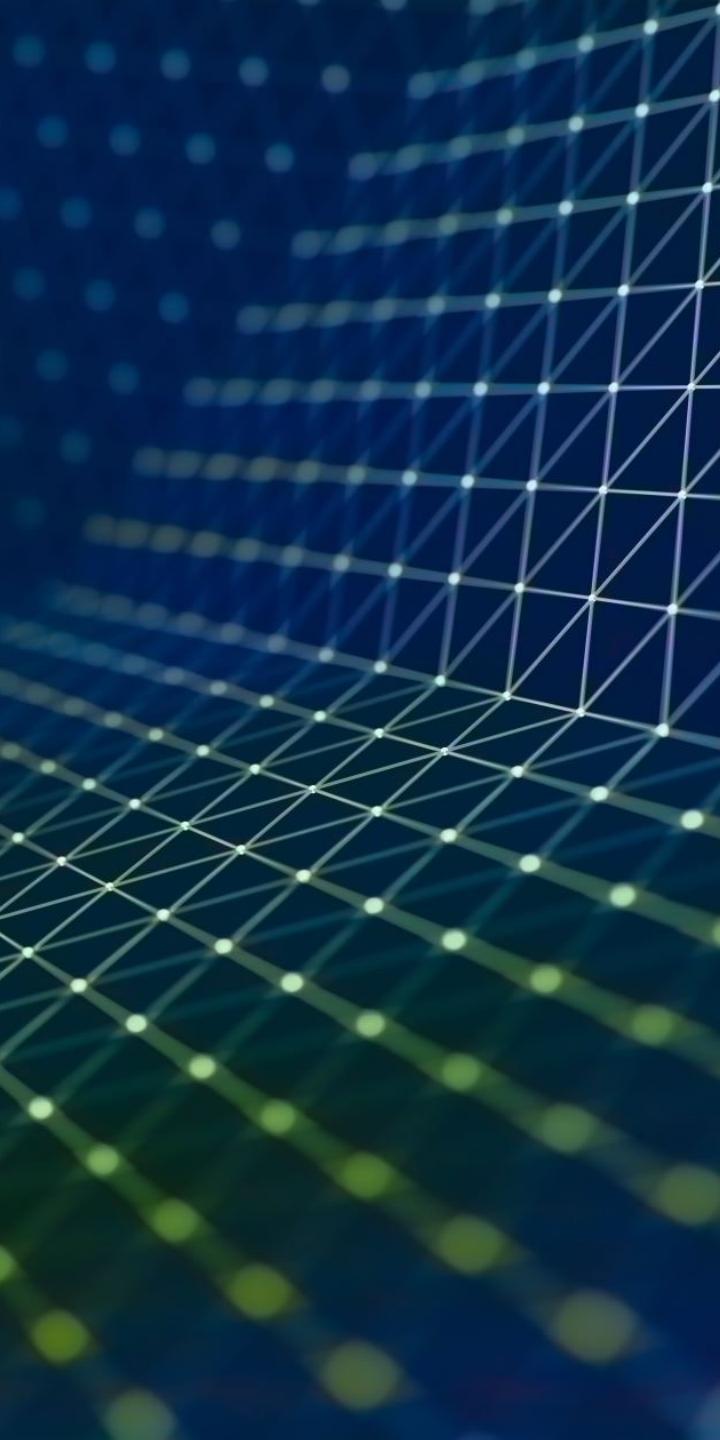


Exercises: <https://ua-researchcomputing-hpc.github.io/Intro-to-HPC/>

A dark blue background featuring a complex, glowing network of white and green lines forming a grid-like structure, representing a high-performance computing cluster.

Intro to HPC*

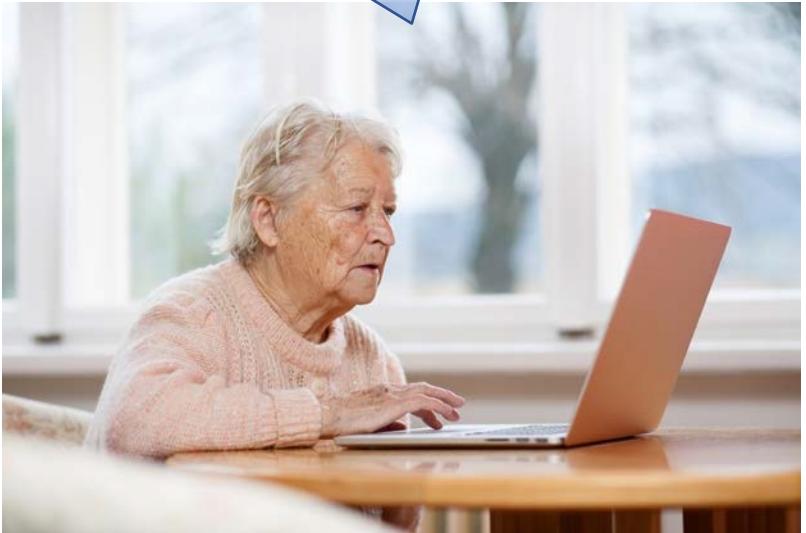
*HPC – high-performance computing

- Why use HPC?
- Anatomy of the HPC cluster
- Basics of working with the Linux shell
- Submitting jobs

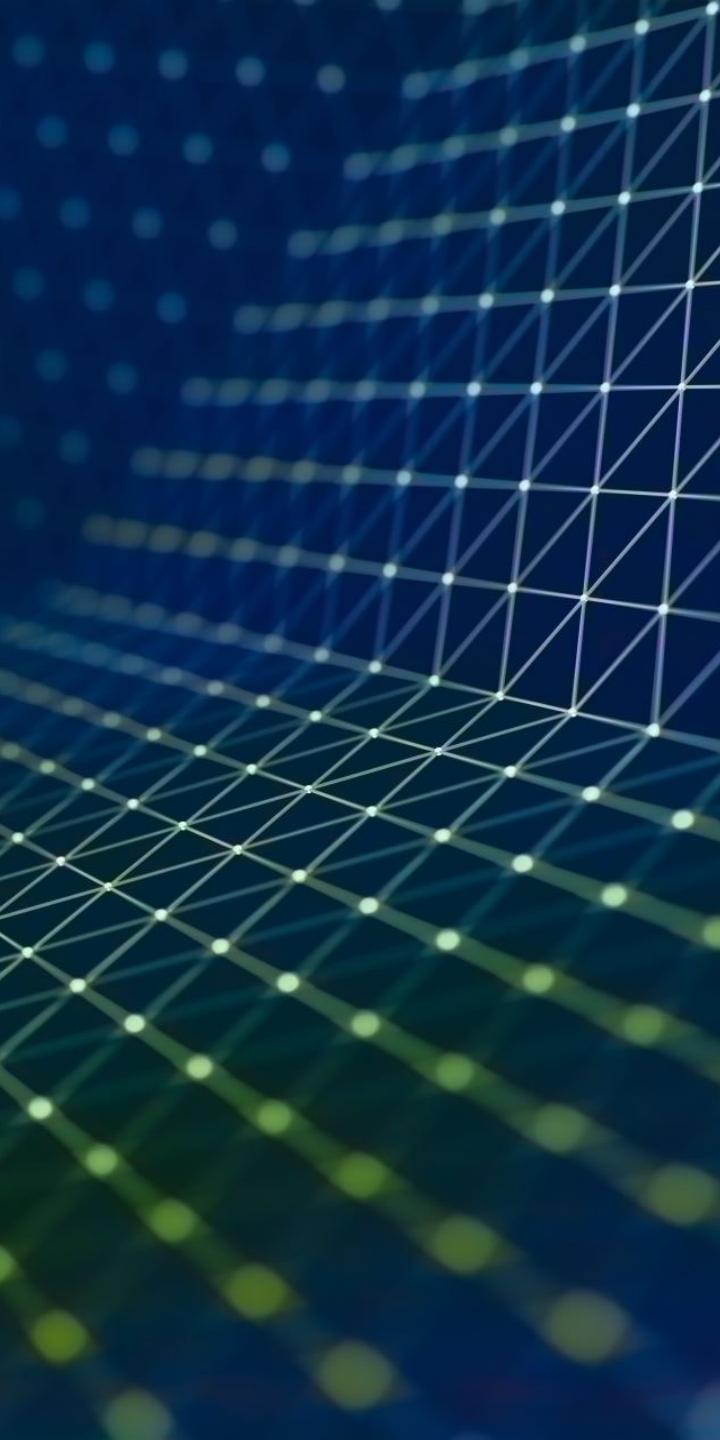
Why HPC?



Research is
easy!



It's still
running...



Why HPC?

Problems

- Computation takes too long
- Computation is too big
- Too many computations



Why HPC?

Problems

- Computation takes too long
→ Get a more powerful computer
- Computation is too big
→ Link multiple computers
- Too many computations
→ Use a separate one for each job

Why HPC?

- Modern instrument for High-Performance Computing is a **cluster**, consisting of lots of connected individual computers (nodes).
- Supercomputer is a commonly used nickname.





Laptop



Supercomputer

Why HPC?



