

high-throughput computing

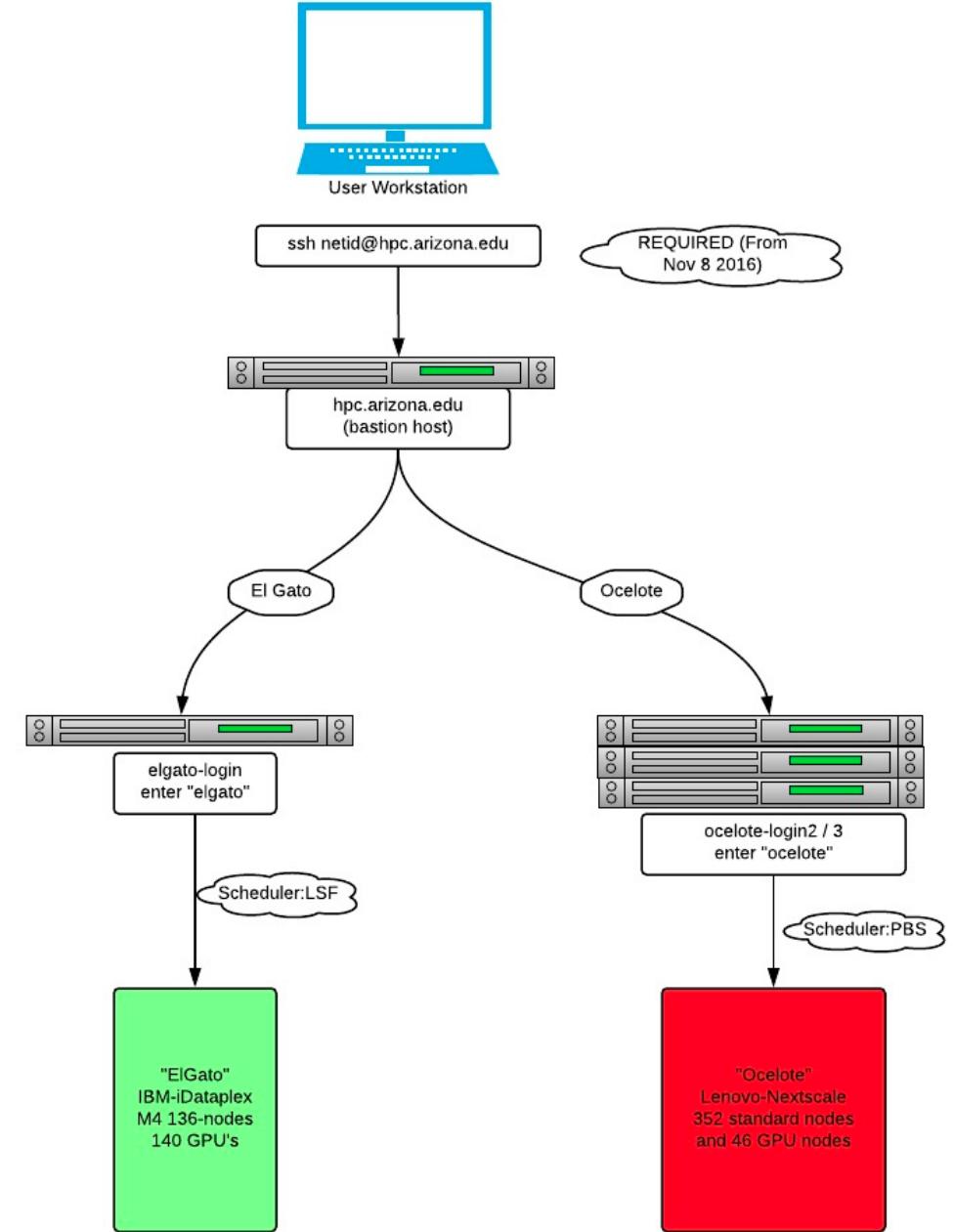


HPC accounts

- UA HPC resources are available to all the students, faculty and staff at no cost
- Students require a sponsor for an HPC account, faculty and staff can sponsor themselves
- accounts.arizona.edu
 - > manage your accounts
 - > HPC account
 - > Notify your sponsor of your request at the HPC sponsorship page

