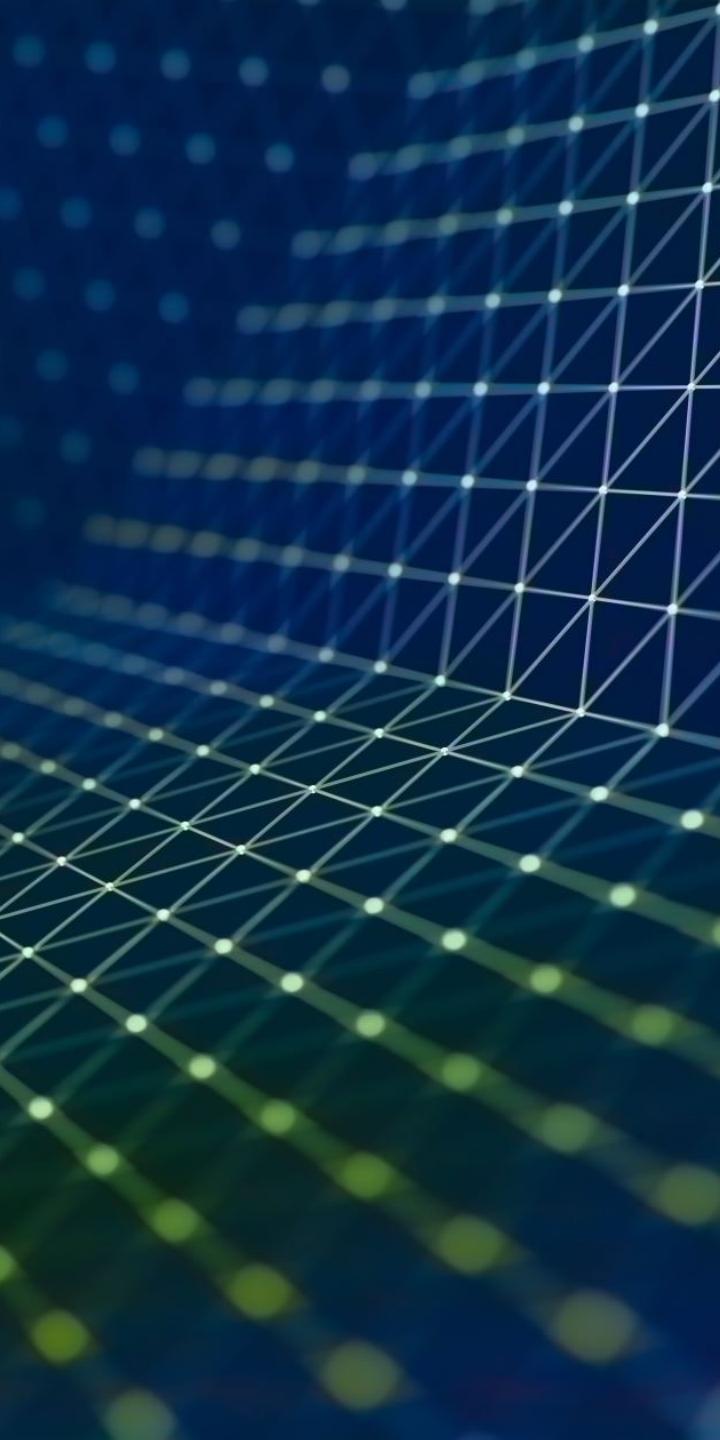


Intro to HPC

Research
Technologies
Department
University of
Arizona

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*

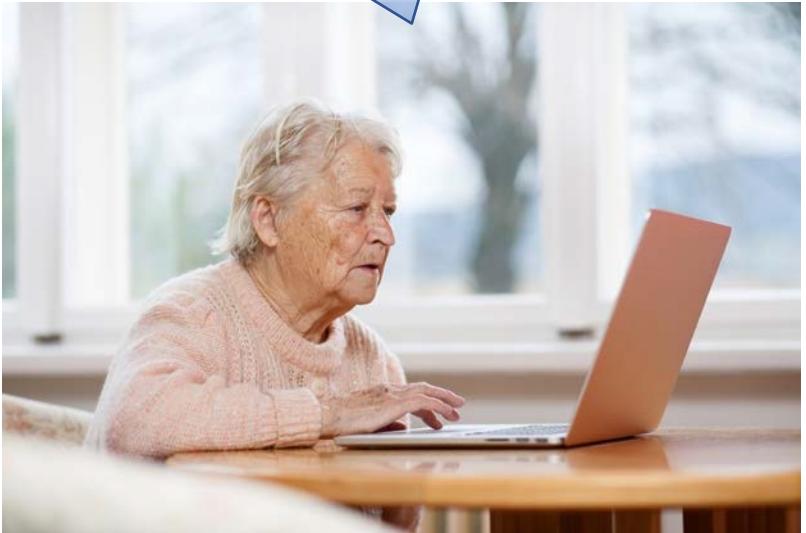
*HPC – high-performance computing

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

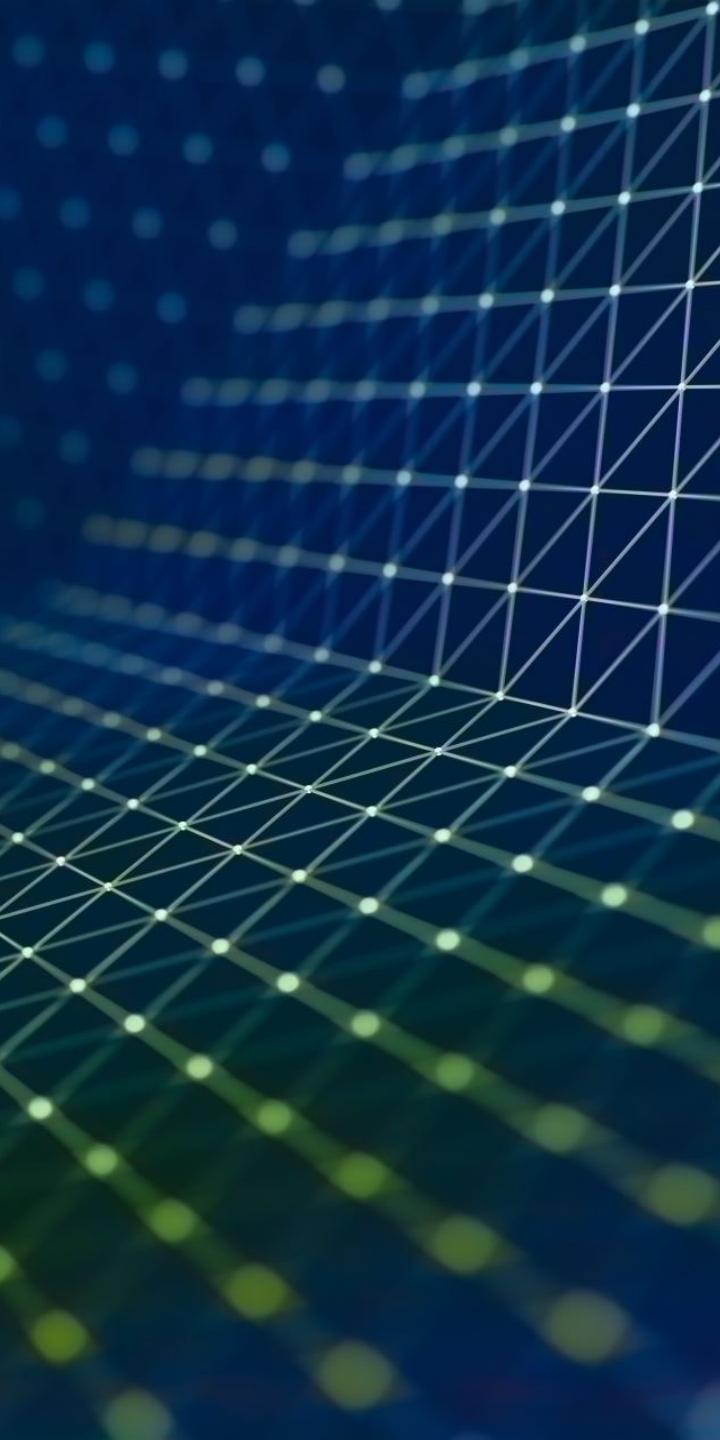
Why HPC?



