Introduction to HPC

Research Technologies Department
University of Arizona

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

Intro to HPC*

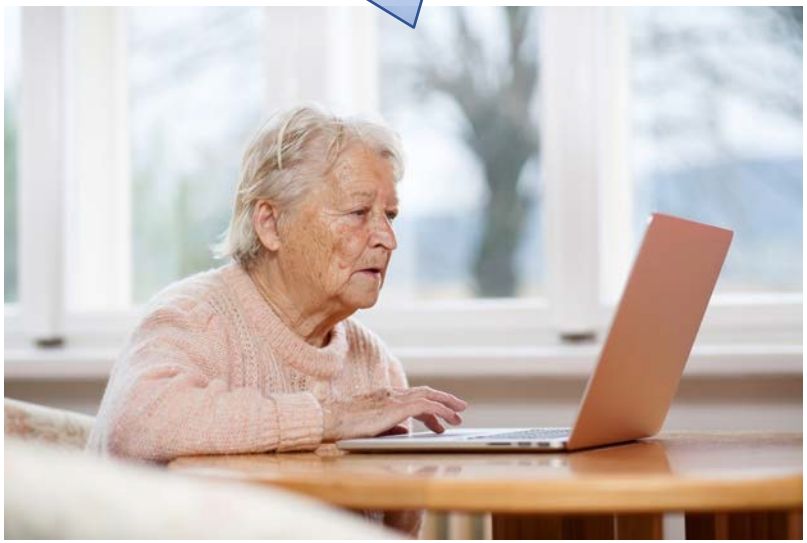
*HPC – high-performance computing

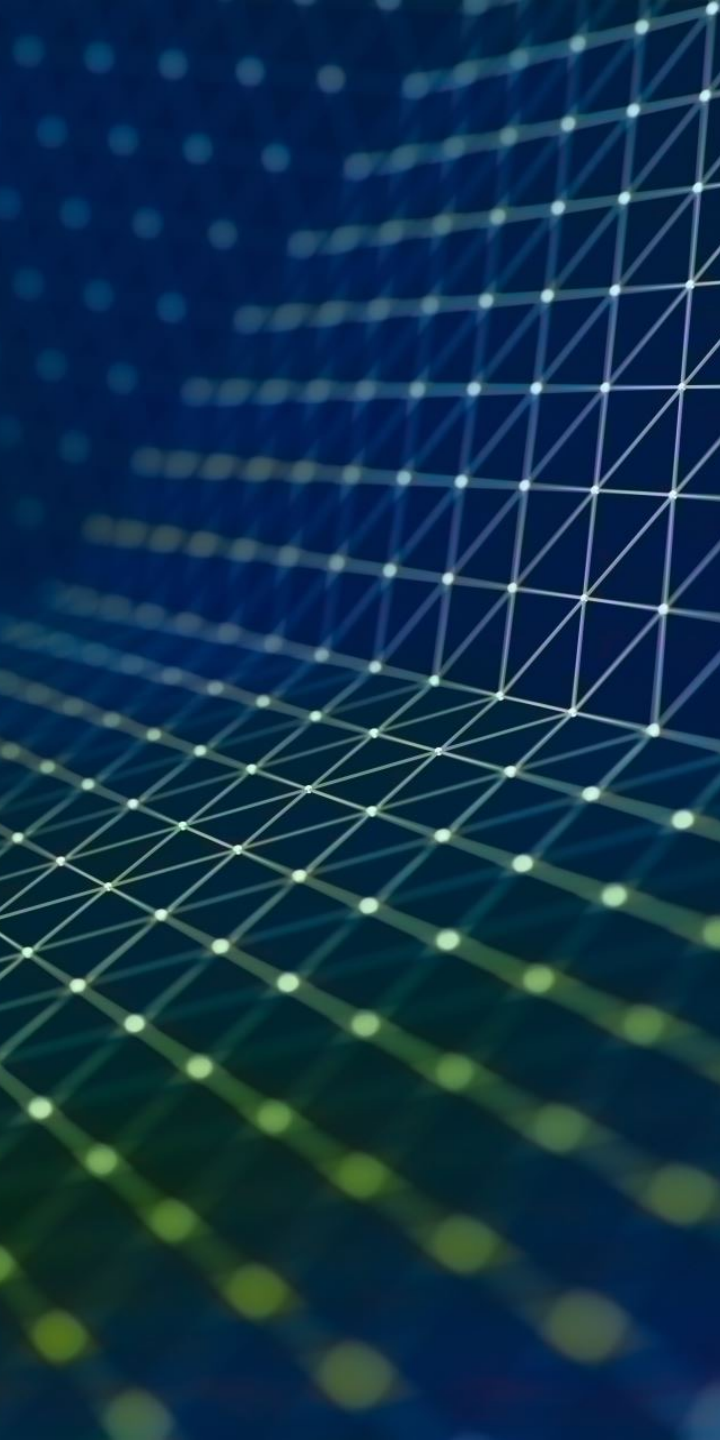
- Why use HPC?
- Anatomy of the HPC cluster
- Basics of working with the Linux shell
- Submitting jobs

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?

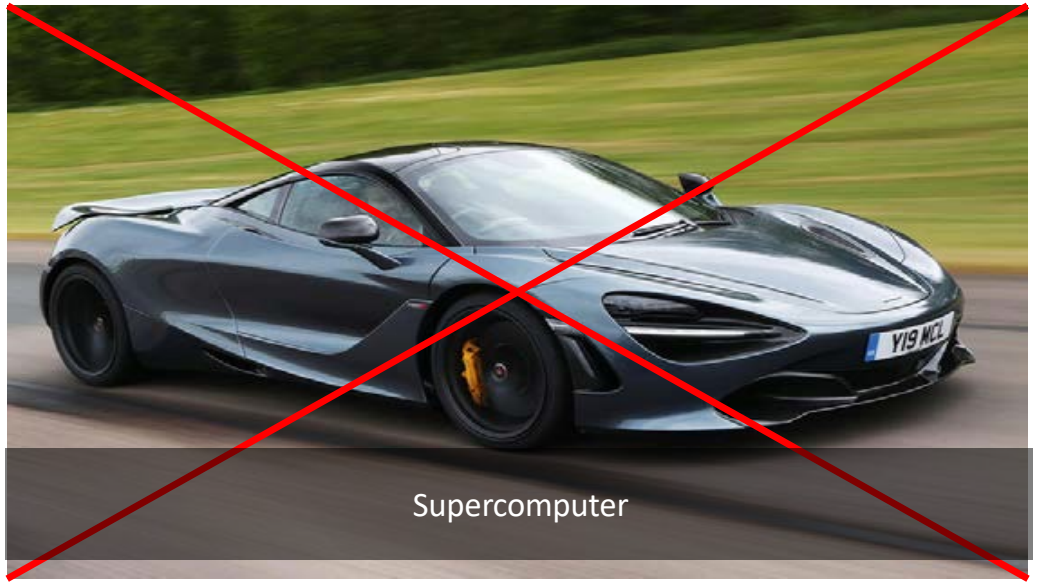
Problems

- 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).

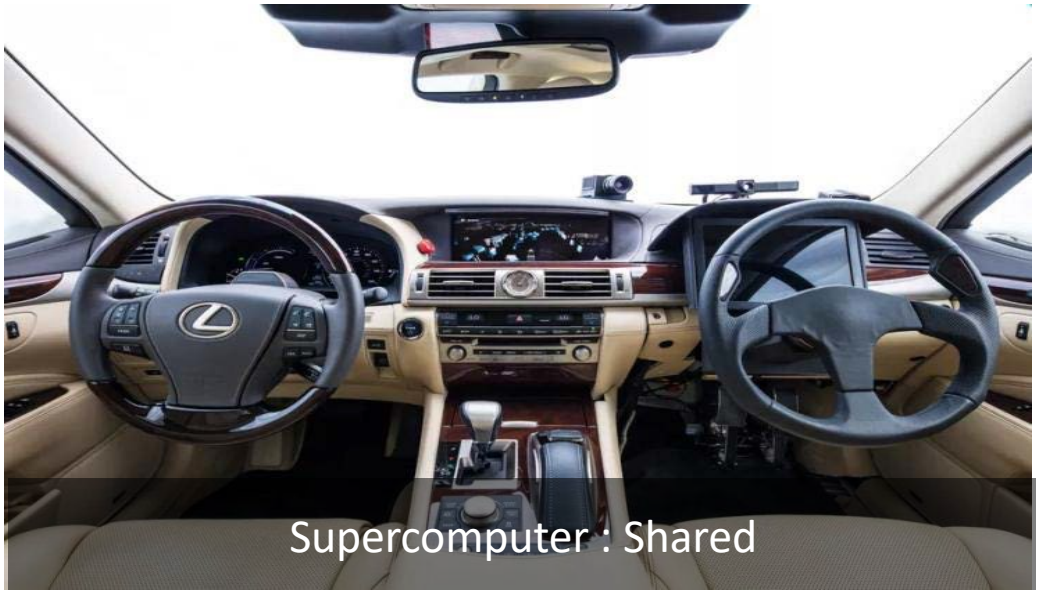
- Supercomputer is a commonly used nickname.