HPC systems in UofA

- Ocelote:
 - ~400 compute nodes
 - 28 cores per node
 - 6GB of memory per core
 - 46 GPU nodes
- El Gato



Accessing the HPC system

- Software for SSH connection:
 - Windows – Putty
 - Mac – Terminal

<https://softwarelicense.arizona.edu/>
> Students
 >SSH

```
wncs-MacBook-Pro:~ dshyshlov$ ssh dshyshlov@hpc.arizona.edu
Password:
Duo two-factor login for dshyshlov

Enter a passcode or select one of the following options:

1. Duo Push to XXX-XXX-0896
2. Phone call to XXX-XXX-0896
3. SMS passcodes to XXX-XXX-0896 (next code starts with: 7)

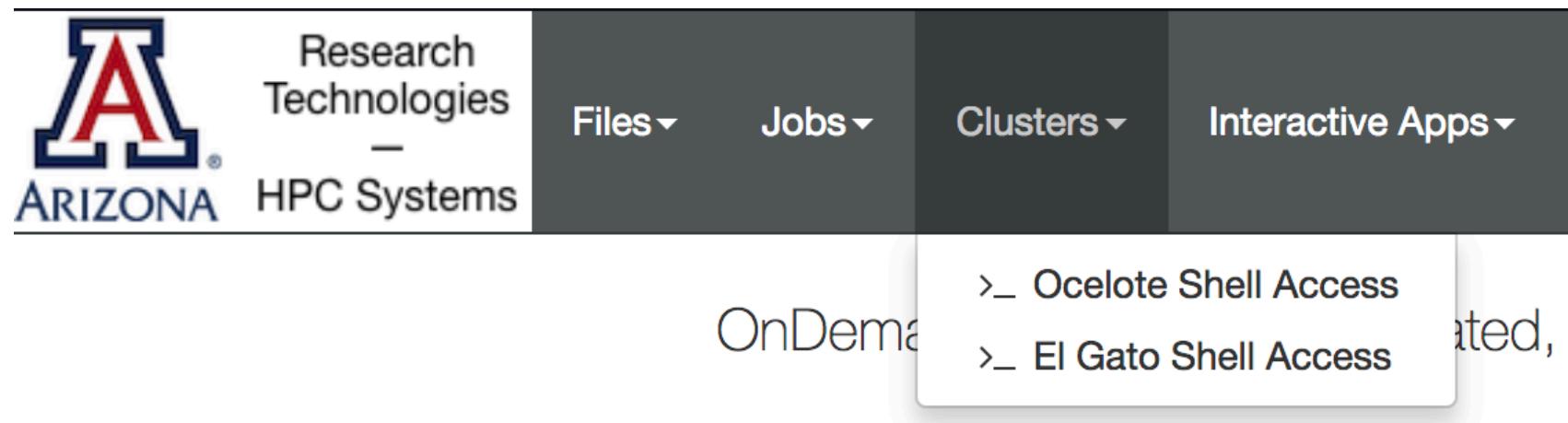
Passcode or option (1-3): 1
Success. Logging you in...
Last login: Wed Jan 31 16:36:22 2018 from dhcp-10-132-181-137.uawifi.arizona.edu
This is a bastion host used to access the rest of the environment.

Shortcut commands to access each resource
-----
Ocelote:          El Gato:
$ ocelote        $ elgato

[dshyshlov@gatekeeper ~]$ ocelote
Last login: Wed Jan 31 09:13:57 2018 from gatekeeper.hpc.arizona.edu
[dshyshlov@login3 ~]$
```