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

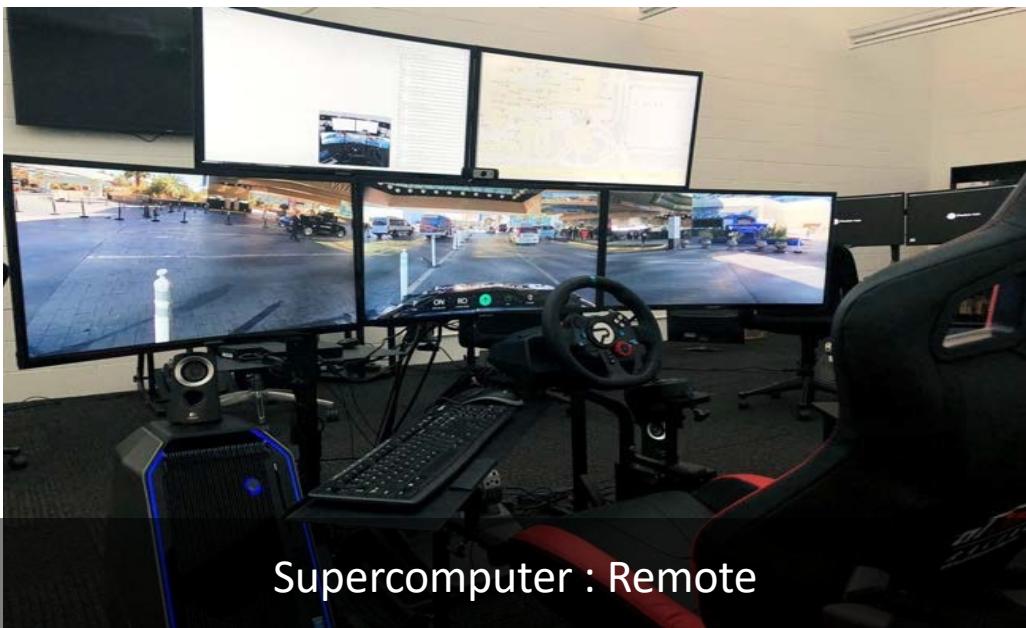


Supercomputer : Shared

Why HPC?



Laptop : Local



Supercomputer : Remote

Why HPC?



Laptop : Interactive



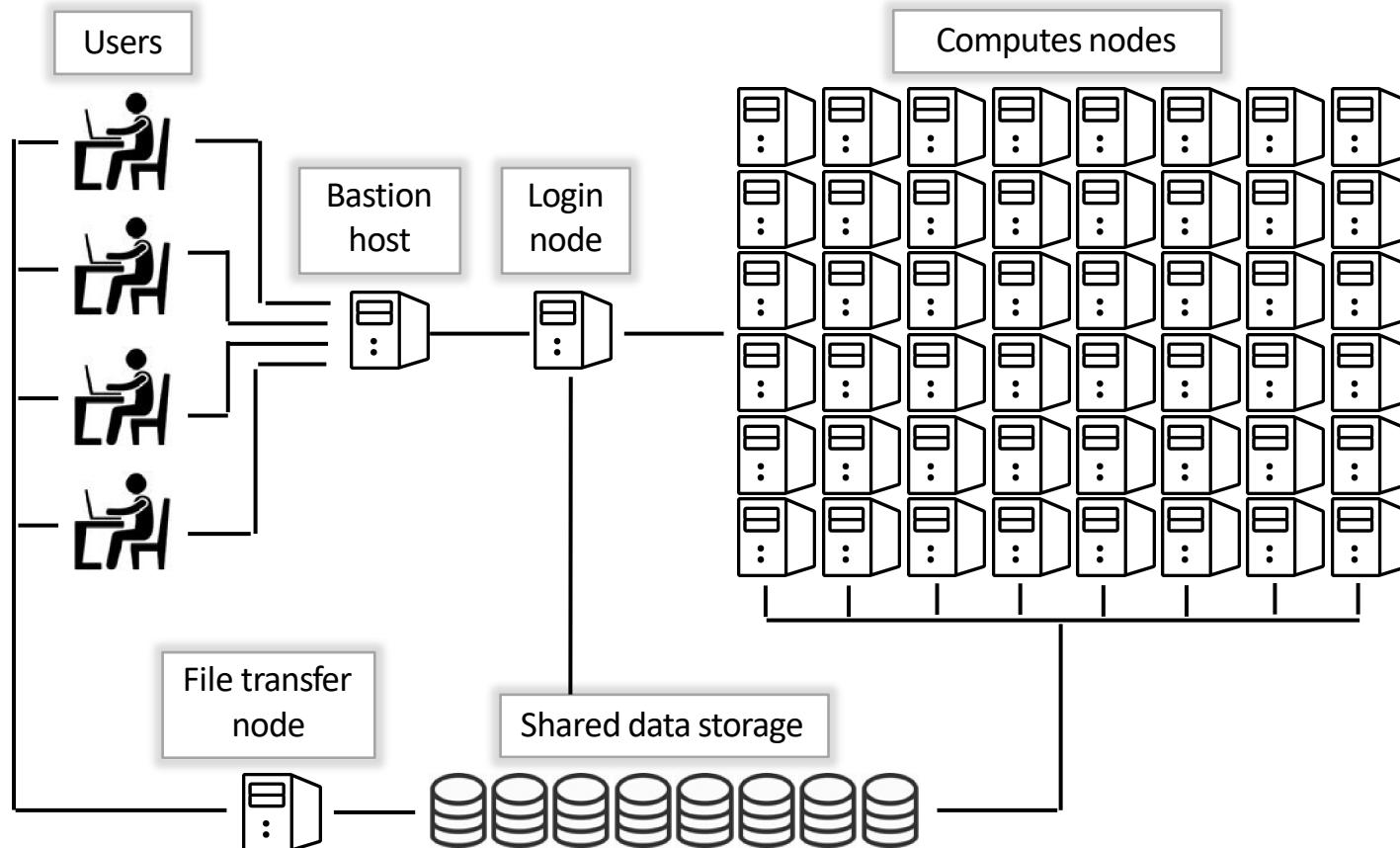
Supercomputer : Batch

Why HPC?