Laptop

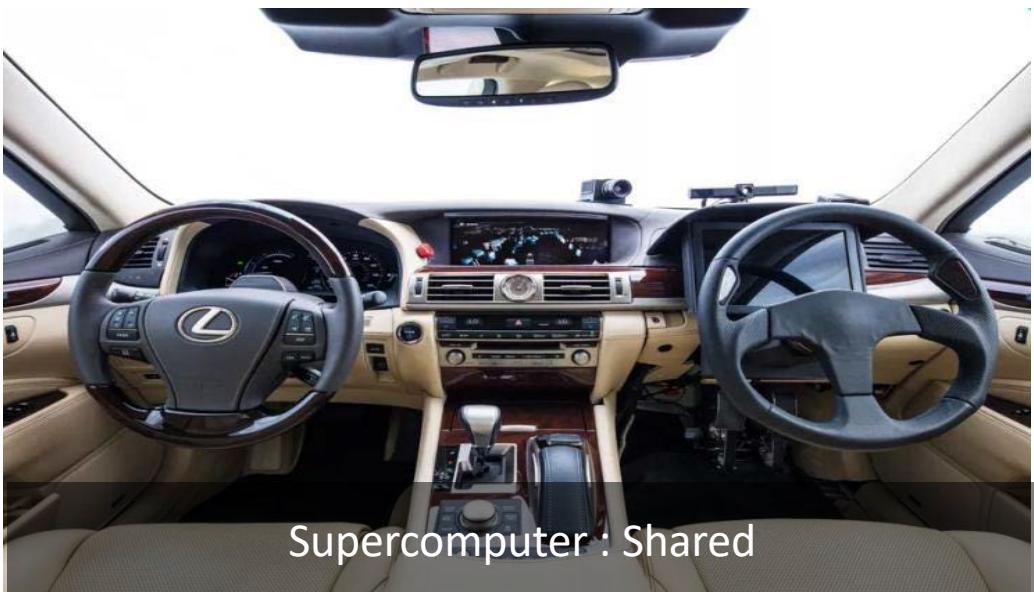


Supercomputer

Why HPC?



Laptop : Personal

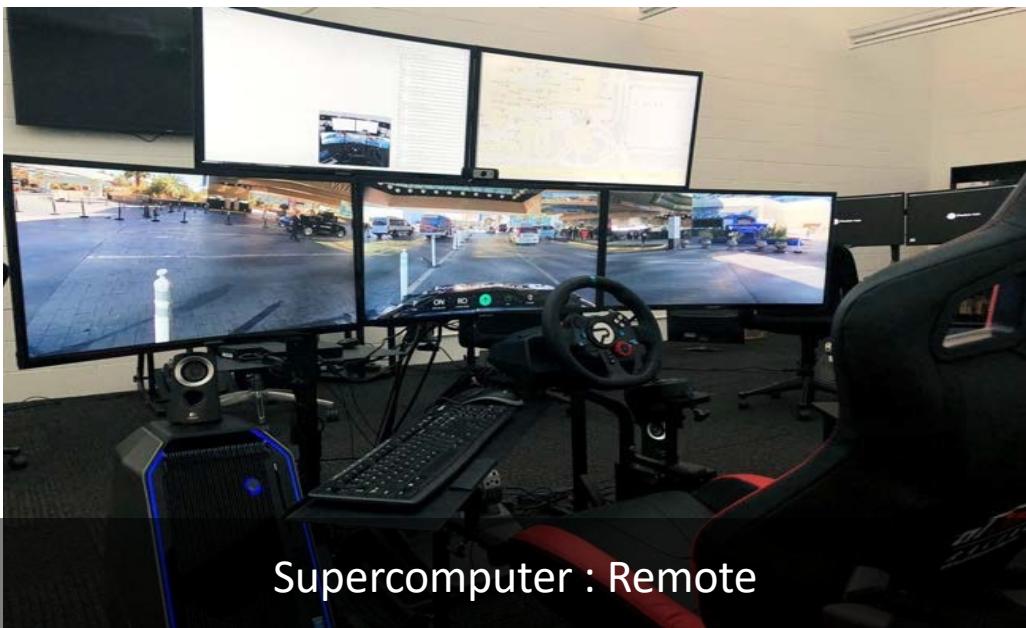


Supercomputer : Shared

Why HPC?



Laptop : Local



Supercomputer : Remote

Why HPC?



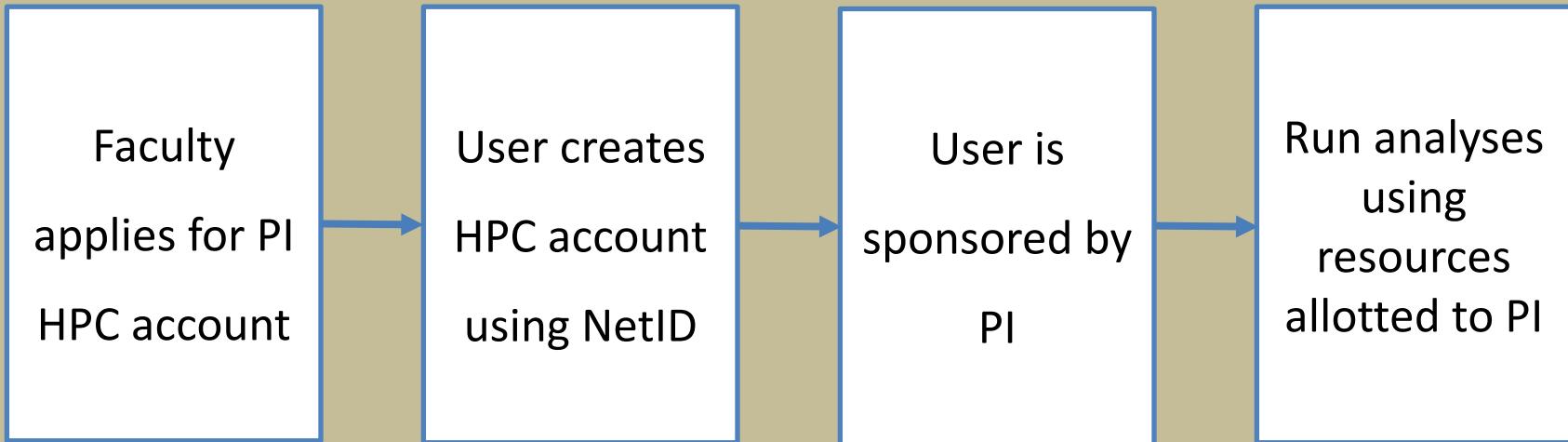
Laptop : Interactive



Supercomputer : Batch

Why HPC?

Gaining Access to UA HPC



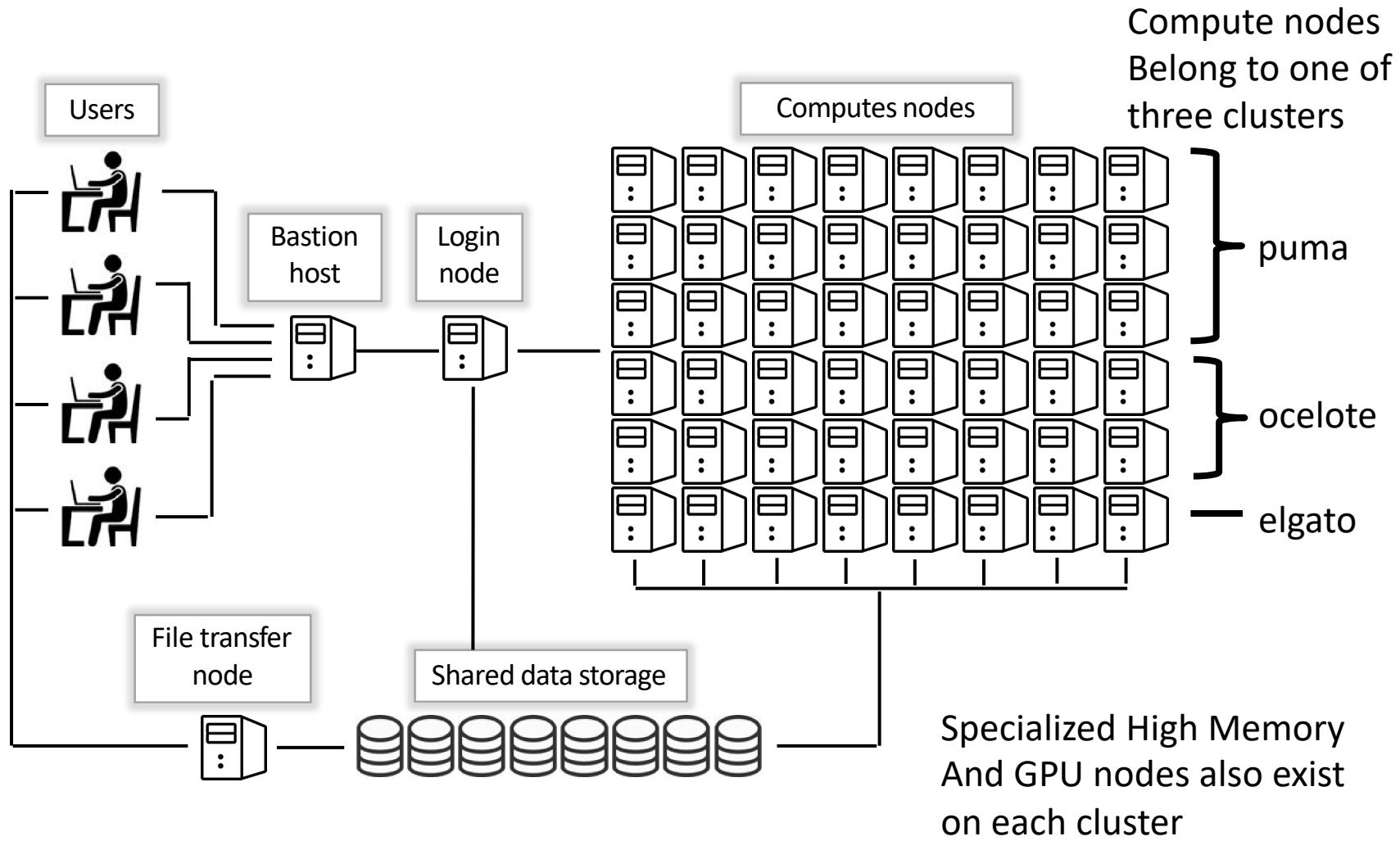
Instructions for PIs and sponsored researchers are here:

<https://public.confluence.arizona.edu/display/UAHPC/Account+Creation>



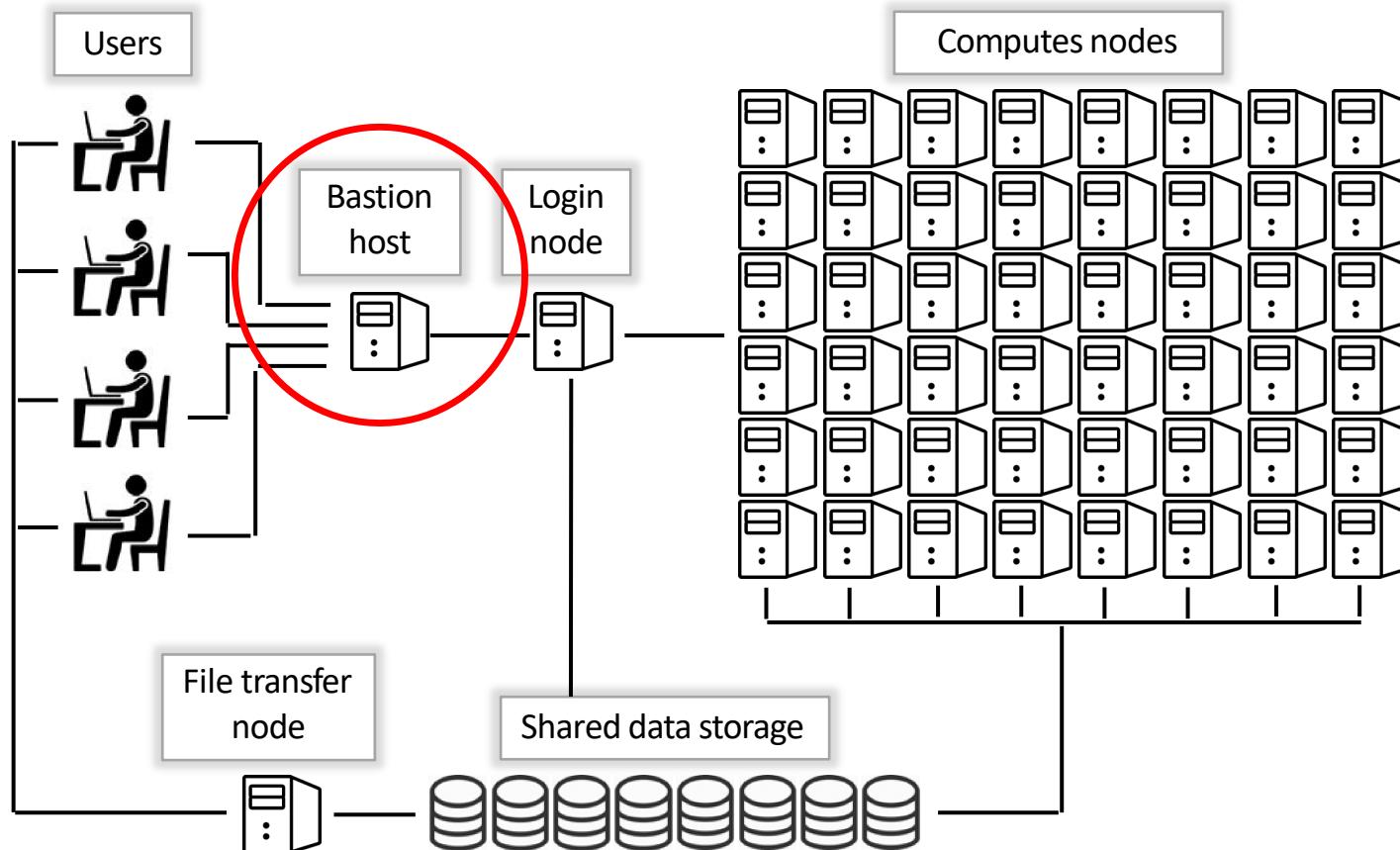
Ocelote

The diagram of the UA HPC System



Connecting to UA HPC – 2 Methods

ssh netid@hpc.arizona.edu
shell



Connecting from the command line

On Laptop:

```
~/ $ ssh chrisreidy@hpc.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

```
[chrisreidy@gatekeeper ~]$ shell  
Last login: Mon Nov  8 20:16:14 2021 from  
gatekeeper.hpc.arizona.edu
```

```
***
```

```
(puma) [chrisreidy@junonia 08:35:32 ~]$ ocelote
```

```
(ocelote) [chrisreidy@ junonia Intro_to_HPC]$ interactive
```

MacOS

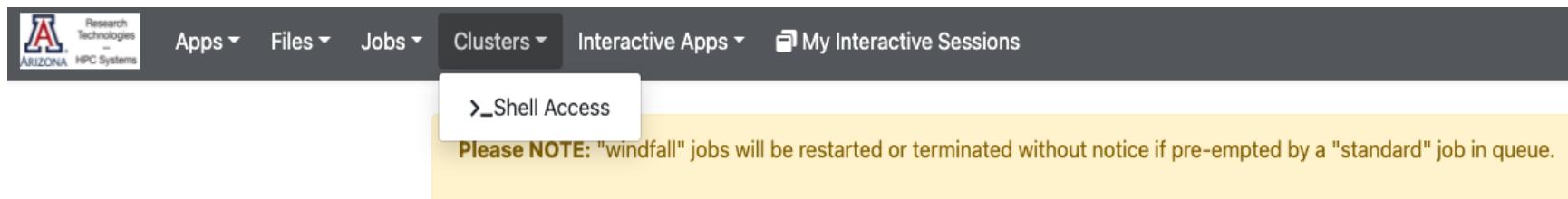
- Includes Terminal app

Windows

- Putty
- MinGW
- Git Bash

Connecting with Web Browser

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

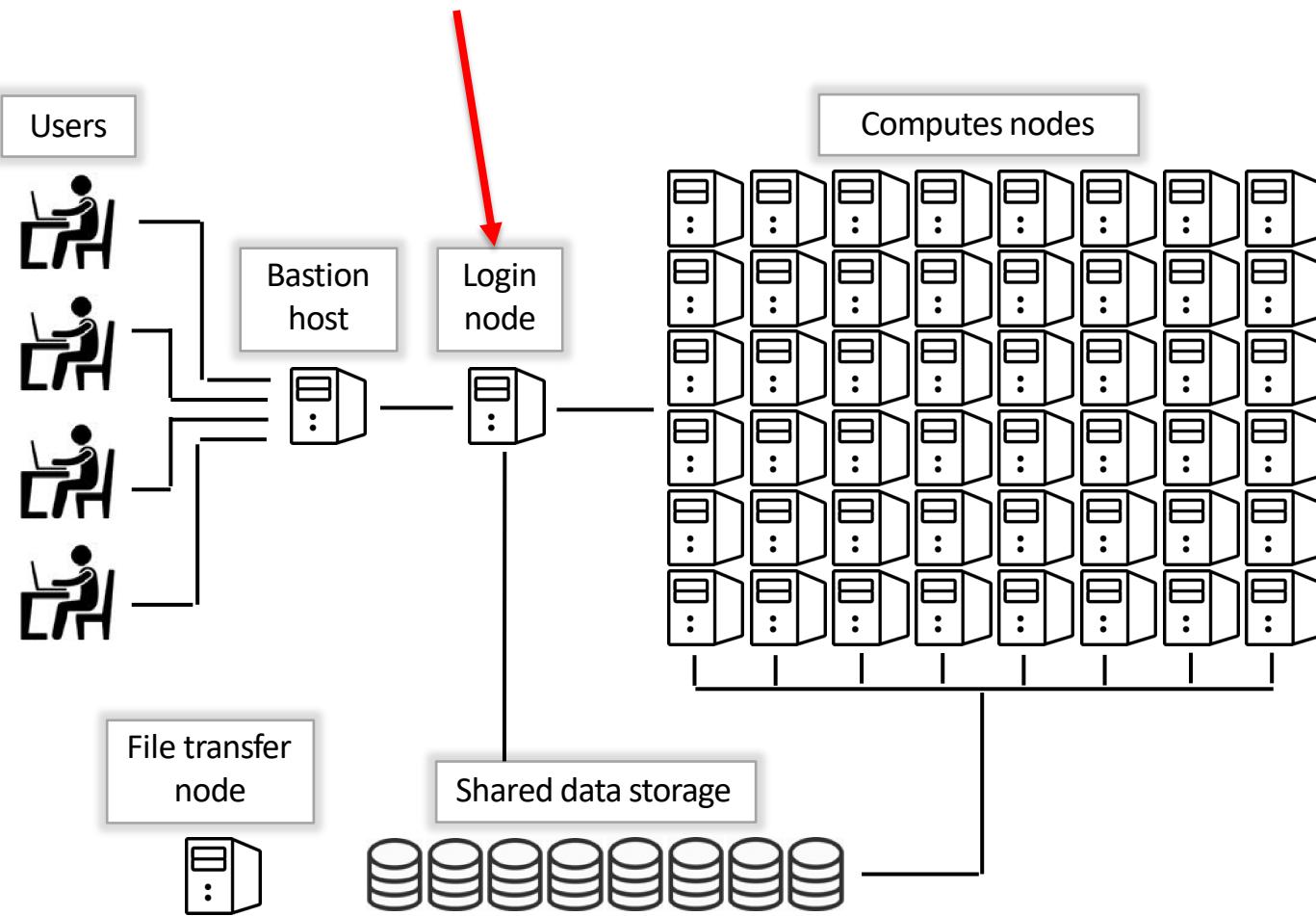


OnDemand provides an integrated, single access point for all of your HPC resources.

- Exercise - connect to UA HPC.

Login node