OpenOnDemand

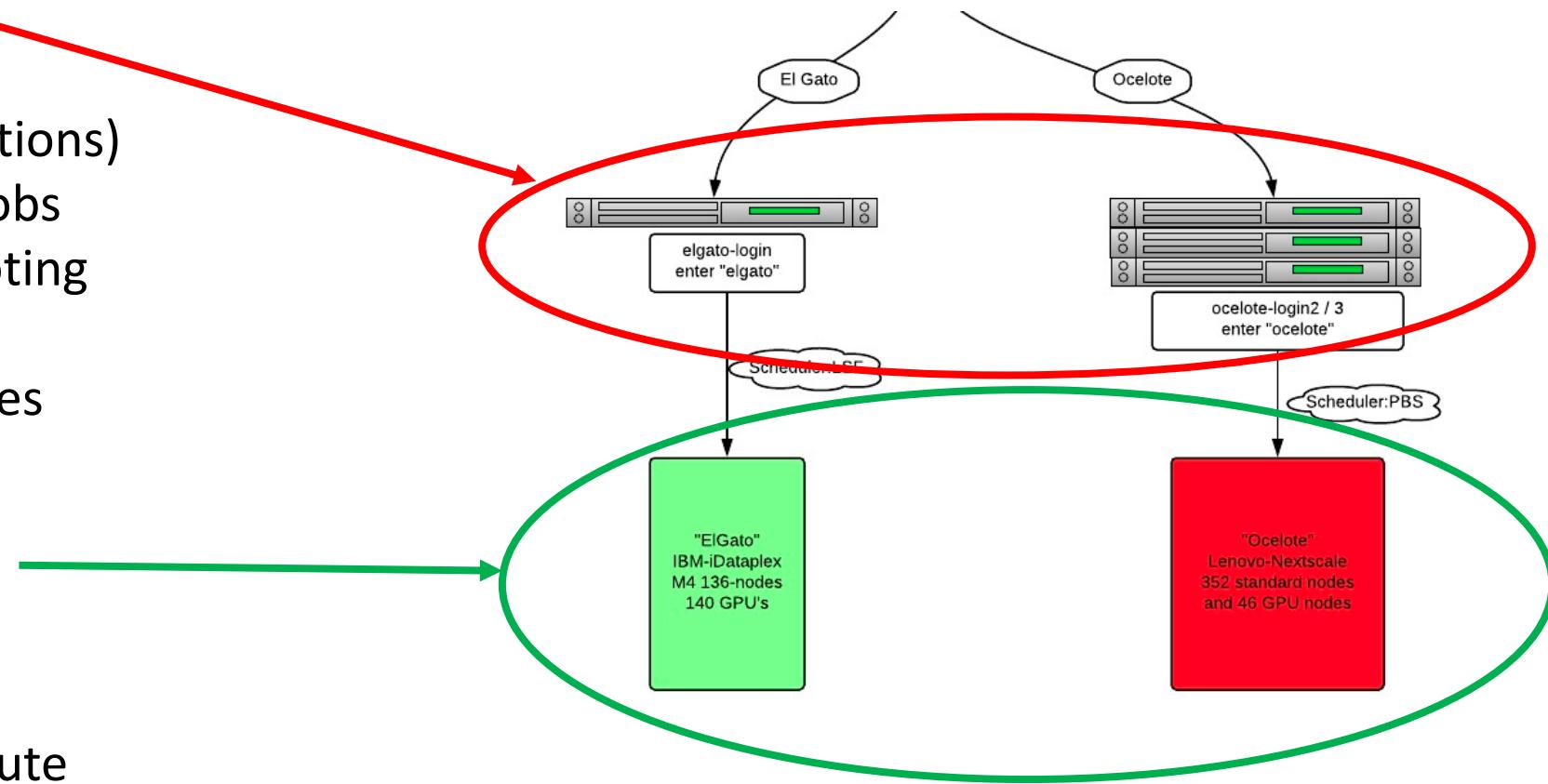
- Access to the HPC resources through the web browser
- ood.hpc.arizona.edu