Why HPC?

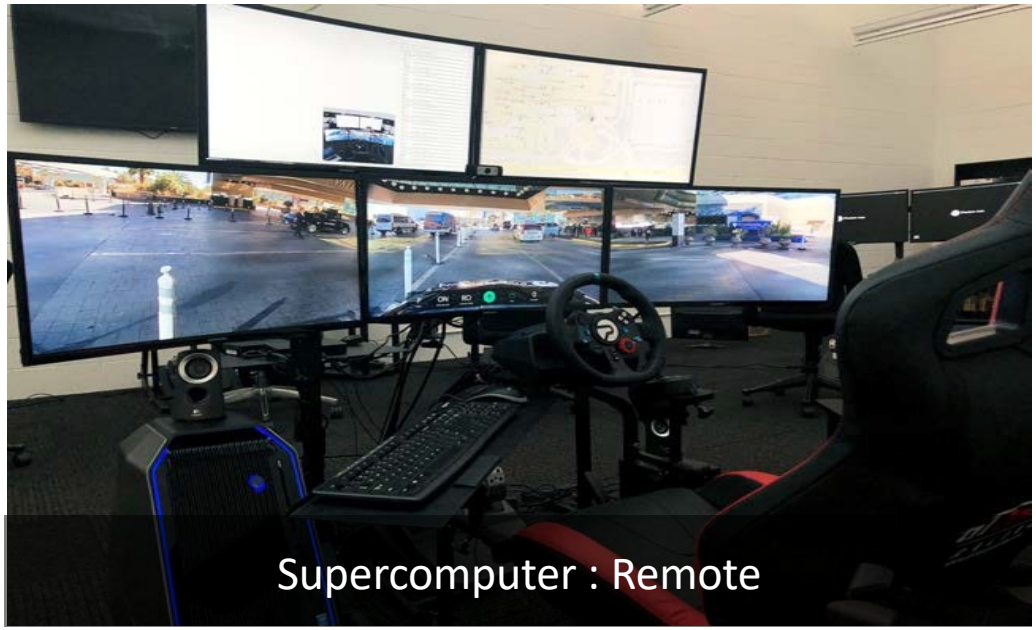
Why HPC?

Laptop : Personal



Supercomputer : Shared

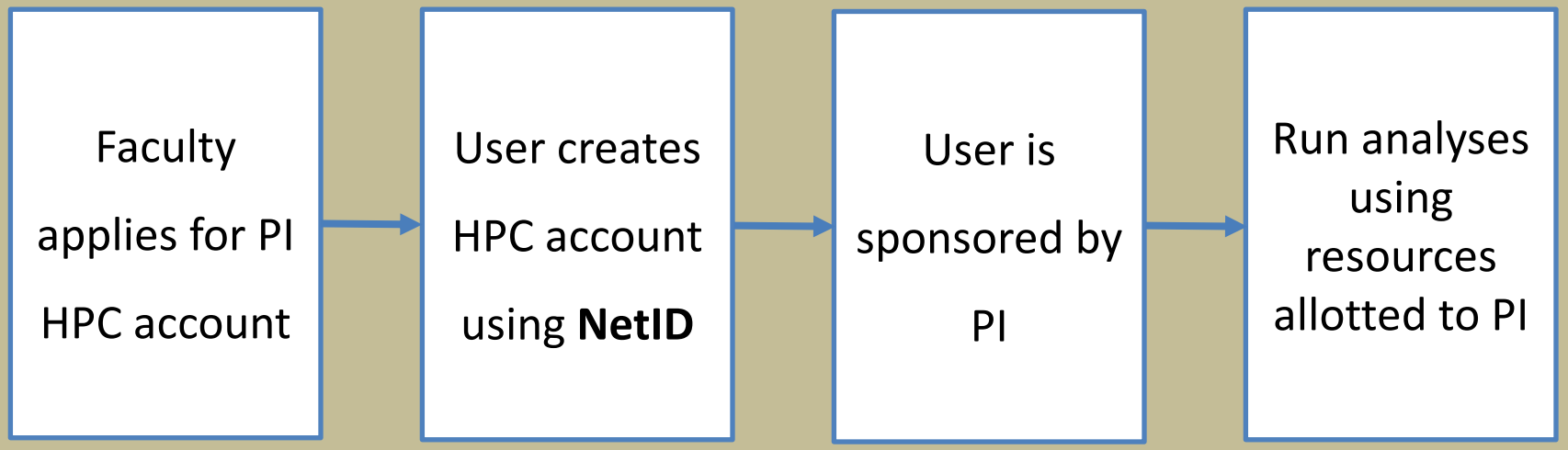
Why HPC?



Why HPC?

Why HPC?

Gaining Access to UA HPC



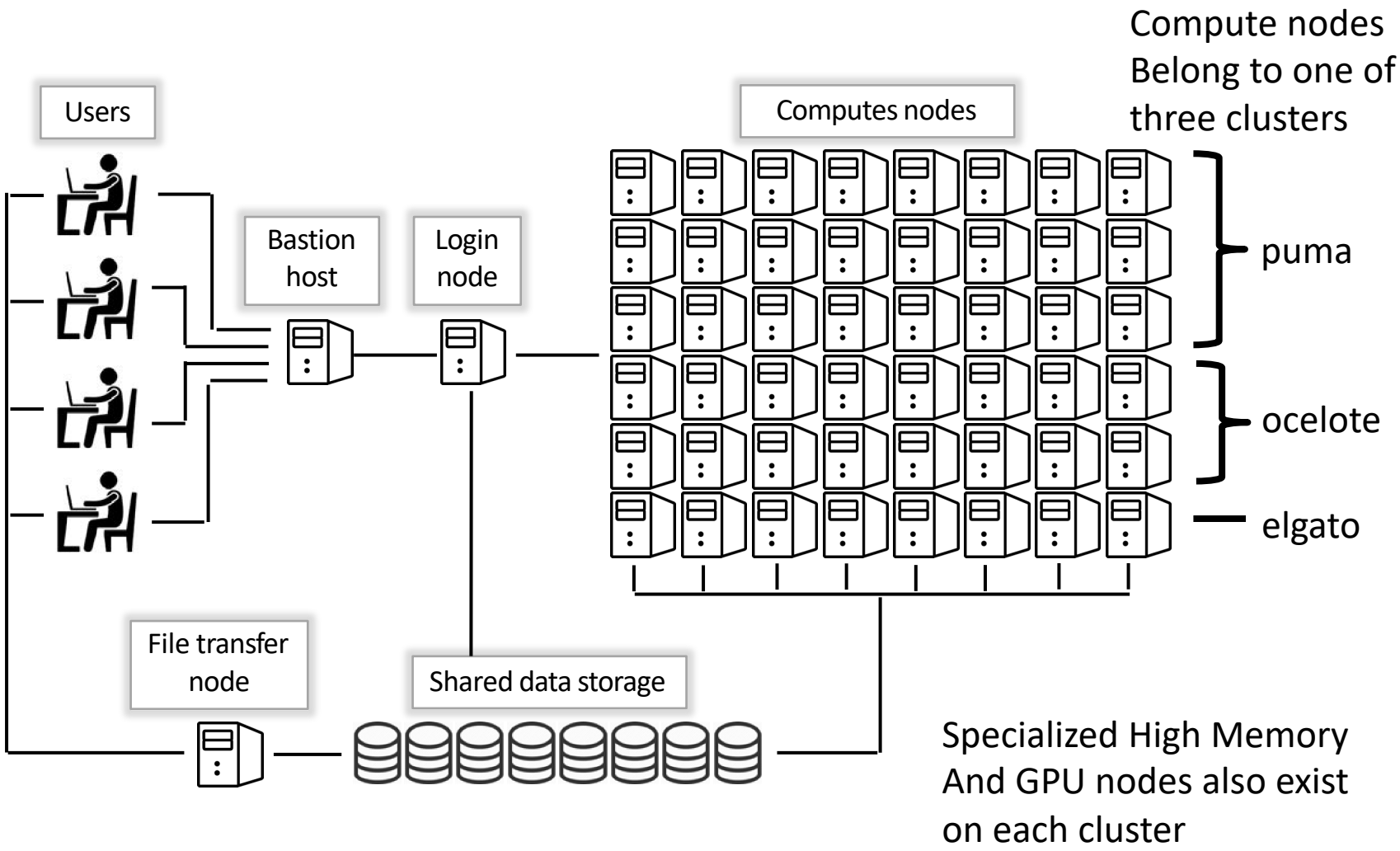
Instructions for PIs and sponsored researchers are here:

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


Sponsors
Karen Williams | Interim CIO; Dean, University Libraries
Dr. Kimberly Espy | Senior Vice President, Research
Dr. Skip Garcia | Senior Vice President, Health Sciences
high-throughput computing

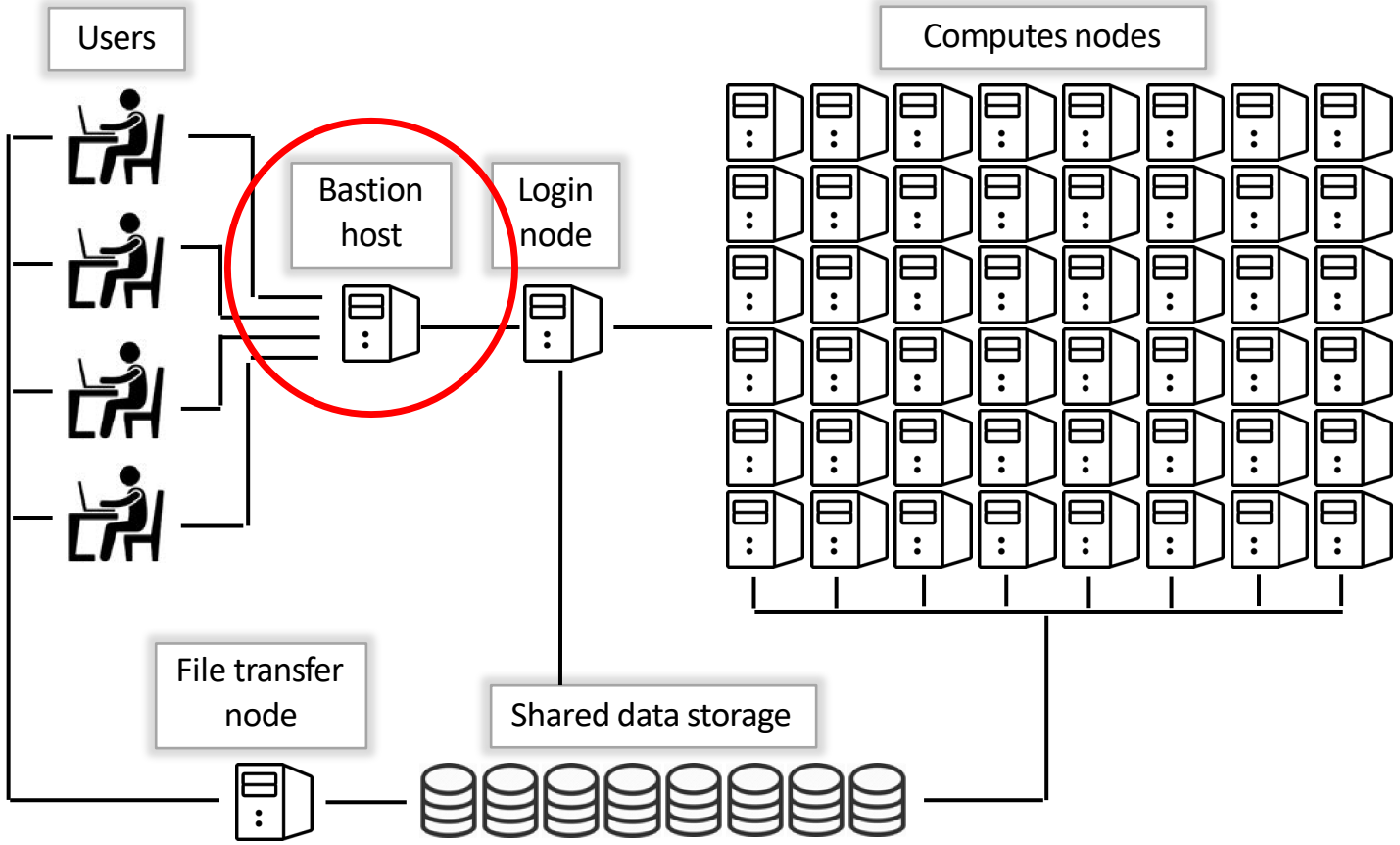
Ocelote

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

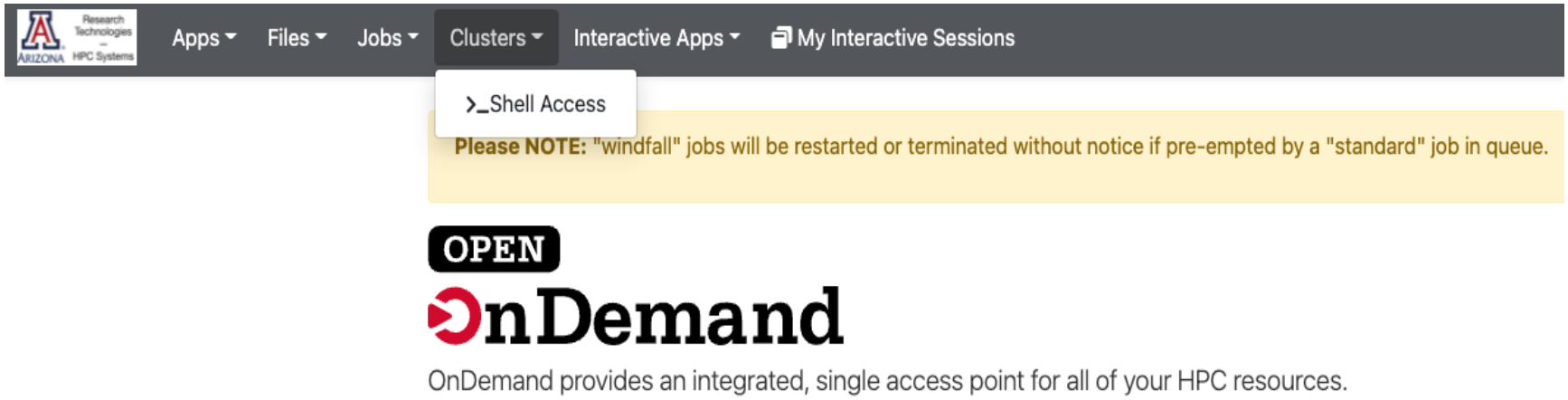
- Includes Terminal app

Windows

- Putty
- MinGW
- Git Bash

Connecting with Web Browser

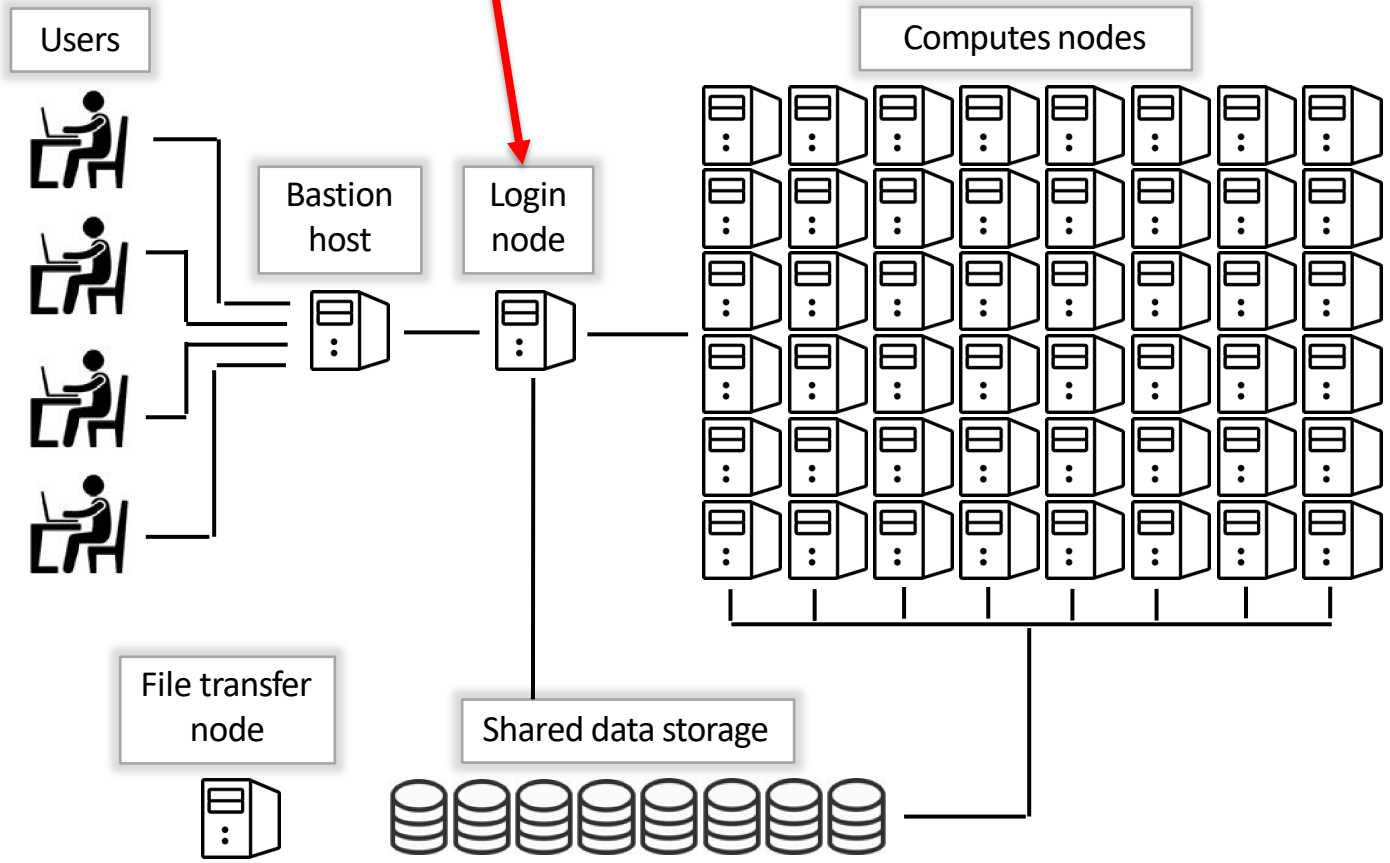
- Open **ood.hpc.arizona.edu** in your web browser and login with your NetID and password.
- From the “Clusters” drop-down menu “Shell Access"