```
(puma) [chrisreidy@wentletrap 16:03:26 ~]$ ls
```



The command line

Your NetID
(who are you)

Name of the current
directory

```
(puma) [chrisreidy@gentlettrap 16:03:26 ~]$ ls
```

Cluster your
jobs will be
submitted to

Node name
(where are you)

Prompt
(what are you going to do)



Login Node aka Submit Node



Compute Nodes

Login
Node

Login node

- The login node is a computer intended for users to prepare and manage computations:
 - submit jobs
 - edit files
 - manage files
 - compile codes - **NO**
 - small-scale testing - **NO**
- **DO NOT** run any calculations on the login node



The command line

```
(puma) [chrisreidy@junonia 14:16:33 ~]$ whoami  
chrisreidy  
(puma) [chrisreidy@junonia 14:16:38 ~]$
```

Command

Output

For companion information on the hands-on practice:
<https://ua-researchcomputing-hpc.github.io/Intro-to-HPC/>

The command line

```
(puma) [chrisreidy@junonia 14:16:38 ~]$ pwd  
/home/u13/chrisreidy  
(puma) [chrisreidy@junonia 14:21:41 ~]$
```

Path to Working Directory

Name of the current directory

- ~ is a shortcut for your /home directory

The command line

- List all the files and directories

```
(puma) [chrisreidy@junonia 14:21:41 ~]$ ls
```

- Make a directory

```
(puma) [chrisreidy@junonia ~]$ mkdir intro-to-hpc
```

- List all the files and directories again

```
(puma) [chrisreidy@junonia 14:21:41 ~]$ ls
```

Command Line

- Change directory

```
(puma) [chrisreidy@junonia 14:41:30 ~]$ cd intro-to-hpc/  
(puma) [chrisreidy@junonia 14:48:36 intro-to-hpc]$
```

- Go back a level

```
(puma) [chrisreidy@junonia 14:49:48 intro-to-hpc]$ cd ..  
(puma) [chrisreidy@junonia 14:49:51 ~]$
```

- Change directory using absolute path

```
(puma) [chrisreidy@junonia 14:49:51 ~]$ cd ~/intro-to-hpc/  
(puma) [chrisreidy@junonia 14:51:21 intro-to-hpc]$
```

Command Line

- Copy a file Note the period at the end

```
$ cp /xdisk/chrisreidy/workshops/LICENSE .
```

- List all the files and directories again

```
(puma) [chrisreidy@junonia 14:21:41 ~]$ ls
```

- View contents of the file on the screen

```
$ cat LICENSE
```

Working with a Linux shell

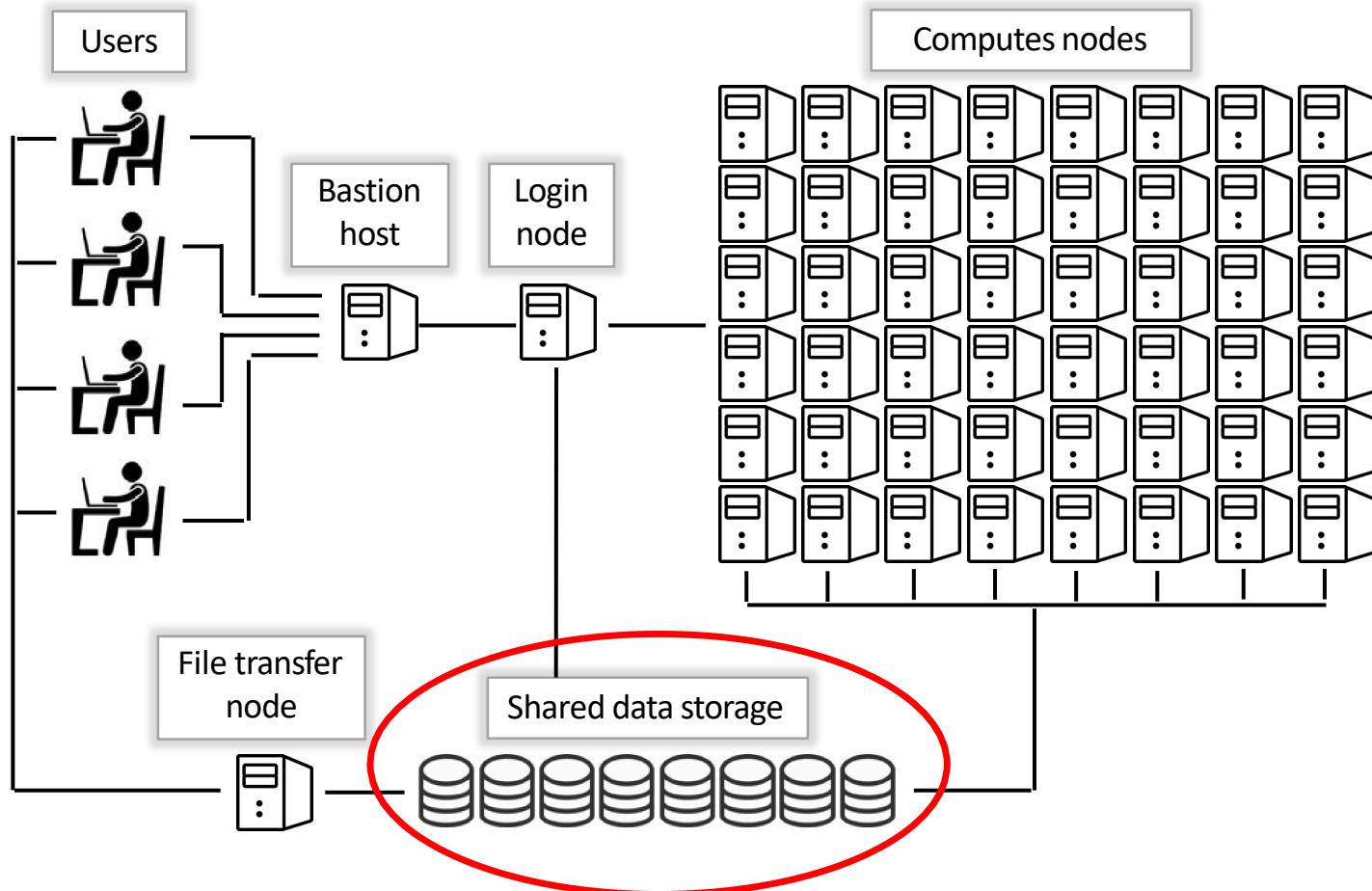
For more information on the Linux command line,
follow the links in our documentation:

[https://public.confluence.arizona.edu/display/UAHPC/
Training#Training-LinuxSelfGuided](https://public.confluence.arizona.edu/display/UAHPC/Training#Training-LinuxSelfGuided)



Linux

Storage



/home/u1/netid

/groups/PI

/xdisk/PI

Storage

- Every user gets two default storage locations :
 - /home
 - the default home directory
 - 50GB
 - Not backed up
 - /groups/PI
 - shared by the PI's group
 - 500GB
 - Not backed up

Storage

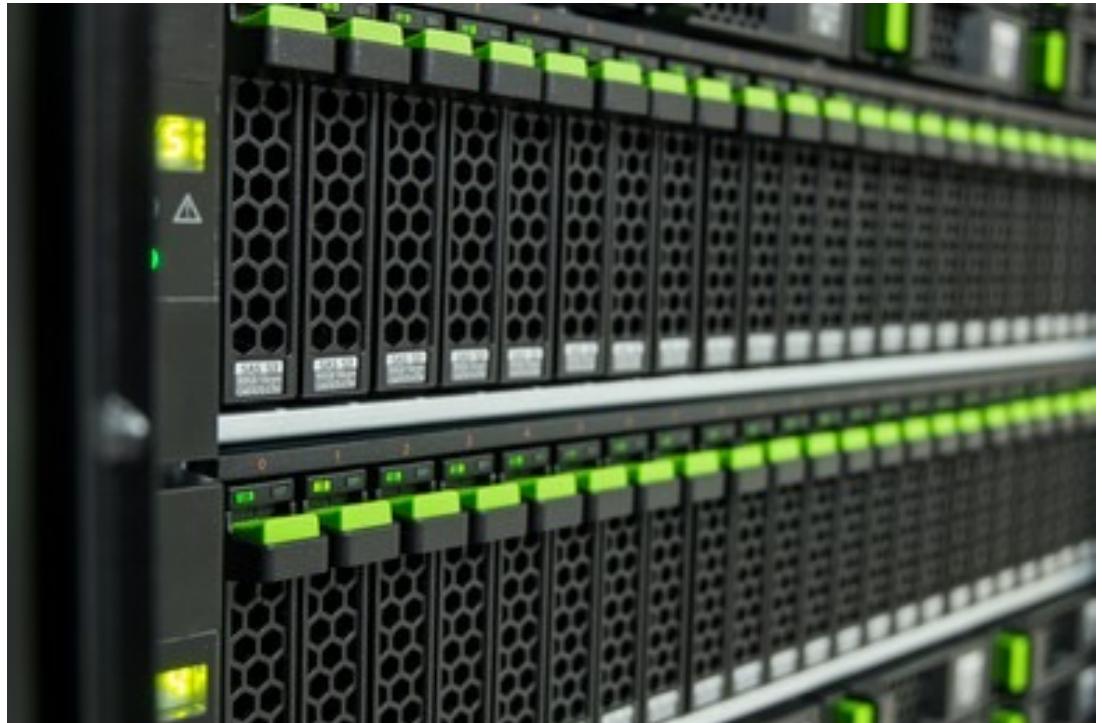
- Command to list all the available storage options –
uquota