Login nodes VS Compute nodes

- Login nodes are for:
 - editing code, scripts
 - submitting jobs (calculations)
 - checking status of the jobs
 - testing and troubleshooting
 - interactive tasks
 - Ocelote has 3 login nodes

- Compute nodes are for running jobs
 - ideal for batch jobs
 - Ocelote has ~400 compute nodes

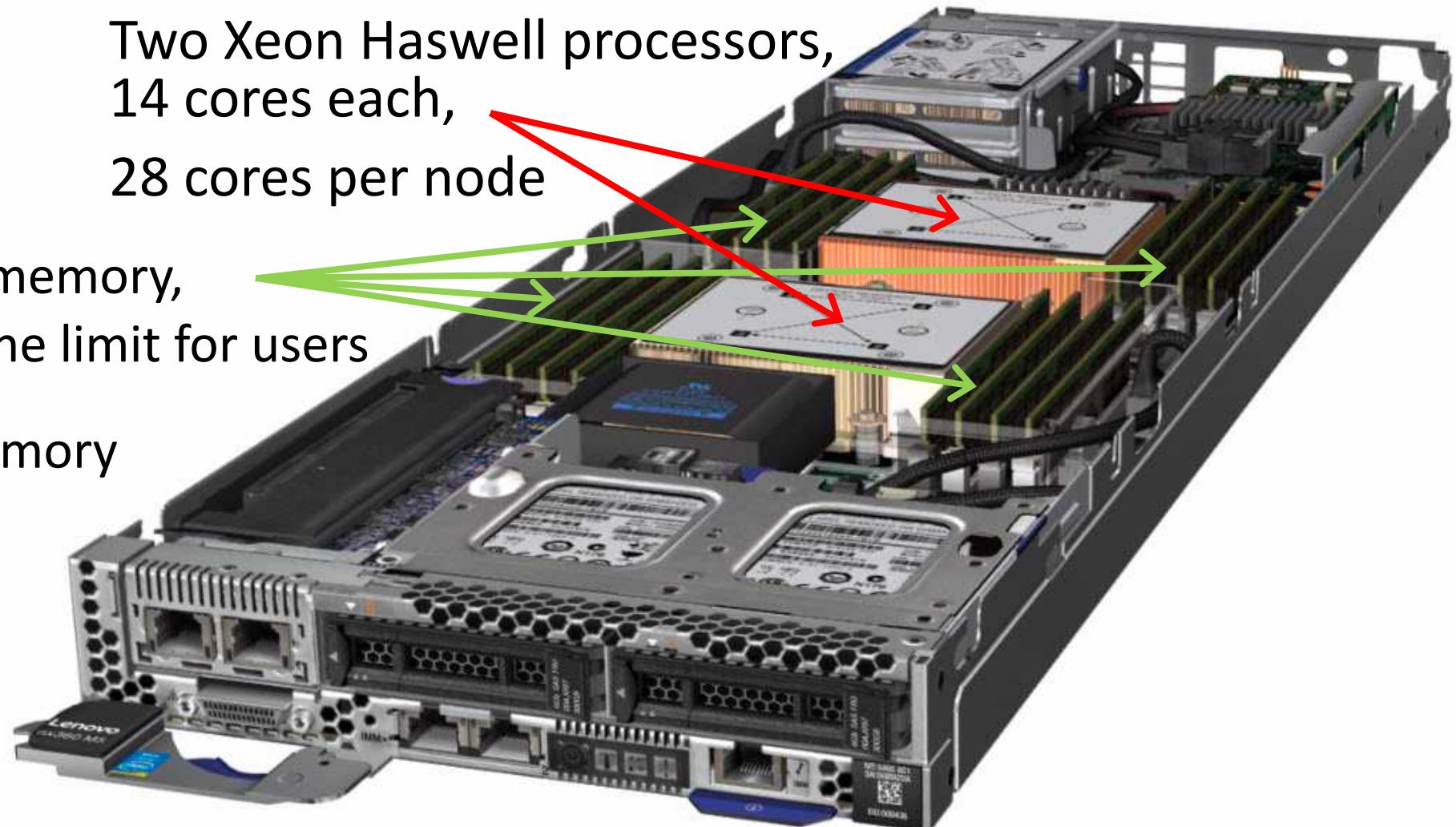


Anatomy of a computing node

Two Xeon Haswell processors,
14 cores each,
28 cores per node

192 GB of memory,
168 GB is the limit for users

6 GB of memory
per core



Storage and Allocation

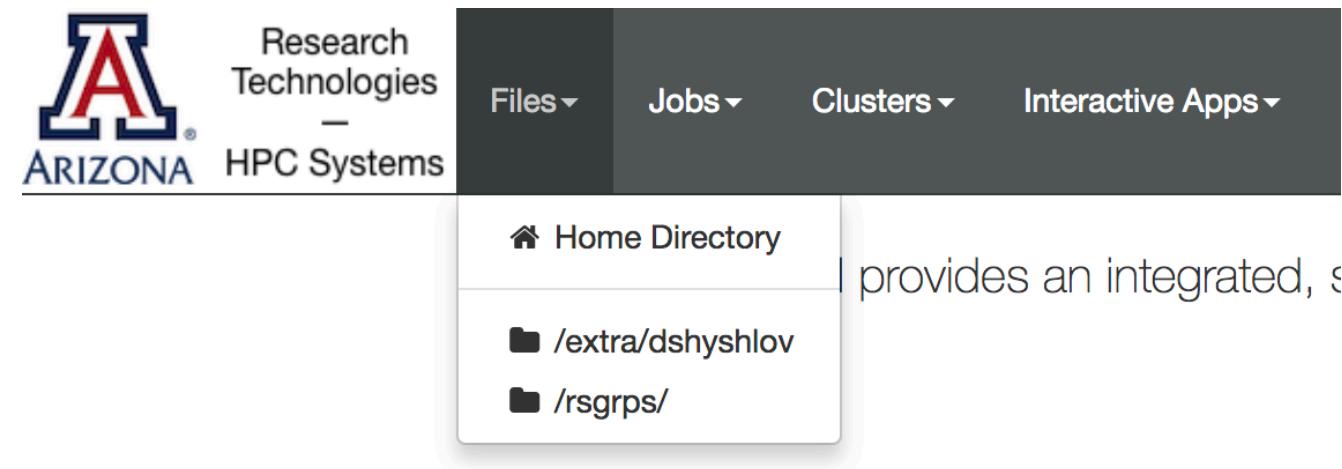
- Storage:
 - Home directory – 15GB
 - /extra – 200GB
 - /xdisk – temporary storage up to 1TB
 - /rsgrps – rented storage by research groups
 - /tmp – local scratch, ~850GB on each node, useful for temporary files used during the job execution
 - *uquota* – Linux command to display your used/available storage
- Allocation
 - standard – limited to 24,000 hours/group/month
 - windfall – unlimited, jobs can be preempted
 - *va* – Linux command to display available allocation

File transfer

- There are special nodes for data transfer
 - **filexfer.hpc.arizona.edu**
 - old hostname sftp.hpc.arizona.edu still works as well
- Connecting to file transfer node
 - sftp **NetID@filexfer.hpc.arizona.edu**
- File transfer software
 - WinSCP (Windows), Cyberduck (Windows and Mac), Fugu (Mac)
 - <https://softwarelicense.arizona.edu/ssh-clients-windows-and-mac>
- Other ways of file transfer:
 - Globus (large files), scp, rsync, irods

File transfer with OpenOnDemand

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



File Explorer v1.3.6

/home/u1/dshyshlov/

name size modified date

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>	..
gui_tmp	<dir>	..
iceVirtEnv	<dir>	..
install_test	<dir>	..
intel	<dir>	..
ions	<dir>	..
local	<dir>	..