- 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

Cluster your
jobs will be
submitted to

Node name
(where are you)

Prompt
(what are you going to do)

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

Command

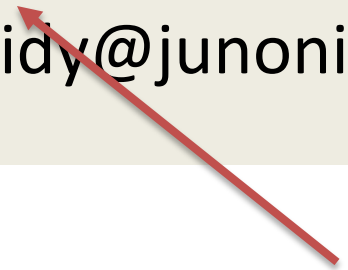
```
(puma) [chrisreidy@junonia 14:16:33 ~]$ whoami
chrisreidy
(puma) [chrisreidy@junonia 14:16:38 ~]$
```

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 ~]$
```



- ~ 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
```

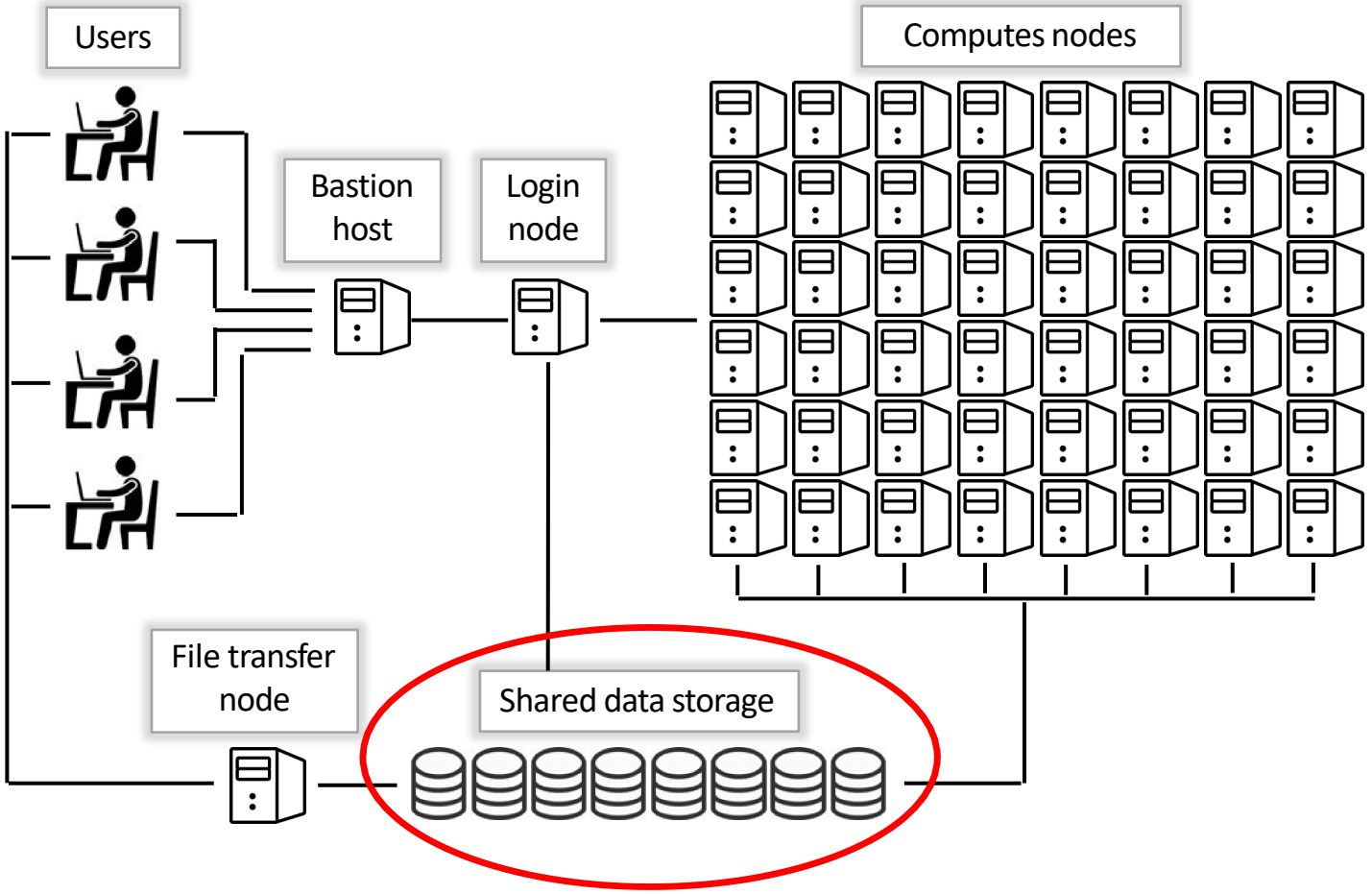
Working with a Linux shell

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

https://public.confluence.arizona.edu/display/UAHPC/Training#Training-LinuxSelfGuided

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 300 days

- /tmp

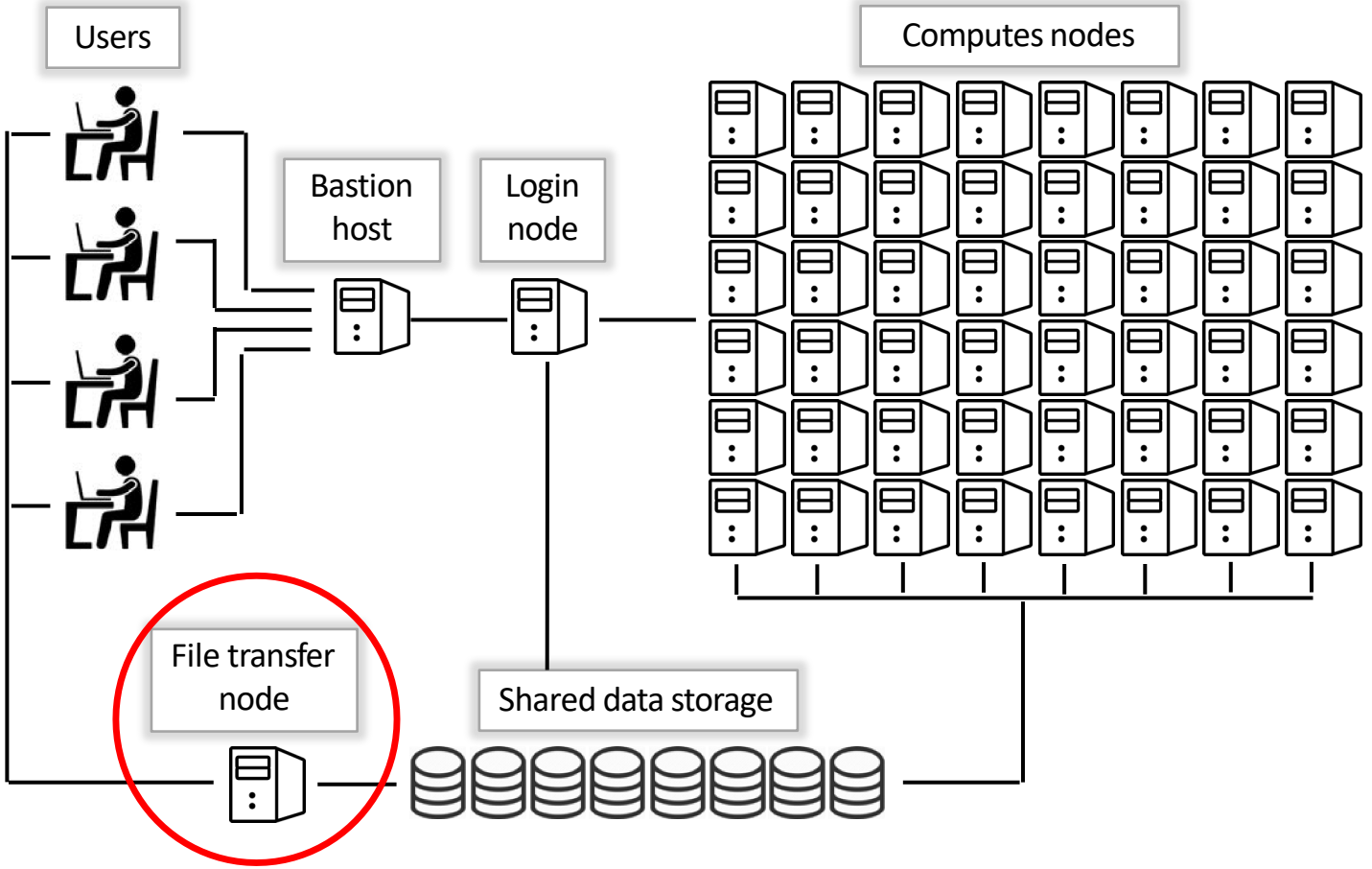
Every Puma node has about 1.4TB on a NVME SSD