```
$ uquota
```

	used	soft limit	hard limit
/groups/chrisreidy	38.1G	500.0G	500.0G
/home	12.9G	50.0G	50.0G
/xdisk/chrisreidy	6.2T	19.5T	19.5T

Storage

- Additional Storage:
- /xdisk/PI
- Upon request, up to 20TB for limited duration with one renewal
- /tmp
- Every Puma node has about 1.4TB on a NVME SSD

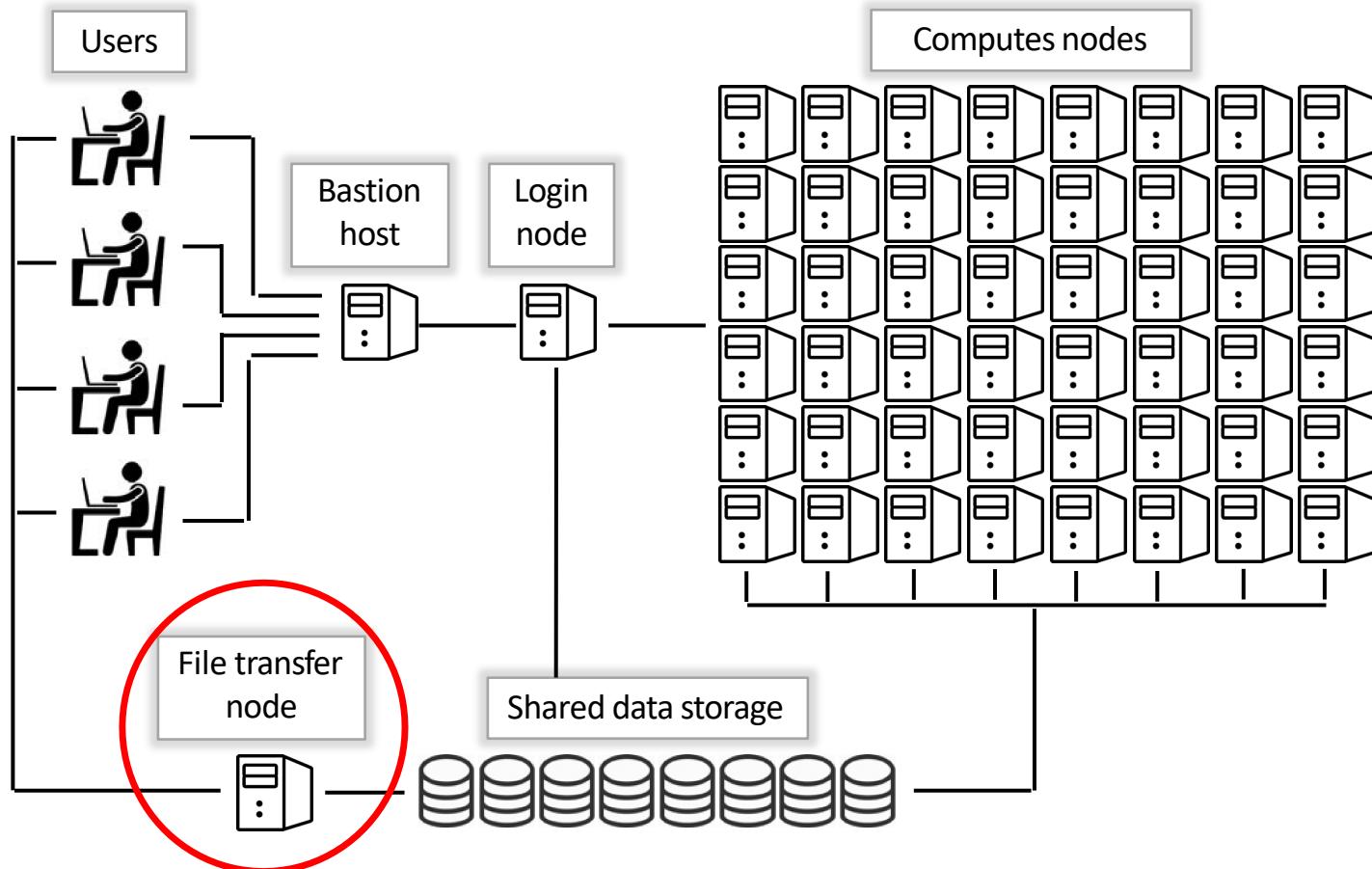


shutterstock.com • 302314952

TIME ALLOCATION

- Every PI gets a monthly allocation of free time, and each user shares that allocation:
- Partitions (queues):
 - standard
 - 100,000 cpu hours on Puma
 - 35,000 cpu hours on Ocelote
 - 7,000 cpu hours on Elgato
 - Limits on GPU nodes
 - Not preempted
 - windfall
 - Unlimited
 - Preemptable

Transferring Files



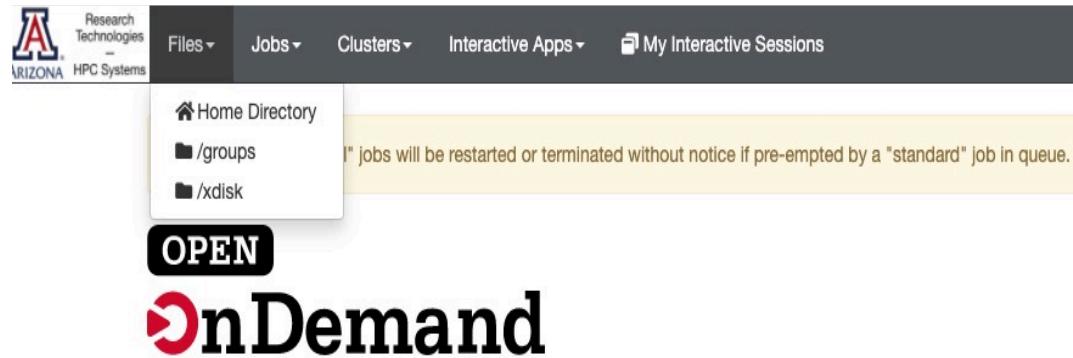
`filexfer.hpc.arizona.edu`

Transferring Files

- UA HPC uses a specific node for file transfer
 - hostname –
`filexfer.hpc.arizona.edu`
- Command line options:
 - `scp`
 - `sftp`
 - `rsync`
 - `Irods`
 - `rclone`
- GUI options
 - Windows based: `WinSCP`
 - Cross-platform: `Cyberduck`
 - `Globus`

Transferring Files with OnDemand

- Display and manage your files
- Edit text files
- Drag and drop files to/from the file explorer

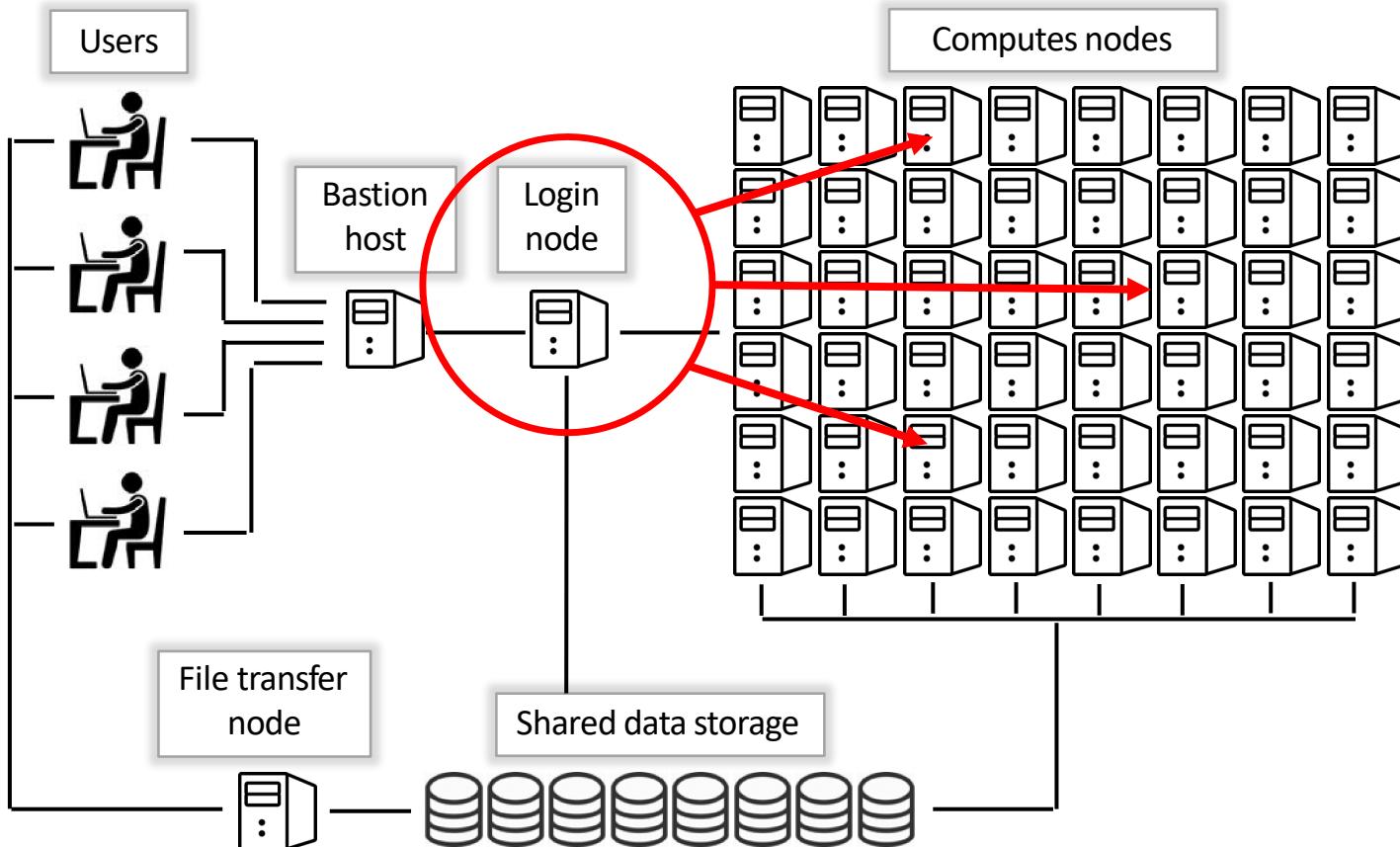


OnDemand provides an integrated, single access point for all of your HPC resources.

The image shows the File Explorer v1.3.6 interface. On the left is a tree view of the 'Home Directory' containing various subfolders like ECOL-346, R, UA-HPC-Intro, etc. The main area shows the path '/home/u1/dshyshlov/'. Below the path are buttons for Go To..., Open in Terminal, New File, New Dir, Upload, Show Dotfiles, and Show Owner/Mode. A toolbar below these buttons includes View, Edit, Rename, Download, Copy, Paste, and (Un)Select All. The main pane lists files and folders with columns for name, size, and modified date. The 'ECOL-346' folder is currently selected, highlighted in blue.

name	size	modified date
..	<dir>	01/31/2018
ECOL-346	<dir>	01/31/2018
R	<dir>	08/28/2017
UA-HPC-Intro	<dir>	09/25/2017
Wolfram Mathematica	<dir>	12/13/2017
bin	<dir>	07/11/2017
blast_data	<dir>	01/31/2018
exercises_unix	<dir>	06/13/2018
extra	<dir>	08/22/2018
gui_tmp	<dir>	
iceVirtEnv	<dir>	
install_test	<dir>	
intel	<dir>	
ions	<dir>	
local	<dir>	

From the login node to compute

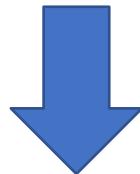


From the login node to compute

- How do we know if there are any available nodes?
- How do we decide who gets what and when?
- How do we ensure that a task gets the resources it needs?
- The Scheduler!
- Software that manages the HPC resources and decides which computation runs where and when.

Scheduler - SLURM

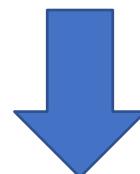
Scheduler receives a request for resources and creates a job



Job is put in the queue, where it waits for the resources



Job is assigned to the compute nodes and performs computation



When job is finished, output and error files are created



Scheduler

- All clusters use SLURM
- Every computation that requests resources from the scheduler is called a *job*.
- *Submitting a job* means requesting resources from the scheduler and giving it a list of commands to run.

SLURM script