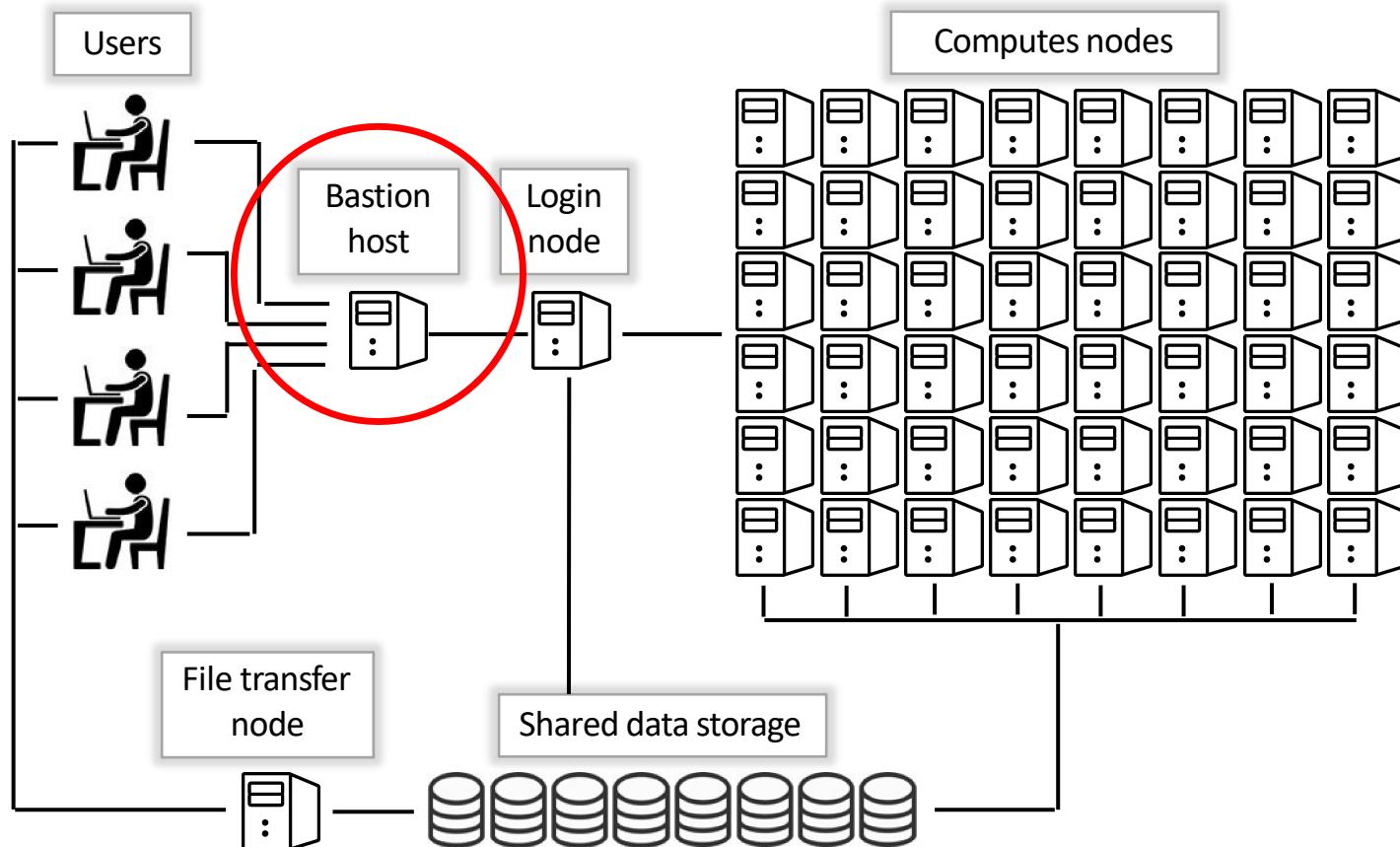
Ocelote

The diagram of the UA HPC cluster



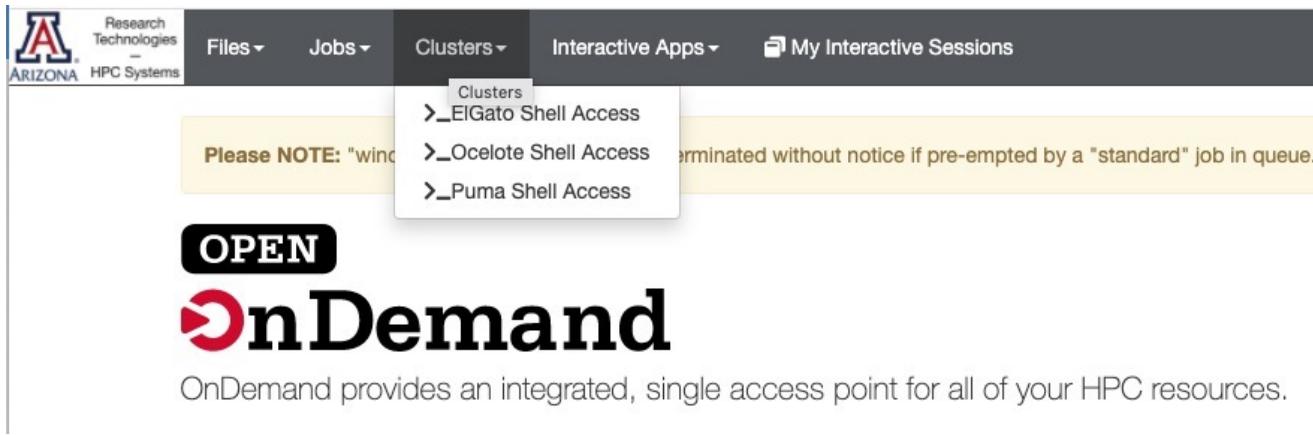
Connecting to Ocelote

ssh netid@hpc.arizona.edu
shell



Connecting to Puma (web browser)

- Open **ood.hpc.arizona.edu** in your web browser and login with your NetID and password.
- From the “Clusters” drop-down menu choose which HPC cluster you would like to access:



- Exercise - connect to Ocelote.

Command line

Your NetID
(who are you)