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
    - 70,000 cpu hours on Ocelote
    - 7,000 cpu hours on Elgato
    - Limits on GPU nodes
    - Not preempted
  - windfall
    - Unlimited
    - Preemptable

Transferring Files



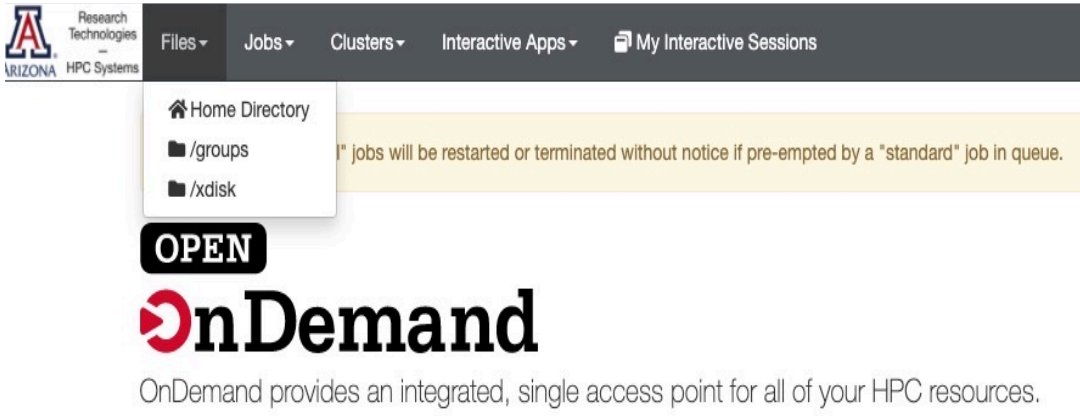
filexfer.hpc.arizona.edu

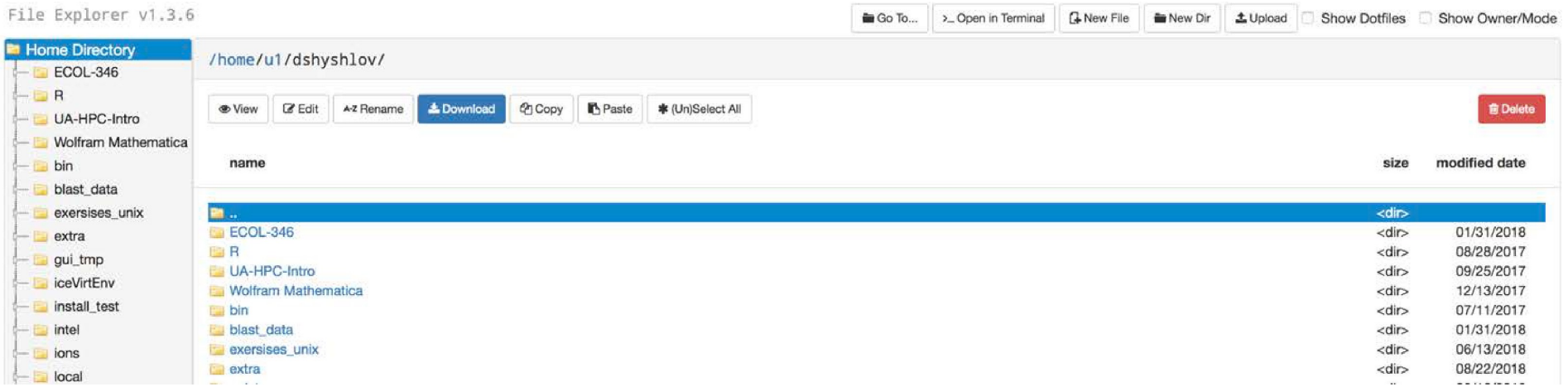
Transferring Files

- 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

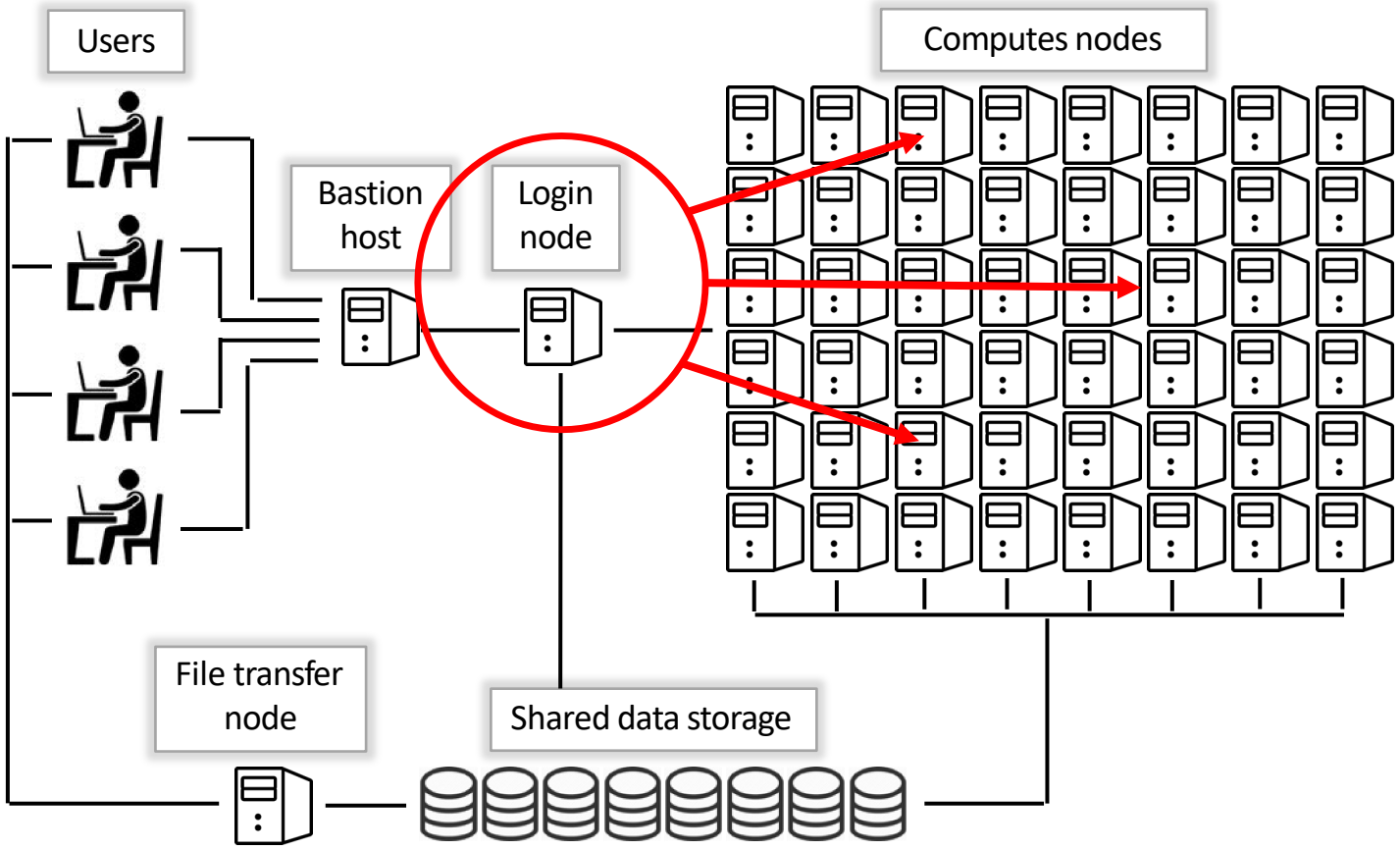
Transferring Files with OnDemand

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





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

```
$ cd cd intro-to-hpc
$ 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

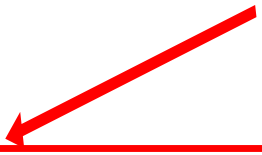
It's a bash shell script