File transfer with Globus

- Parallel data transfer with GridFTP protocol, high-speed and reliable
- Requires setup:
 - <https://docs.hpc.arizona.edu/display/UAHPC/Transferring+Files>
- Client software – Globus Connect Personal
- Every computer with Globus client installed – endpoint
- Keeps data transfer progress in case of interruption, detailed log of the transfer process, email notifications for completed transfer...

File transfer with Globus

- Start file transfer with web interface – www.globus.org/app/transfer

The screenshot shows the Globus Transfer Files web interface. At the top, there is a blue header bar with the Globus logo on the left and navigation links: Manage Data, Publish, Groups, Support, and Account. Below the header, a secondary navigation bar includes Transfer Files, Activity, Endpoints, Bookmarks, and Console. The main area is titled "Transfer Files". It features two sets of input fields for endpoints and paths, each with a "Go" button and a star icon. A central control panel contains a left arrow, a right arrow, and a double arrow. Below these controls, two large boxes are labeled "Start by selecting an endpoint." The entire interface has a clean, modern design with a white background and light gray accents.

File transfer with Globus

The screenshot shows the Globus Transfer Files interface. At the top, there is a navigation bar with links for Manage Data, Publish, Groups, Support, and Account. Below the navigation bar, there are links for Transfer Files, Activity, Endpoints, Bookmarks, and Console.

The main area is titled "Transfer Files". It features two file selection panes:

- Endpoint:** Work Laptop
Path: `/~/`
- Endpoint:** arizona#sdmz-dtn
Path: `/~/`

Between the two panes is a central transfer button consisting of a grey arrow pointing left and a blue arrow pointing right. Above the transfer button, there is a "RECENT ACTIVITY" section with three circular icons showing counts of 0 for each category.

The left pane lists local files and folders:

- select none
- Applications
- CUDA
- Desktop
- Documents
- Downloads
- Dropbox (Personal)
- Dropbox (UA HPC)
- KeplerData
- Movies
- Music
- Pictures
- Public
- PycharmProjects
- VirtualBox VMs
- singularity-vm
- htc2.pbs** 2.02 KB

The right pane lists remote files and folders:

- select all
- ECOL-346
- R
- UA-HPC-Intro
- Wolfram Mathematica
- bin
- blast_data
- exercises_unix
- extra
- gui_tmp
- iceVirtEnv
- install_test
- intel
- ions
- local
- matlab
- modules
- mpi_hello_world
- ondemand
- p27_virtenv
- permtest

Software

- Many software packages are available as modules
 - *module avail* – list all the installed modules
 - *module avail matlab* – list all versions of MATLAB
 - *module load matlab* – load the module (the latest version is usually the default)
 - *module list* – display all the modules loaded in your environment

Exercise

- Copy exercise files:
 - *git clone https://github.com/dshyshlov/UA-HPC-Intro-Matlab*
- List the files and directories:
 - *ls*
- Change directory to UA-HPC-Intro
 - *cd UA-HPC-Intro-Matlab* (use tab for autocompletion)
- List the files again:
 - *ls*

PBS Script

- Parameters for scheduler
- Loading necessary software
- Navigating to the working directory
- Run the program

```
#!/bin/bash
#PBS -N JobName
#PBS -m bea
#PBS -M NetID@email.arizona.edu
#PBS -W group_list=kanchukaitis
#PBS -q standard
#PBS -l select=1:ncpus=28:mem=168gb:pcmem=6gb
#PBS -l walltime=0:1:0
#PBS -l cput=0:28:0

module load matlab

cd ~/UA_HPC_Intro

matlab -nodisplay -nosplash < helloworld.m
```

PBS Script

- Display the content of the PBS script on the screen:
 - *cat script.pbs*
- Edit the PBS script with nano text editor:
 - *nano script.pbs*
- Submit the script with the command:
 - *qsub script.pbs*
- Check the job status:
 - *qstat -u NetID*

Output and Error files

- Check the output file
- Check the error file
- Output and error files can be joined together with the PBS script:
 - #PBS -j oe
- You can also specify the file names:
 - #PBS -o output.txt
 - #PBS -e error.txt

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