Name of the current
directory

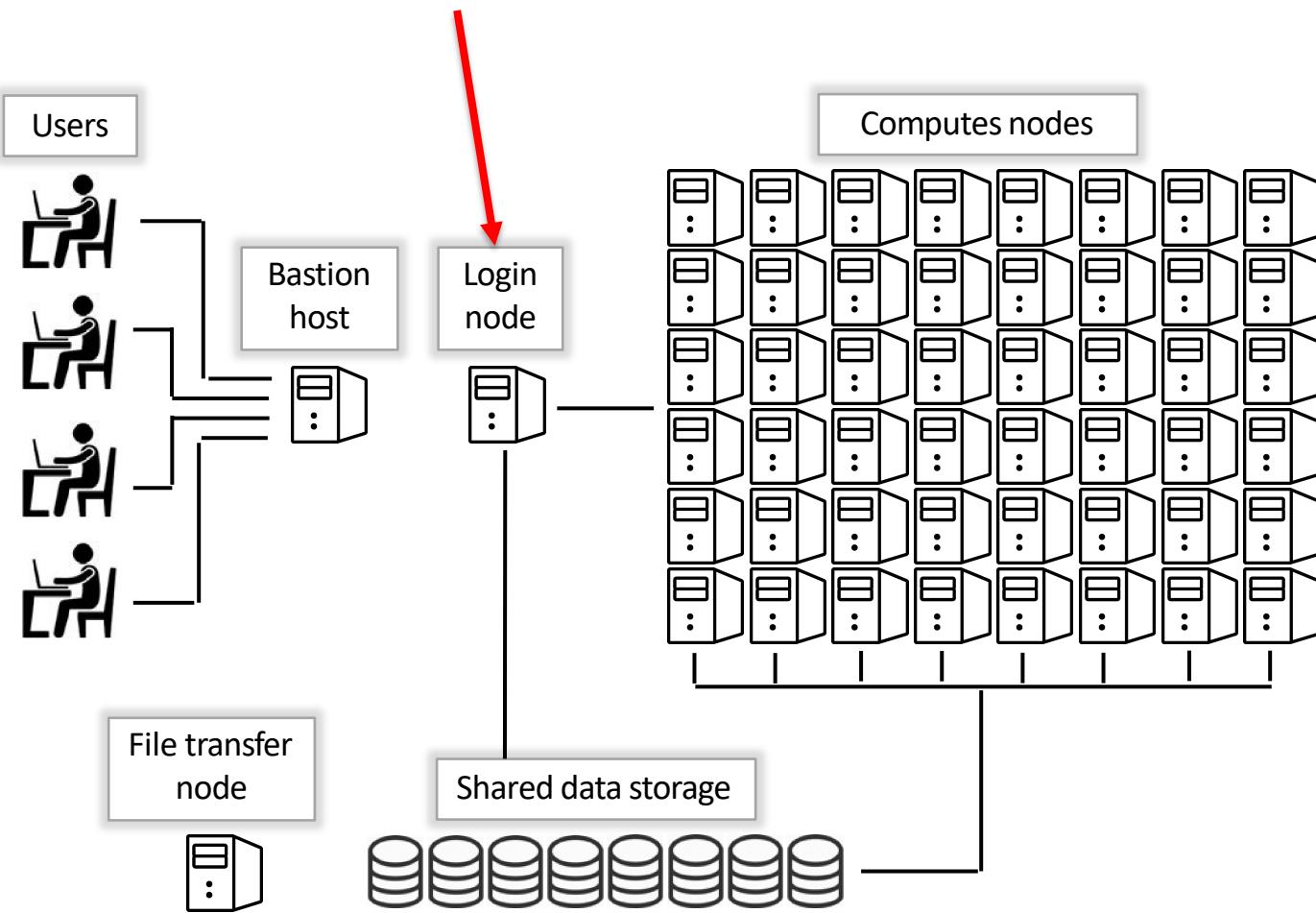
```
(puma) [chrisreidy@wentletrap 16:03:26 ~]$ ls
```

Node name
(where are you)

Prompt
(what are you going to do)

Login node

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





Login Node aka Submit Node



Compute Nodes

Login
Node

Login node

- 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



Working with a Linux shell

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@wentletrap 08:37:20 Intro_to_HPC]\$
interactive

Working with a Linux shell

Command

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

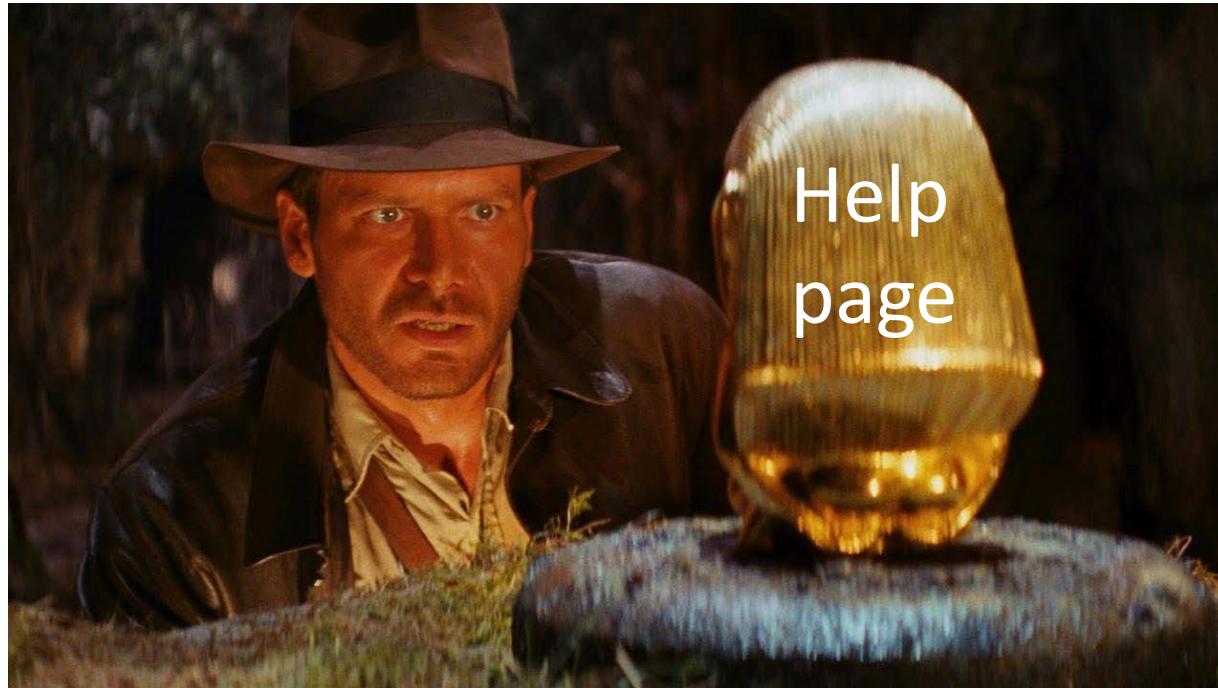
Output

Working with a Linux shell

```
[dshyshlov@login2 ~]$ which --help
```

Usage: /usr/bin/which [options] [--] COMMAND [...]

Help flag



Working with a Linux shell

```
[dshyshlov@login2 ~]$ which whoami  
/usr/bin/whoami  
[dshyshlov@login2 ~]$ █
```

```
[dshyshlov@login2 ~]$ whoareyou  
-bash: whoareyou: command not found  
[dshyshlov@login2 ~]$ █
```

Working with a Linux shell

```
[dshyshlov@login2 ~]$ pwd  
/home/u1/dshyshlov  
[dshyshlov@login2 ~]$ █
```

Path to
Working
Directory

Name of the current
directory

- ~ is a shortcut for your /home directory

Working with a Linux shell

- List all the files and directories

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

- Make a directory

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

- List all the files and directories again

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

Working with a Linux shell

- Change directory

```
[dshyshlov@login2 ~]$ cd Intro_to_HPC  
[dshyshlov@login2 Intro_to_HPC]$ █
```

- Go back a level

```
[dshyshlov@login2 Intro_to_HPC]$ cd ..  
[dshyshlov@login2 ~]$ █
```

- Change directory using absolute path

```
[dshyshlov@login2 ~]$ cd ~/Intro_to_HPC/  
[dshyshlov@login2 Intro_to_HPC]$ █
```