```
#!/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

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
Cancel a queued or running job

$ 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:

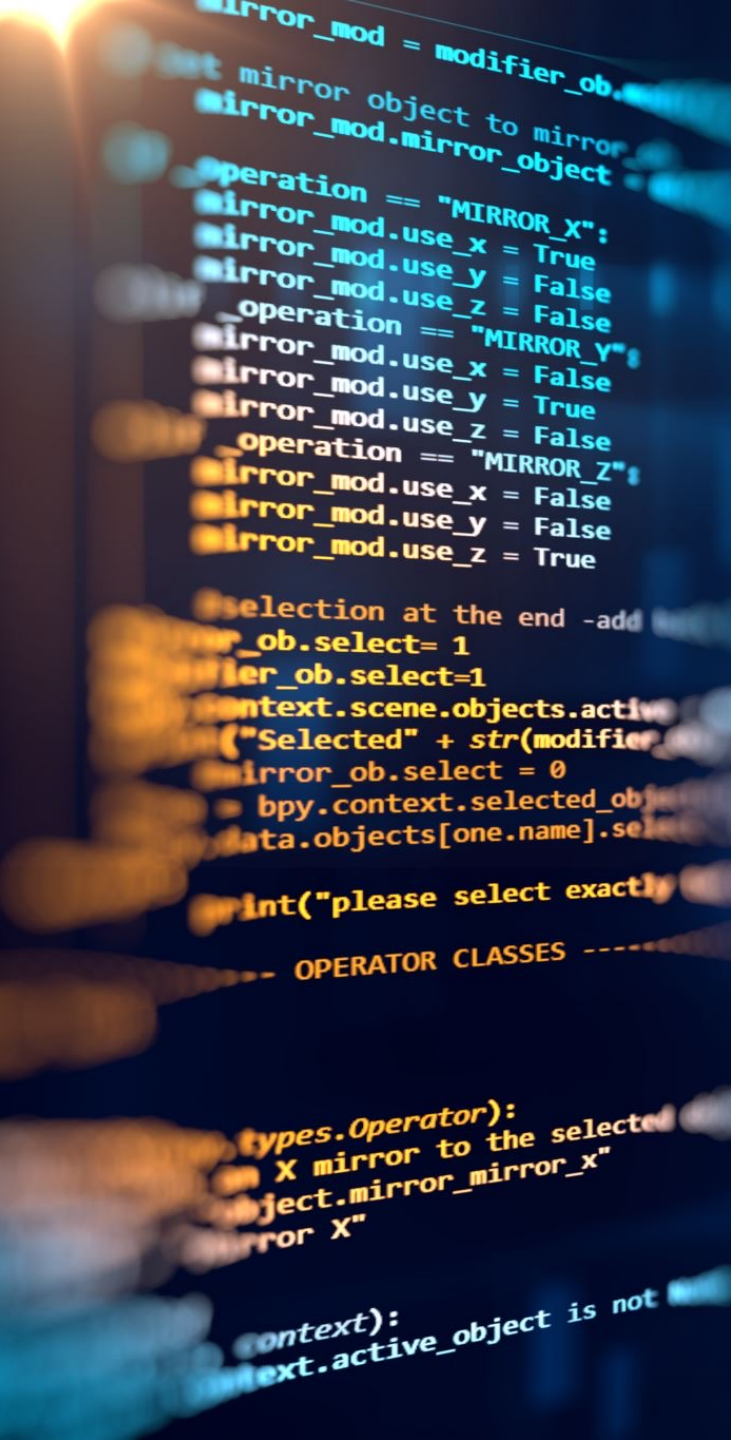
- You need to compile code
- You need test runs
- You need access to modules