```
$ cp /xdisk/chrisreidy/workshops/sample_slurm.script .
$ cat sample_slurm.script

#!/bin/bash
#SBATCH --job-name=test
#SBATCH -e test.e%A
#SBATCH -o test.o%A
#SBATCH --partition=windfall
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --time=00:10:00

echo 'This script is running on:'
hostname
sleep 120
```

SLURM script

```
#!/bin/bash
#SBATCH --job-name=test
#SBATCH -e test.e%A
#SBATCH -o test.o%A
#SBATCH --partition=windfall
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --time=00:10:00
```

```
echo 'This script is running on:'
hostname
sleep 120
```

It's a bash shell script

SLURM script

SLURM directives

```
#!/bin/bash
#SBATCH --job-name=test
#SBATCH -e test.e%A
#SBATCH -o test.o%A
#SBATCH --partition=windfall
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --time=00:10:00
```

```
echo 'This script is running on:'
hostname
sleep 120
```

SLURM script

List of commands to run

```
#!/bin/bash
#SBATCH --job-name=test
#SBATCH -e test.e%A
#SBATCH -o test.o%A
#SBATCH --partition=windfall
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --time=00:10:00
```

```
echo 'This script is running on:'
hostname
sleep 120
```

SLURM script

- Submitting a batch job

```
$ sbatch sample_slurm.script
```

Did you get an error?

If not, you will see:
Submitted batch job 2118950

```
$ squeue -j 2118950
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST(REASON)
2118950	windfall	test	chrisrei	PD	0:00	1	(Priority)

```
$ cat test.o2118950
```

This script is running on:

r1u11n1.puma.hpc.arizona.edu

Detailed performance metrics for this job will be available at

https://metrics.hpc.arizona.edu/#job_viewer?action=show&realm=SUPREMM&resource_id=73&local_job_id=2118950 by 8am on 2021/09/23.

SLURM script

- Modifying your batch job

1/ Change the script to use 4 cores from one node

```
$ vi sample_slurm.script
```

Hint: look at our SLURM documentation here:
<https://public.confluence.arizona.edu/display/UAHPC/Running+Jobs+with+SLURM>

```
$ sbatch sample_slurm.script  
Submitted batch job 2118966
```

2/ Change the script to use the standard queue

Answer:

```
#SBATCH --account=<PI GROUP>  
#SBATCH --partition=standard
```

Note: *partition* is the same as *queue*

SLURM script

- Other SLURM commands

\$ squeue

You might need to know the grep command to handle the hundreds of lines of output

\$ squeue |wc

\$ scancel jobid

\$ scontrol show job 2099296

Show details about a running job

\$ seff 2099296

Show details about a completed job

\$ nodes-busy

\$ system-busy

Shows activity of whole cluster at a glance

Interactive jobs

- Batch vs Interactive

Interactive is used when:

- You need to compile code
- You need test runs
- You need access to modules

Modules are not available on the login nodes

-bash: module: command not found

interactive takes you to a compute node. It is an alias for:

```
$ salloc --job-name=interactive --mem-per-cpu=4GB --nodes=1 --ntasks=1  
--time=01:00:00 --account=windfall --partition=windfall
```

Now your prompt includes the compute node hostname:
[chrisreidy@r3u13n1 chrisreidy]\$

Job Composer with OnDemand

- Create and monitor your jobs

The screenshot shows the OnDemand web interface. At the top, there is a navigation bar with the ARIZONA logo, Research Technologies, and HPC Systems. The navigation items include Apps, Files, Jobs (which is currently selected and highlighted in blue), Clusters, Interactive Apps, and a download icon. A tooltip for the 'Jobs' item displays the text: '① Active Jobs' and 'Job Composer'. Below the navigation bar, there is a yellow banner with the text: 'Please NOTE: Job Composer has been restarted or terminated without notice'. The main area is titled 'Jobs'.

Jobs

The screenshot shows the 'Jobs' index page. At the top left, there is a button labeled '+ New Job'. A modal window is open, titled 'Steps to create a job:', containing the following steps:

1. Create a new job by copying from an existing job template directory or a previously run job directory.
2. Edit the files in the job via the file explorer.
3. Submit the job and monitor the progress from the "Job Composer" index page.

Below the modal, there is a table header with columns: ID, Cluster, Status, and a search bar. The table body is currently empty, showing 'Showing 0 to 0 of 0 entries'. At the bottom of the page, there are 'Previous' and 'Next' buttons.