Working with a Linux shell

- Copy a file

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

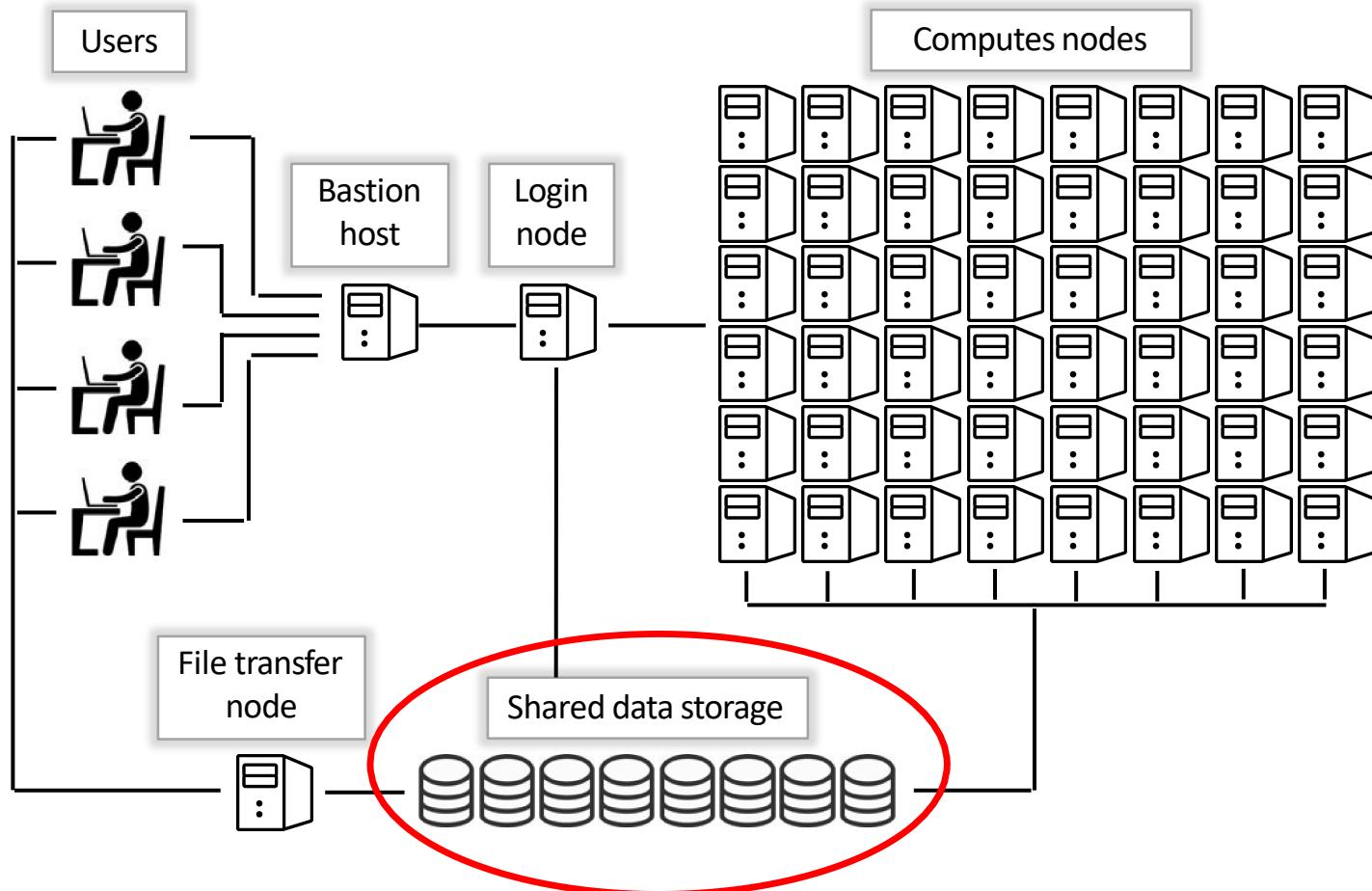
- List all the files and directories again

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

- View contents of the file on the screen

```
$ cat LICENSE
```

Storage



/home/u1/netid /groups/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	9.9T	9.9T

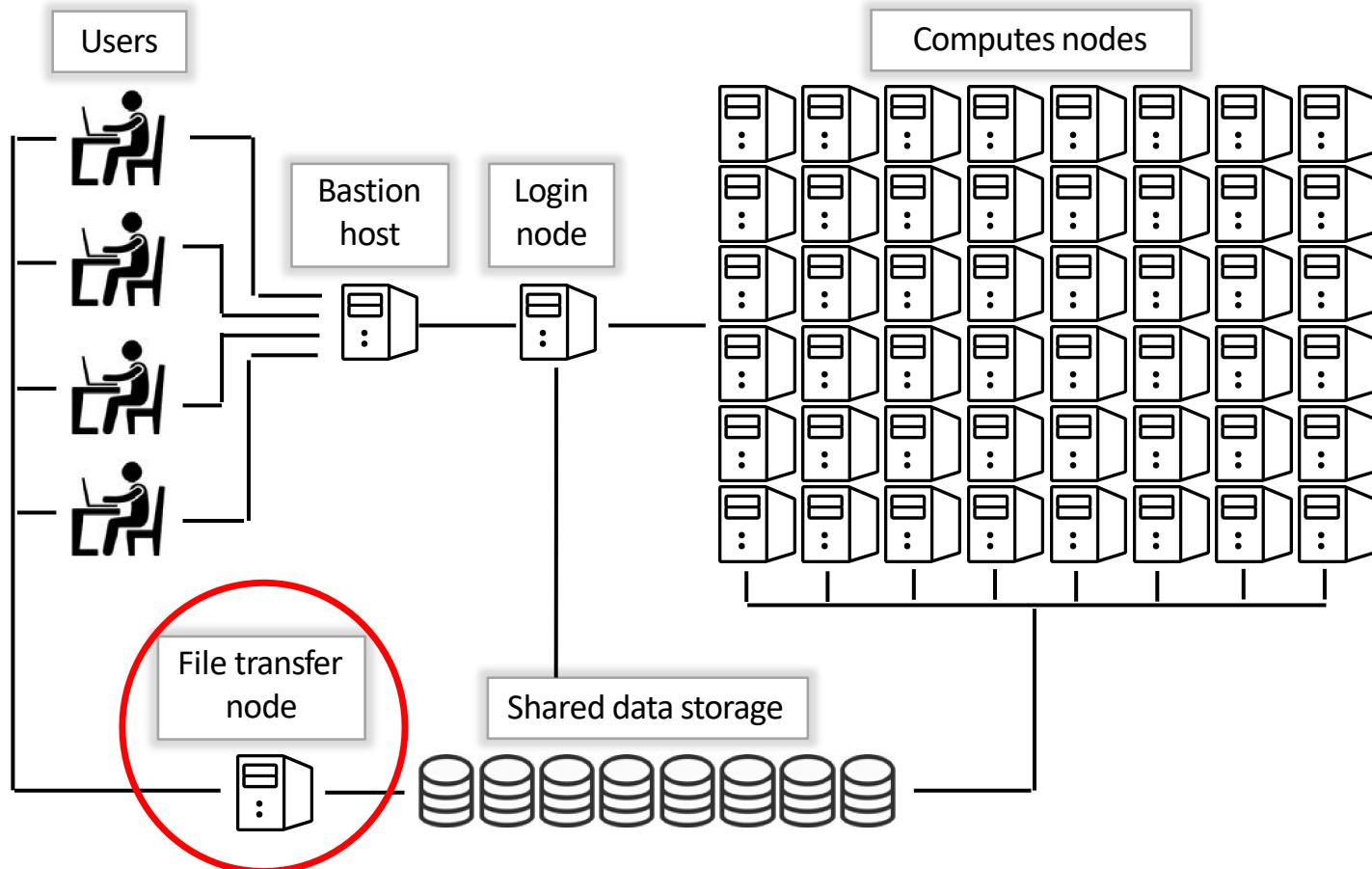
Storage

- Additional Storage:
- /xdisk
- 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

Transferring Files



`filexfer.hpc.arizona.edu`

Transferring Files

- Puma and Ocelote have two specific nodes 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 (web browser)