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]$



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

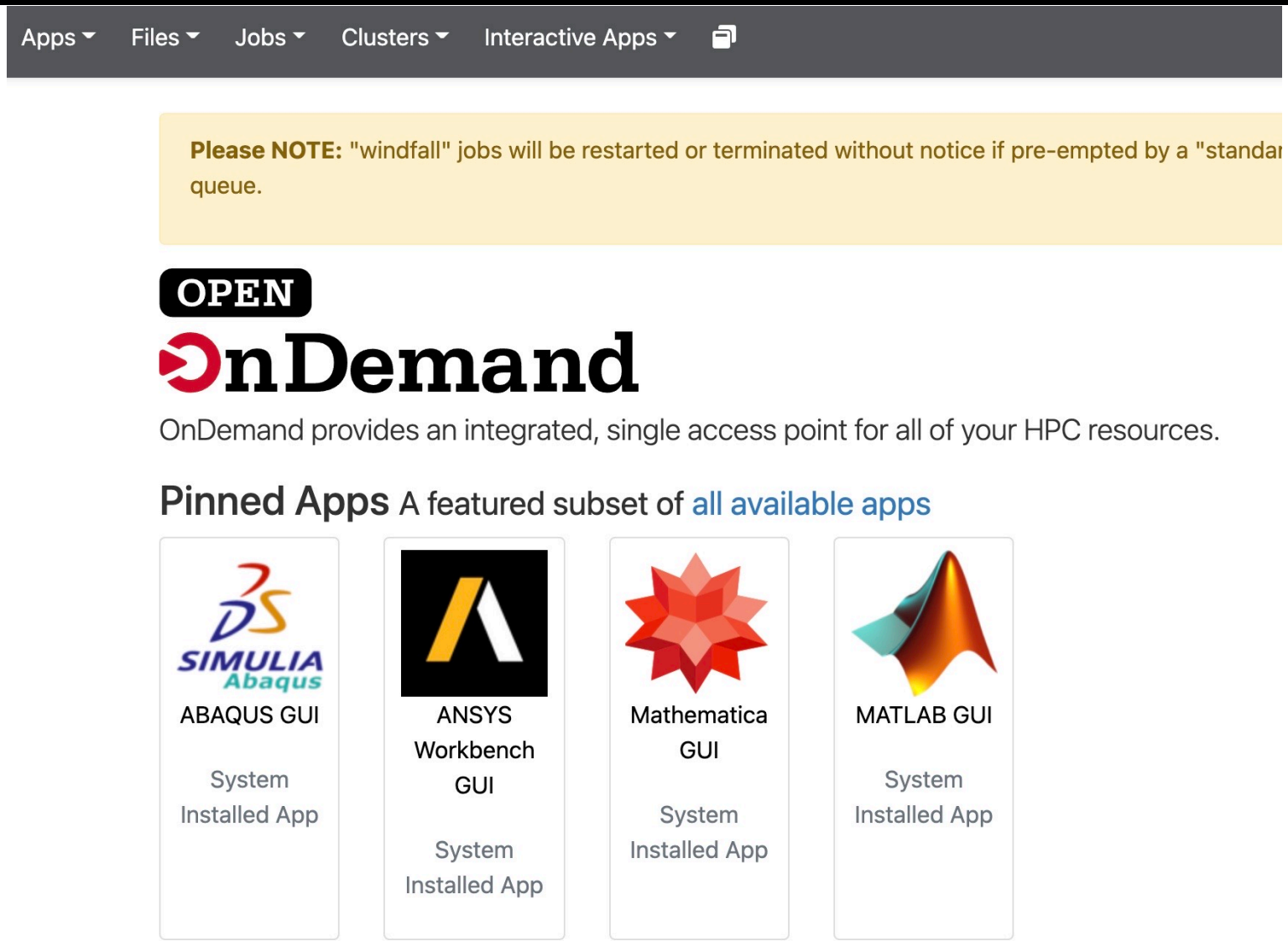
$ shell

$ ocelote

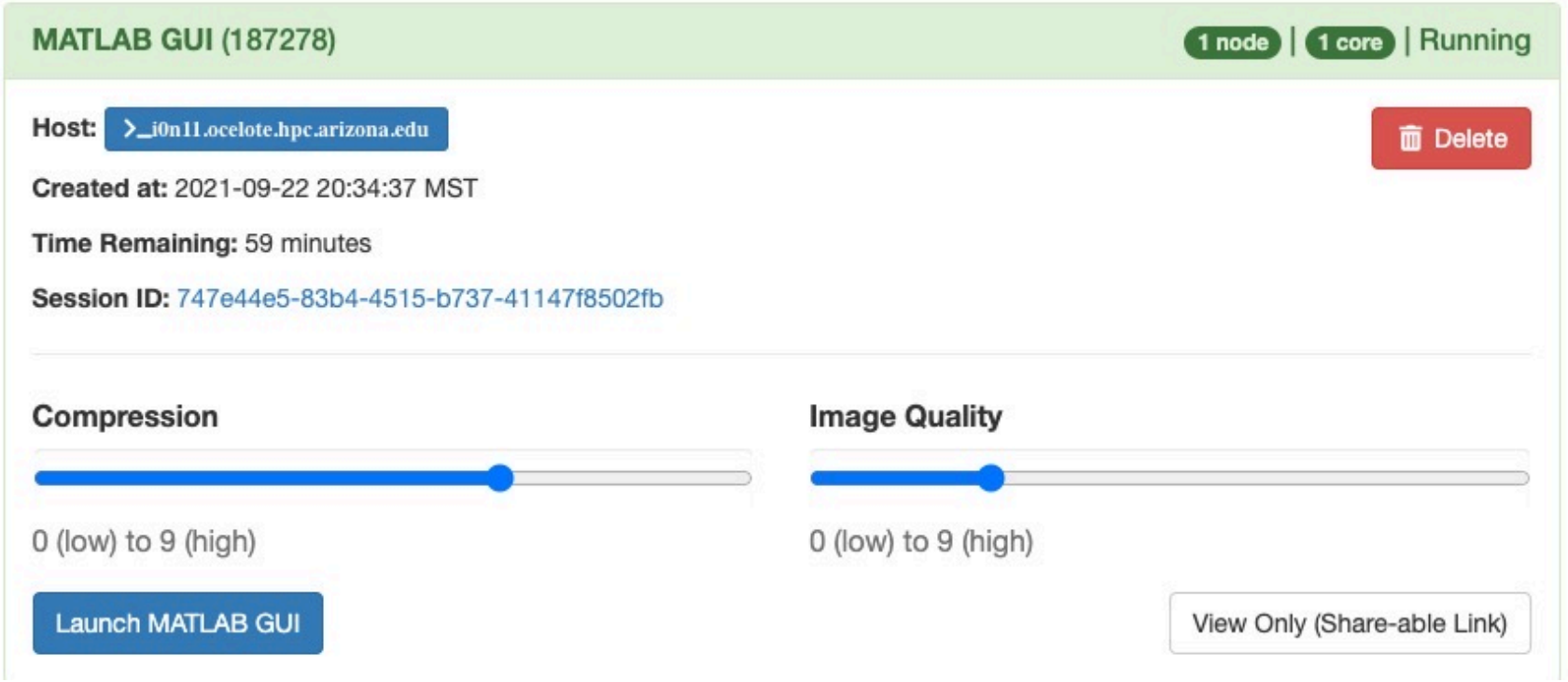
$ interactive

$ module avail

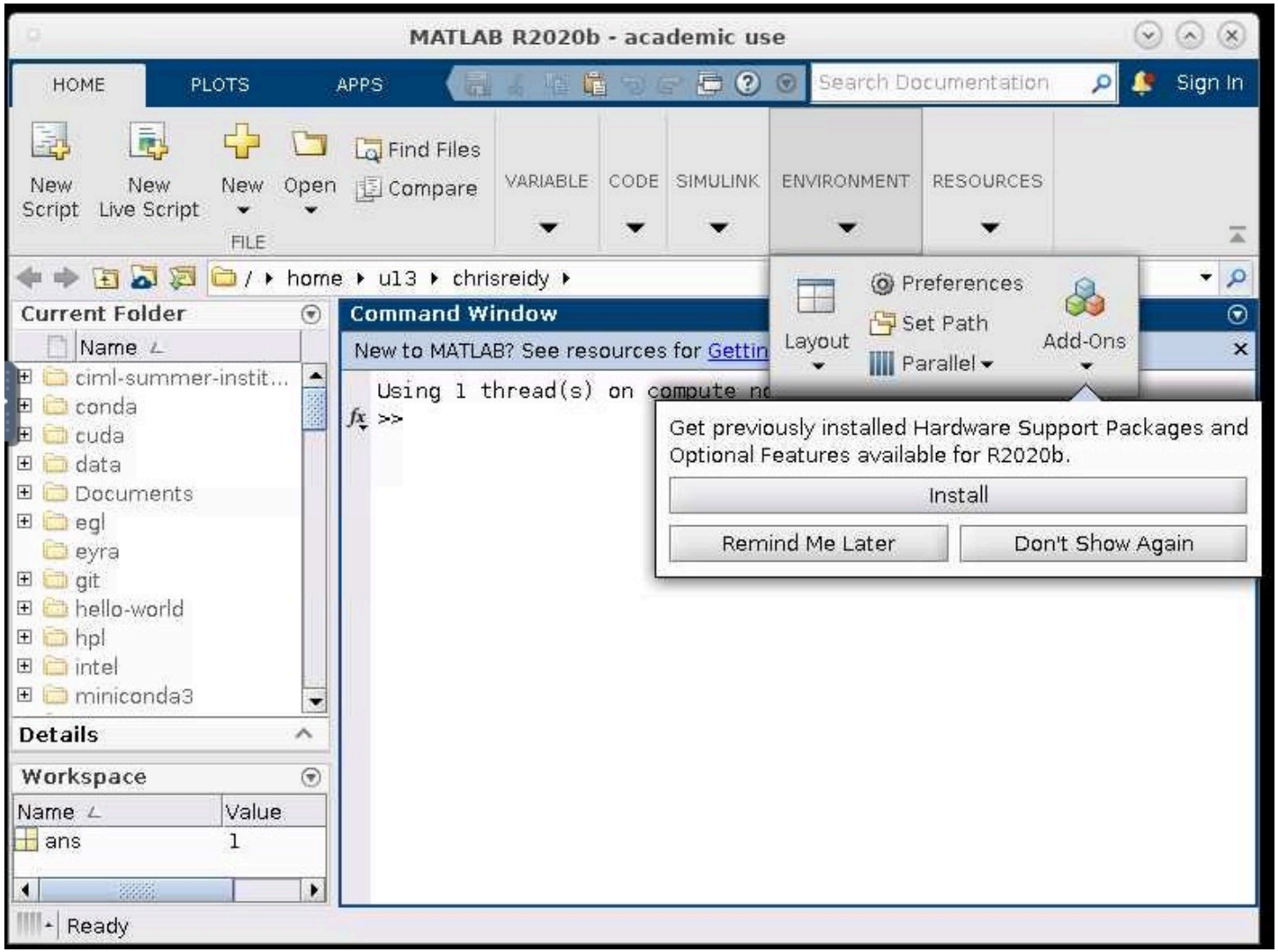
Accessing Software with OnDemand
ood.hpc.arizona.edu