Accessing Software Modules

- Much software is available as “modules”
- 100 Applications from Abaqus to Xcrysden

To see the list:

Either

<https://public.confluence.arizona.edu/display/UAHPC/Software+Resources>

Or

\$ shell

\$ ocelote

\$ interactive

\$ module avail

```
mirror_mod = modifier_obj
# Set mirror object to mirror
mirror_mod.mirror_object = mirror_object
operation = "MIRROR_X":
    mirror_mod.use_x = True
    mirror_mod.use_y = False
    mirror_mod.use_z = False
operation == "MIRROR_Y":
    mirror_mod.use_x = False
    mirror_mod.use_y = True
    mirror_mod.use_z = False
operation == "MIRROR_Z":
    mirror_mod.use_x = False
    mirror_mod.use_y = False
    mirror_mod.use_z = True

selection at the end -add
modifier_obj.select= 1
modifier_obj.select=1
context.scene.objects.active = modifier_obj
("Selected" + str(modifier_obj))
modifier_obj.select = 0
bpy.context.selected_objects.append(modifier_obj)
data.objects[one.name].select = 1
print("please select exactly one object")
print("operator classes")
- OPERATOR CLASSES ---

types.Operator:
    X mirror to the selected object.mirror_mirror_x"
    "or X"
context):
    ext.active_object is not None
    print("operator classes")
```

Accessing Software with OnDemand

Apps ▾ Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾ 

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

OPEN

 **OnDemand**

OnDemand provides an integrated, single access point for all of your HPC resources.

Pinned Apps A featured subset of [all available apps](#)



ABAQUS GUI
System
Installed App



ANSYS
Workbench
GUI
System
Installed App



Mathematica
GUI
System
Installed App



MATLAB GUI
System
Installed App

Accessing Software with OnDemand

MATLAB GUI (187278) 1 node | 1 core | Running

Host: >_j0n11.ocelote.hpc.arizona.edu Delete

Created at: 2021-09-22 20:34:37 MST

Time Remaining: 59 minutes

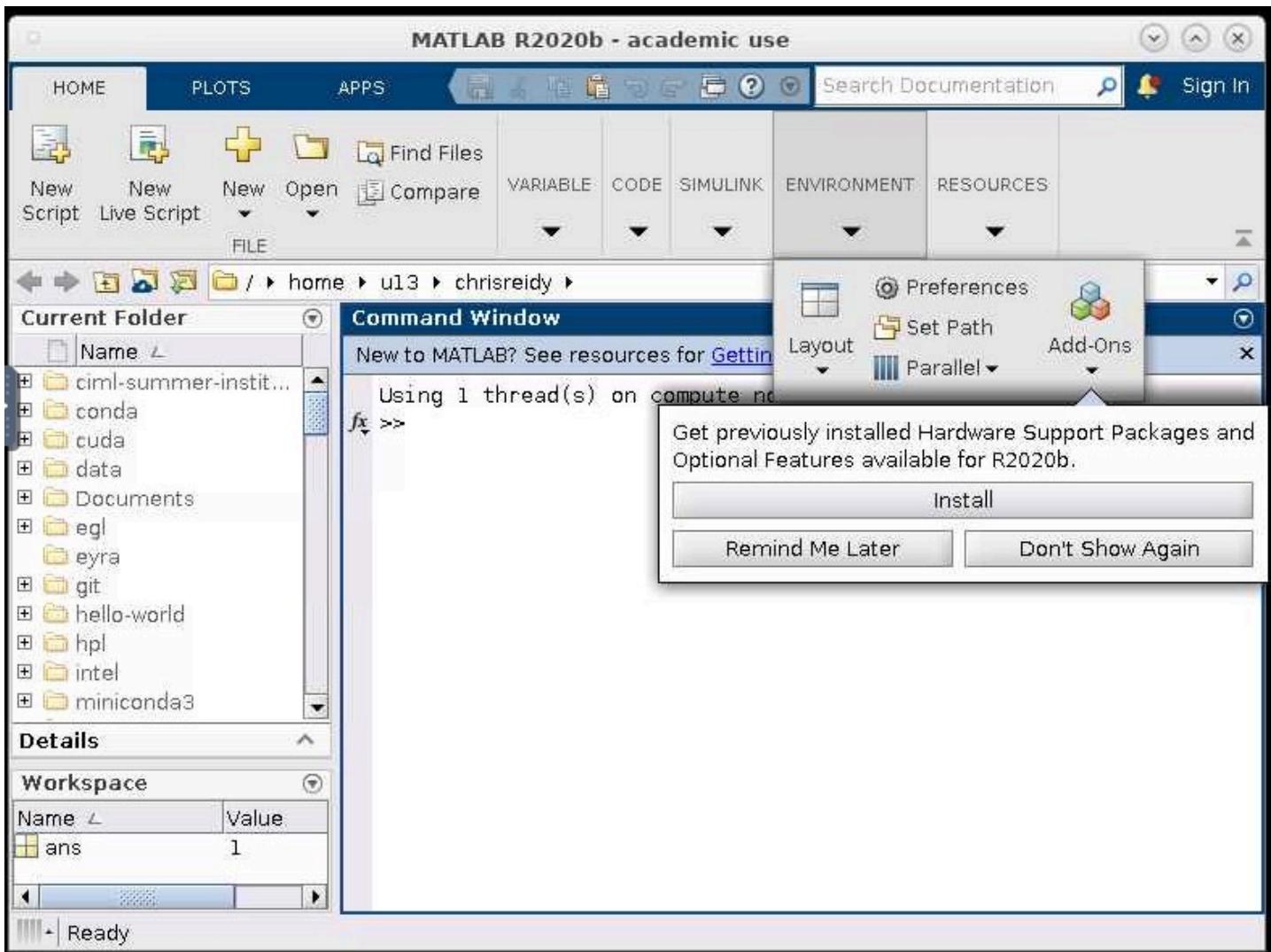
Session ID: 747e44e5-83b4-4515-b737-41147f8502fb

Compression  0 (low) to 9 (high)

Image Quality  0 (low) to 9 (high)

Launch MATLAB GUI View Only (Share-able Link)

Accessing Software with OnDemand



Accessing Software Command Line

- \$ ocelote
- \$ interactive
- r3u11n1 \$ module avail
- r3u11n1 \$ module avail python
- r3u11n1 \$ module load python/3.8
- r3u11n2 \$ \$ python3
- Python 3.8.2 (default, Mar 16 2021, 17:11:14)
- [GCC 8.3.0] on linux
- Type "help", "copyright", "credits" or "license" for more information.
- >>> import numpy as np
- >>> quit()

Accessing Software Command Line

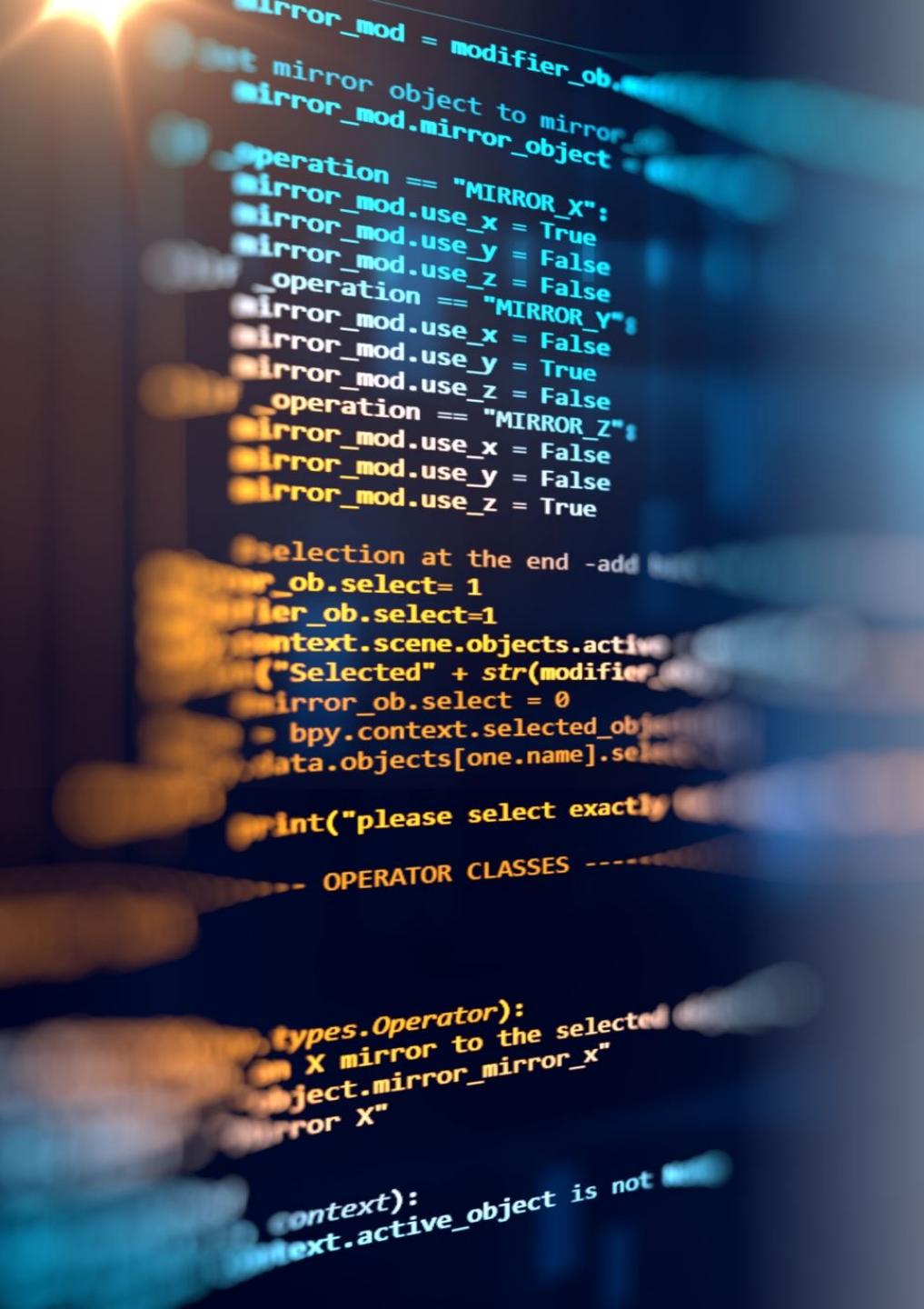
What modules do:

- Set your command path:
- \$ echo \$PATH
- Set your library path:
- \$ echo \$LD_LIBRARY_PATH

Try this from a compute node:

- \$ which freesurfer
- \$ module load freesurfer
- \$ which freesurfer

Now try the two *echo* commands



mirror_mod = modifier_obj
mirror object to mirror
mirror_mod.mirror_object = ob

operation == "MIRROR_X":
 mirror_mod.use_x = True
 mirror_mod.use_y = False
 mirror_mod.use_z = False

operation == "MIRROR_Y":
 mirror_mod.use_x = False
 mirror_mod.use_y = True
 mirror_mod.use_z = False

operation == "MIRROR_Z":
 mirror_mod.use_x = False
 mirror_mod.use_y = False
 mirror_mod.use_z = True

selection at the end -add
 ob.select= 1
 ob.select=1
context.scene.objects.active =
 ("Selected" + str(modifier))
 mirror_ob.select = 0
 bpy.context.selected_objects.append(mirror)
 data.objects[one.name].select = 1

int("please select exactly one object")

-- OPERATOR CLASSES --

types.Operator:
 X mirror to the selected
 object.mirror_mirror_x"
 mirror X"

context:
 context.active_object is not None

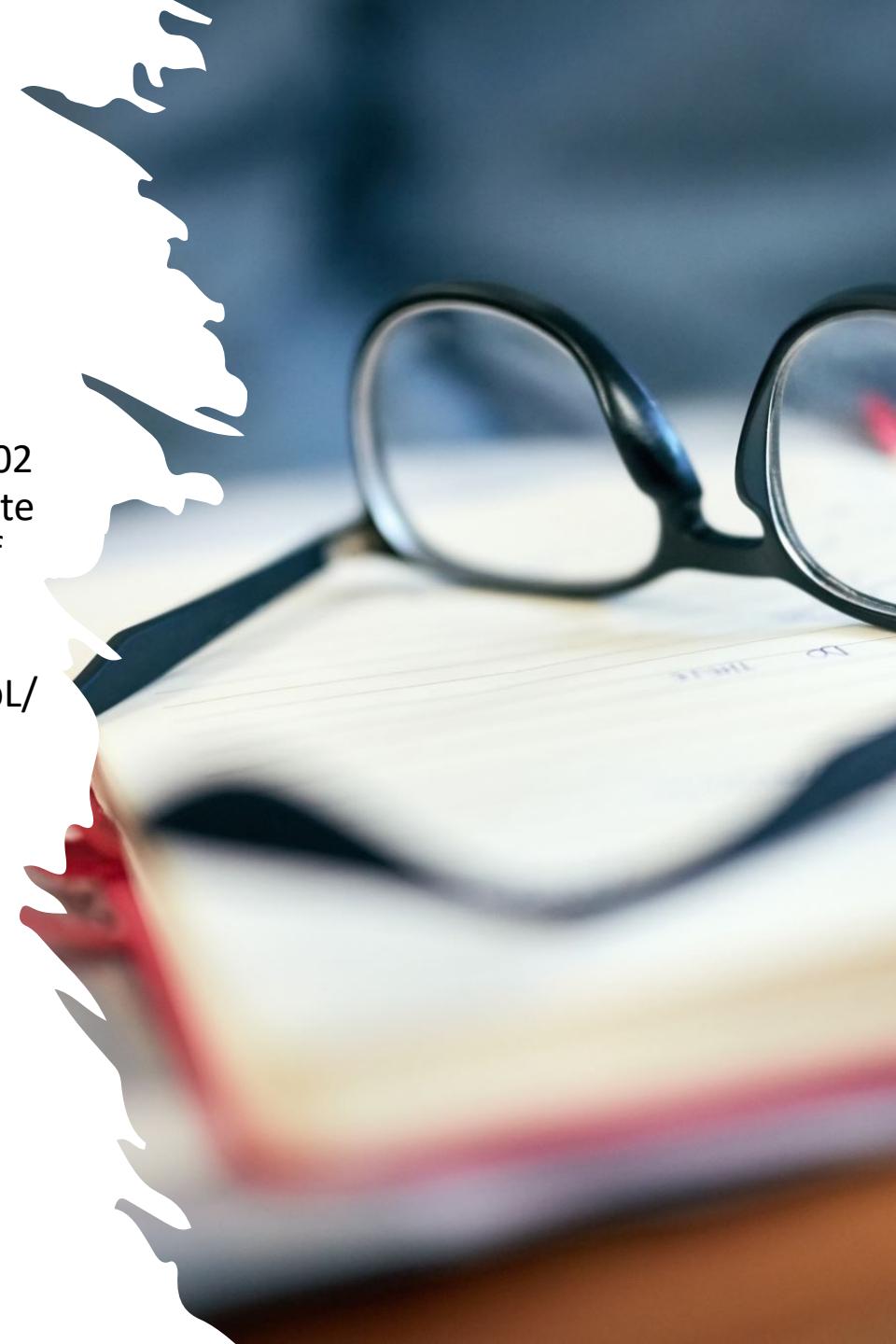
Accessing Software – Command Line

module command options

```
Loading / Unloading commands:  
add | load      modulefile [...] Load modulefile(s)  
rm | unload     modulefile [...] Remove modulefile(s)  
purge           Unload all loaded modulefiles  
reload | refresh          Unload then load all loaded modulefiles  
switch | swap   [mod1] mod2    Unload mod1 and load mod2  
  
Listing / Searching commands:  
list            [-t|-l]        List loaded modules  
avail          [-d|-L] [-t|-l] [mod ...] List all or matching available modules  
aliases          List all module aliases  
whatis          [modulefile ...] Print whatis information of modulefile(s)  
apropos | keyword | search str  Search all name and whatis containing str
```

Getting help

- HPC documentation docs.hpc.arizona.edu
- Support ticket
https://uarizona.service-now.com/sp?id=sc_cat_item&sys_id=2983102adbd23c109627d90d689619c6&sysparm_category=84d3d1acdbc8f4109627d90d6896191f
- Office Hours
<https://gather.town/app/dVsAprPNBVml9NpL/hpc-office-hours>
- HPC consulting
hpc-consult@list.arizona.edu
- Visualization consulting
vislab-consult@list.arizona.edu
- Statistics consulting
stat-consult@list.arizona.edu





ResB(aZ)²

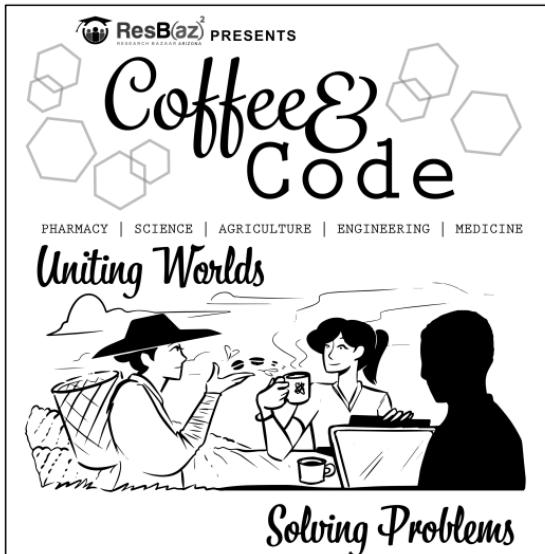
RESEARCH BAZAAR ARIZONA

The Research Bazaar is a worldwide festival promoting the digital literacy emerging at the center of modern research. Check us out @resbazaz 

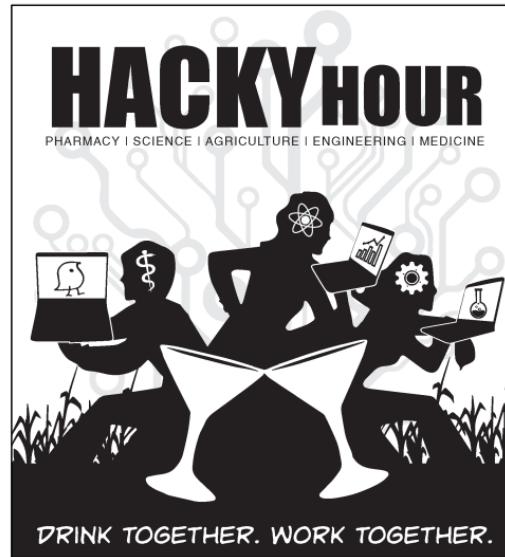
Need help with science or computers? Tired of quietly suffering trying to figure it out?
Come hang out with us; it's free!* Just want to hang out? Also free!*

Not into the bar scene?

Not into mornings?



Weekly, Tuesdays 8-10
Catalyst Café (Keating Building)
1657 E Helen St



Weekly, Thursdays 4-7
Snakes & Lattes (Main Gate Square)
988 E University Blvd

* No beverages are provided. But it's still fun and fairly cheap one way or the other.*

* Neither fun nor cheap is a guarantee. But if you are still reading this, and it's funny: we feel more confident about the first part.