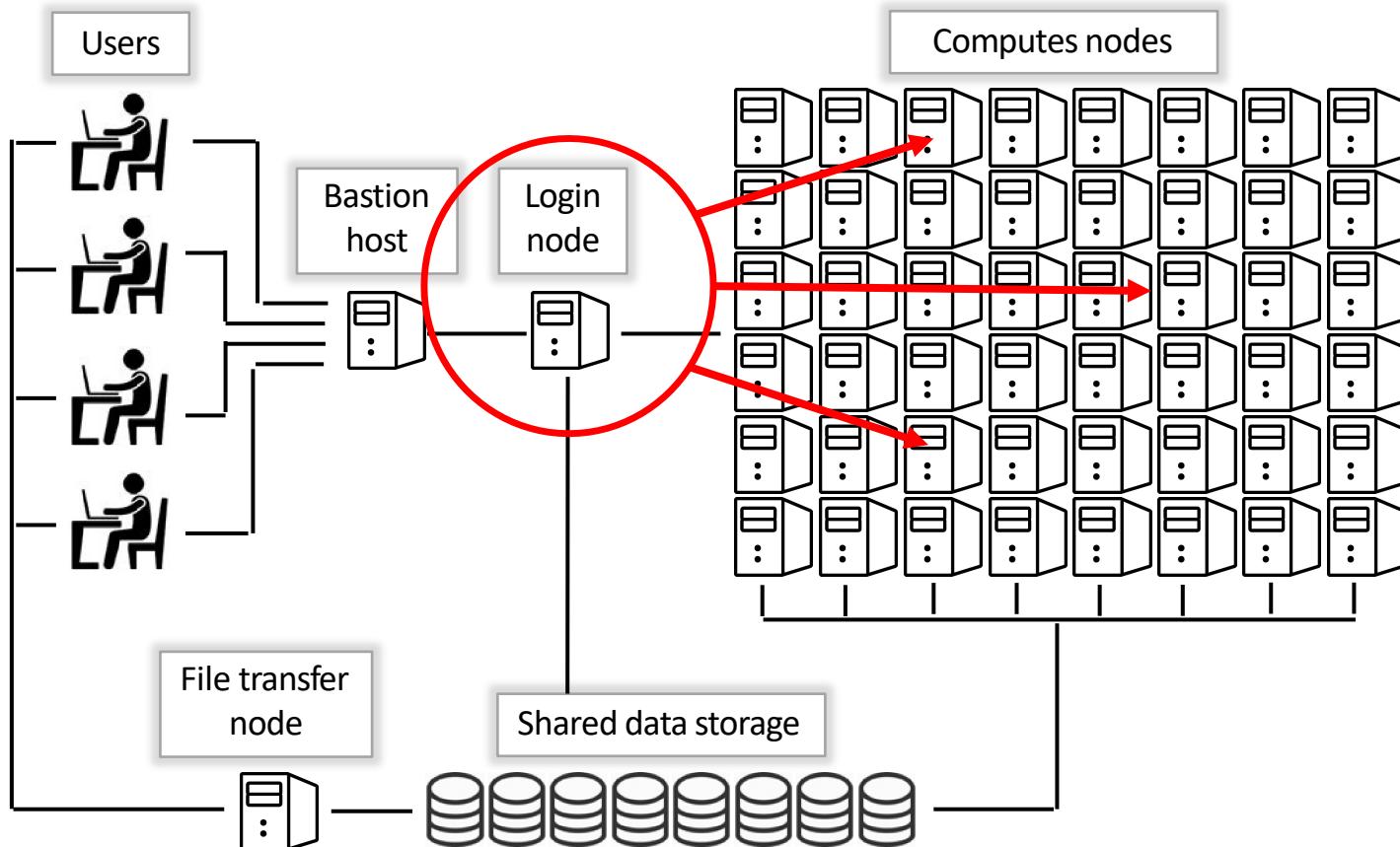
- Display and manage your files
- Edit text files
- Drag and drop files to/from the file explorer

The screenshot shows the OnDemand web interface. At the top, there is a navigation bar with the University of Arizona logo, followed by links for Research Technologies, HPC Systems, Files, Jobs, Clusters, Interactive Apps, and My Interactive Sessions. A dropdown menu under 'Files' shows options like Home Directory, /groups, and /xdisk, with 'OPEN' highlighted. Below the navigation bar, the text "I" jobs will be restarted or terminated without notice if pre-empted by a "standard" job in queue." is displayed. The main area features a large red 'OnDemand' logo. Below it, the text "OnDemand provides an integrated, single access point for all of your HPC resources." is shown.

The screenshot shows the File Explorer v1.3.6 interface. The top bar includes a 'Home Directory' button, a path field showing '/home/u1/dshyshlov/', and various file operations buttons: Go To..., Open in Terminal, New File, New Dir, Upload, Show Dotfiles, and Show Owner/Mode. Below the toolbar is a search bar labeled 'name'. The main area displays a list of files and directories with columns for name, size, and modified date. The 'Home Directory' section on the left lists subfolders like ECOL-346, R, UA-HPC-Intro, Wolfram Mathematica, bin, blast_data, exercises_unix, extra, gui_tmp, iceVirtEnv, install_test, intel, ions, local, and local. The main list shows the contents of the current directory, including .., ECOL-346, R, UA-HPC-Intro, Wolfram Mathematica, bin, blast_data, exercises_unix, extra, and .. again at the bottom.

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

From the login
node to compute

Useful Status commands:

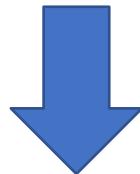
- nodes-busy
- system-busy
- cluster-busy (*work in progress*)

Job status

- job-history *jobid*
- seff *jobid*

Scheduler - SLURM

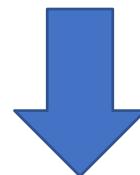
Scheduler receives a request for resources and creates a job



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 --mail-type=ALL
#SBATCH --mail-user=netid@email.arizona.edu
#SBATCH --partition=windfall
#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 --mail-type=ALL
#SBATCH --mail-user=netid@email.arizona.edu
#SBATCH --partition=windfall
#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 --mail-type=ALL
#SBATCH --mail-user=netid@email.arizona.edu
#SBATCH --partition=windfall
#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 --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(REAON)
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

Change the script to use 4 cores from one node

```
$ vi sample_slurm.script
```

Hint: look at "other common options"

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

```
$ cat test.o2118966
```

This script is running on:

r2u13n1.puma.hpc.arizona.edu

Detailed performance metrics for this job will be available at

https://metrics.hpc.arizona.edu/#job_viewer?action=show&realm=SUPREM M&resource_id=73&local_job_id=2118966 by 8am on 2021/09/23.