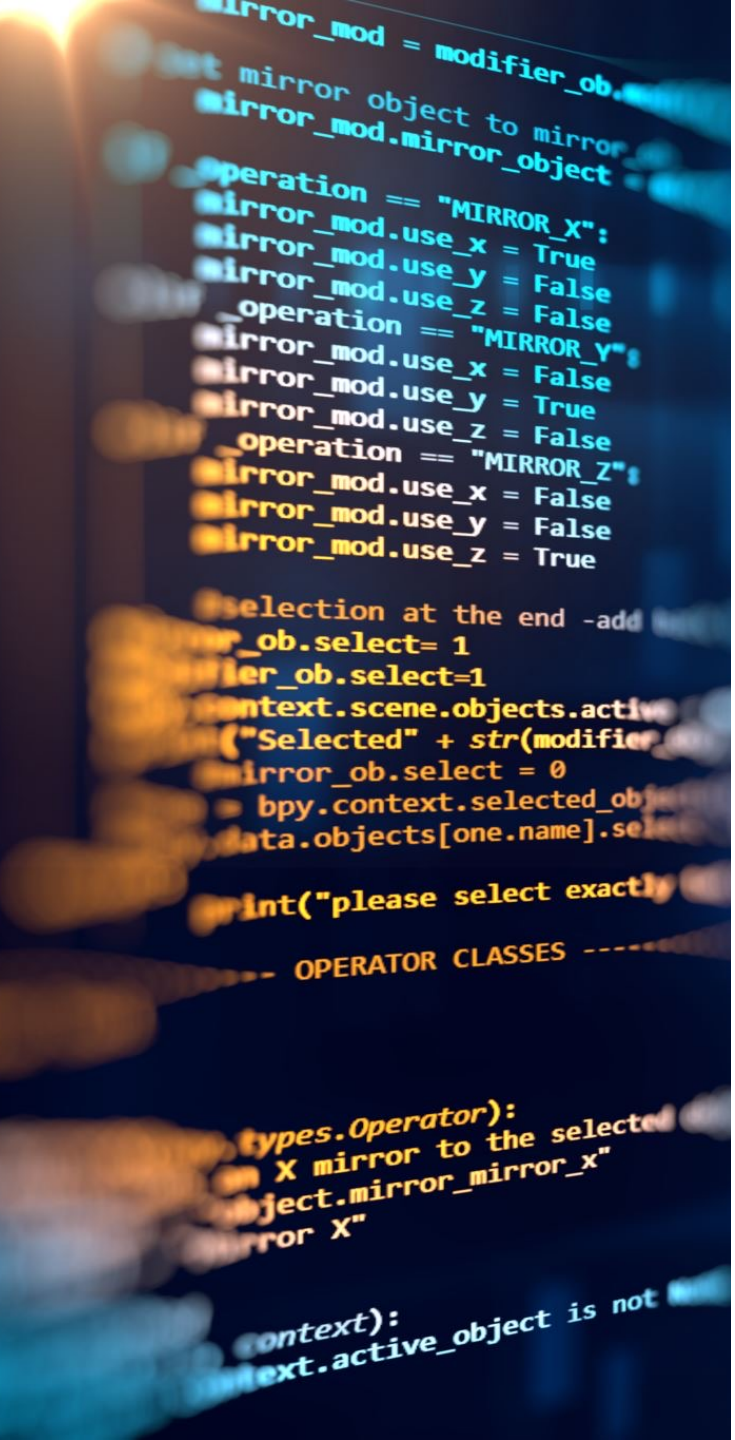


Accessing Software with OnDemand



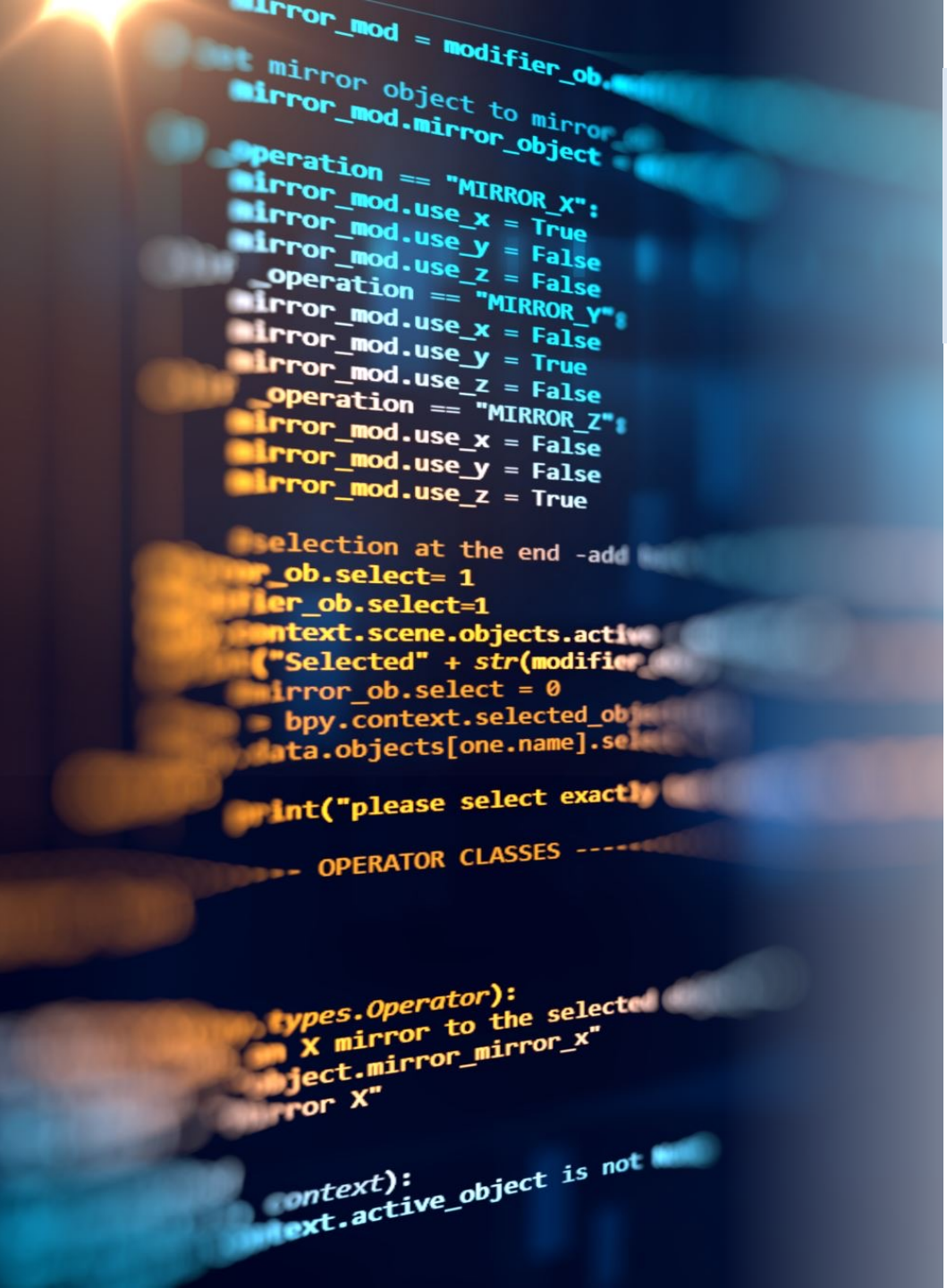
Accessing Software with OnDemand





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

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/dVsAprPNBVmI9NpL/hpc-office-hours
- HPC consulting hpc-consult@list.arizona.edu
- Visualization consulting vislab-consult@list.arizona.edu
- Statistics consulting stat-consult@list.arizona.edu

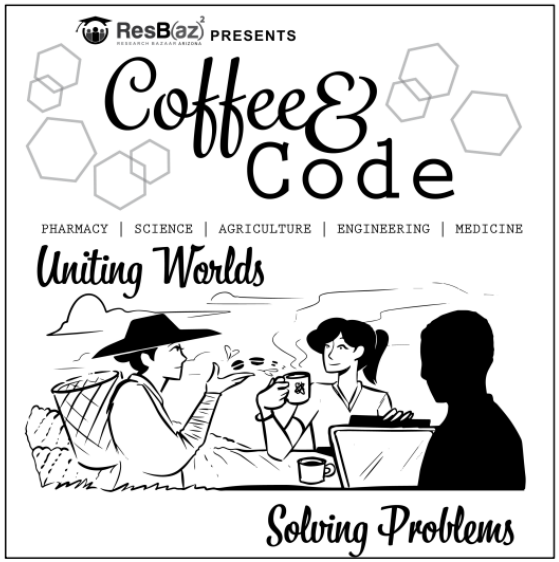
ResB(az)^2

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

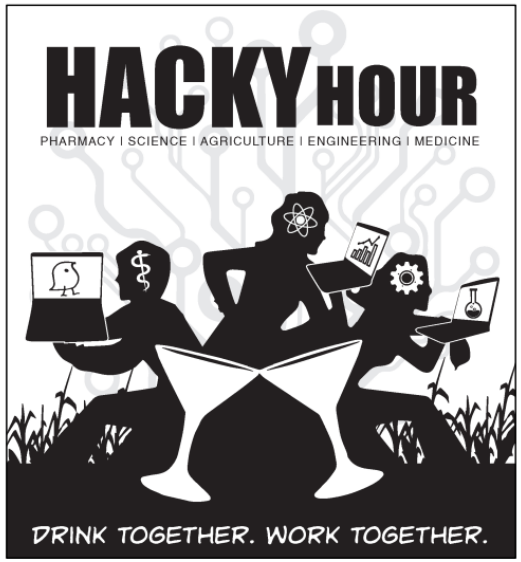
Need help with science or computers? Tired of quietly suffering trying to figure it out? Come hang out with us; it's free!* Just want to hang out? Also free!*

Not into the bar scene?



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

Not into mornings?



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.