SLURM script

- Other SLURM commands

\$ squeue

You might need to know grep 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]\$

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>

On

\$ shell

\$ ocelote

\$ interactive

\$ module avai

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

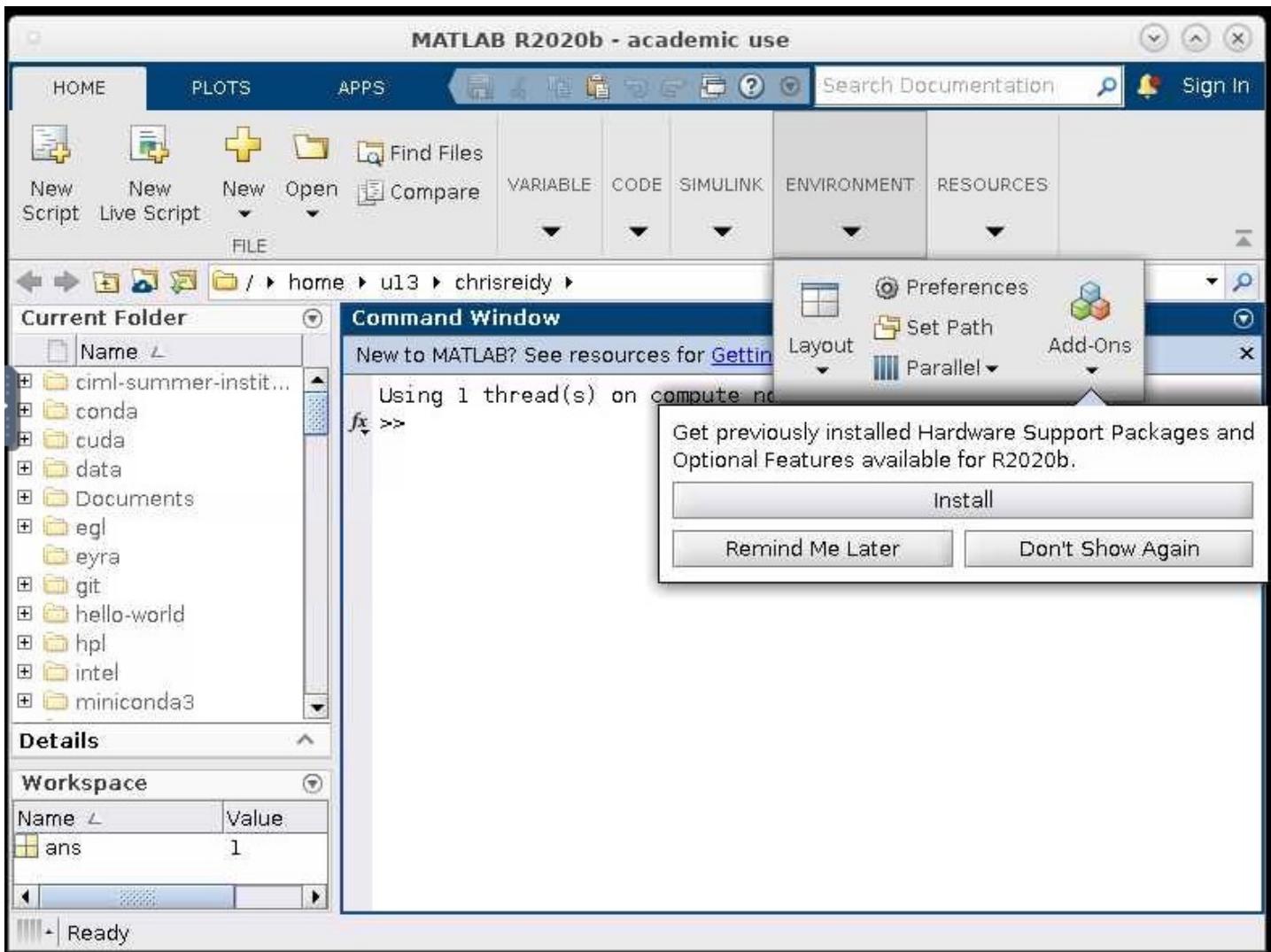
Session ID: 747e44e5-83b4-4515-b737-41147f8502fb

Compression  0 (low) to 9 (high)

Image Quality  0 (low) to 9 (high)

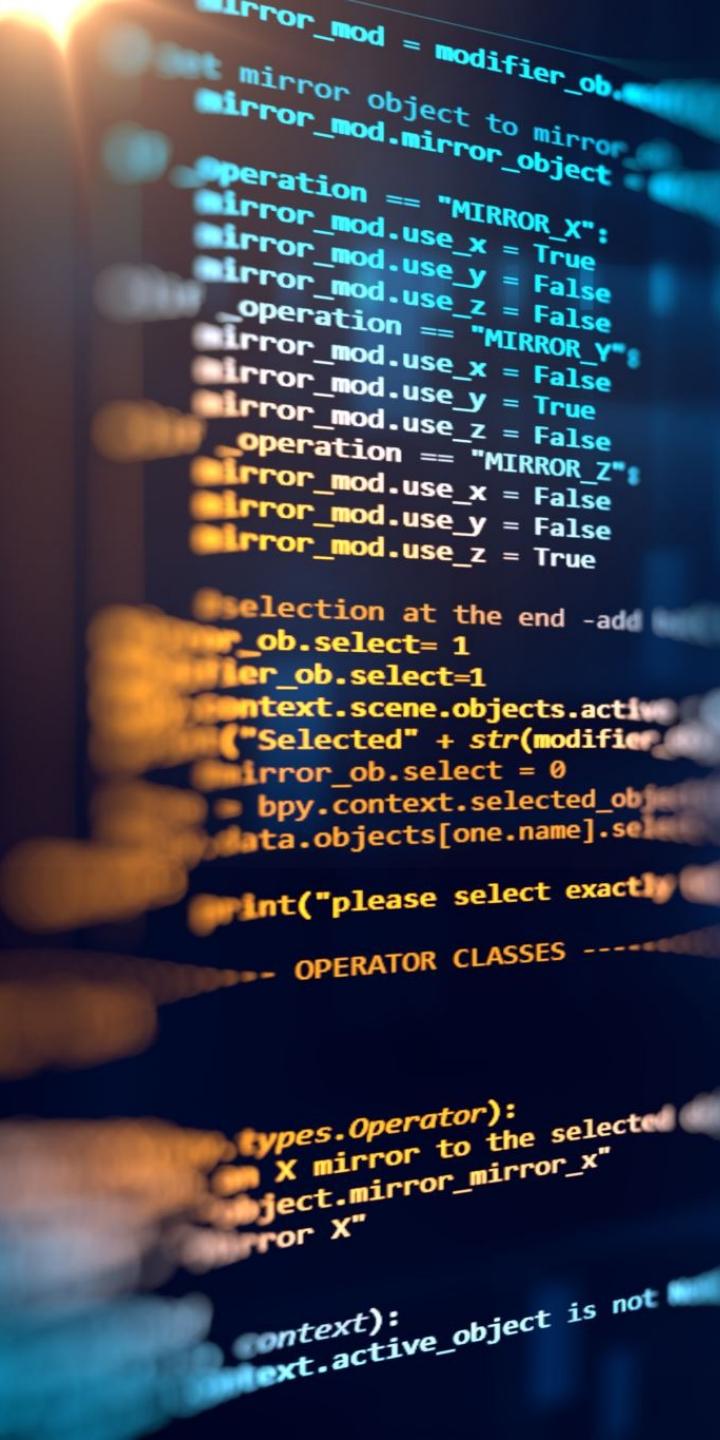
Launch MATLAB GUI View Only (Share-able Link)

Accessing Software with OnDemand



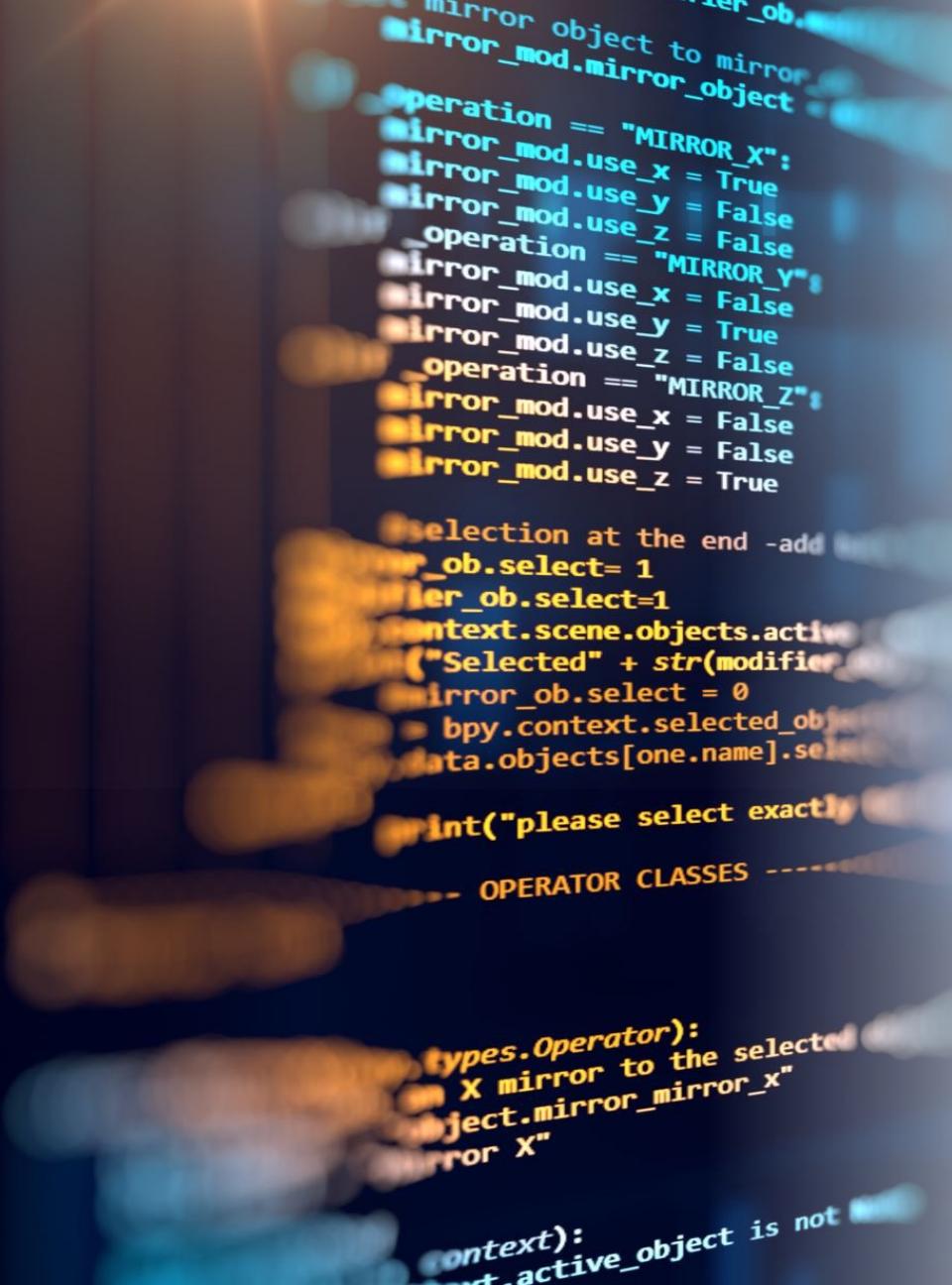
Accessing Software – Command Line

- \$ 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

- Modules:
 - Set your command path:
 - \$ echo \$PATH
- Set your library path:
 - \$ echo \$LD_LIBRARY_PATH
- which freesurfer
 - module load freesurfer
 - which freesurfer



The image shows a close-up of a person's hand pointing their index finger towards a computer monitor. The monitor displays a portion of a Python script, specifically the 'operator' class from Blender's source code. The code is color-coded, with blue for comments, yellow for strings, and various colors for different variable names and keywords. The script handles operations like mirroring objects in 3D space (X, Y, Z axes) and selecting objects. The background is dark, making the bright screen stand out.

```
    mirror_mod = modifier_obj
    # mirror object to mirror
    mirror_mod.mirror_object = None
    if operation == "MIRROR_X":
        mirror_mod.use_x = True
        mirror_mod.use_y = False
        mirror_mod.use_z = False
    elif operation == "MIRROR_Y":
        mirror_mod.use_x = False
        mirror_mod.use_y = True
        mirror_mod.use_z = False
    elif operation == "MIRROR_Z":
        mirror_mod.use_x = False
        mirror_mod.use_y = False
        mirror_mod.use_z = True

    # selection at the end - add
    mirror_ob.select = 1
    other_ob.select = 1
    context.scene.objects.active = eval(
        ("Selected" + str(modifier_index)))
    mirror_ob.select = 0
    bpy.context.selected_objects.append(data.objects[one.name])
    data.objects[one.name].select = 1
    print("please select exactly one object")
    return {'FINISHED'}
```

-- OPERATOR CLASSES --

```
types.Operator):
    """ X mirror to the selected object.mirror_mirror_x"""
    mirror_x = types.BoolProperty(name="mirror X",
        description="mirror X", default=False)
    @classmethod
    def poll(cls, context):
        if context.object is None or context.active_object is not
```

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
```



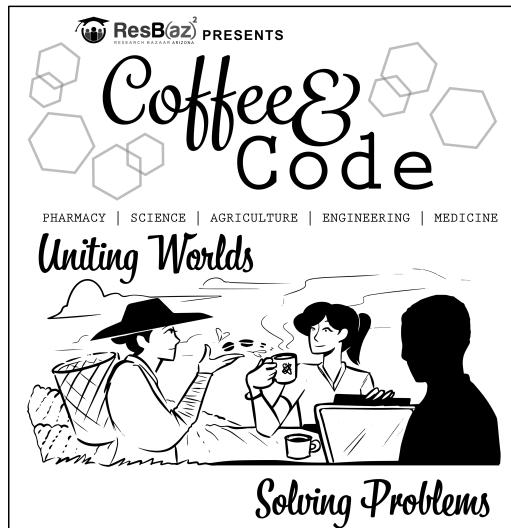
ResB(az)²

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 

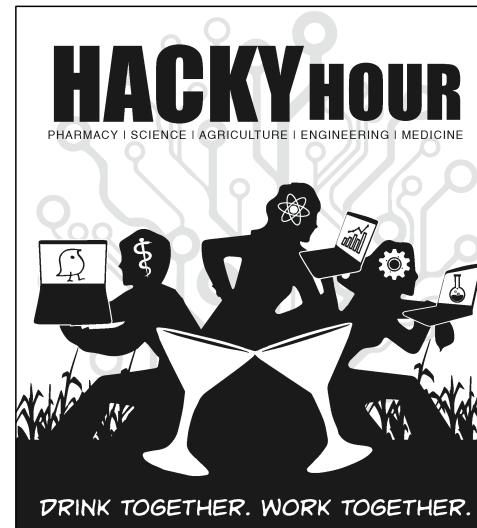
Need help with science or computers? Tired of quietly suffering trying to figure it out?
Come hang out with us; it's free!* Just want to hang out? Also free!*

Not into the bar scene?



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

Not into mornings?



Weekly, Thursdays 4-7
Gentle Ben's (Main Gate Square)
865 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.



Getting help

- HPC documentation –
docs.hpc.arizona.edu
- HPC consulting – hpc-consult@list.arizona.edu
- Visualization consulting –
vislab-consult@list.arizona.edu
- Statistics consulting –
stat-consult@list.arizona.edu