



Research Computing Governance Committee  
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high-throughput computing



high performance computing



Visualization Consultation

# UA HPC Introduction

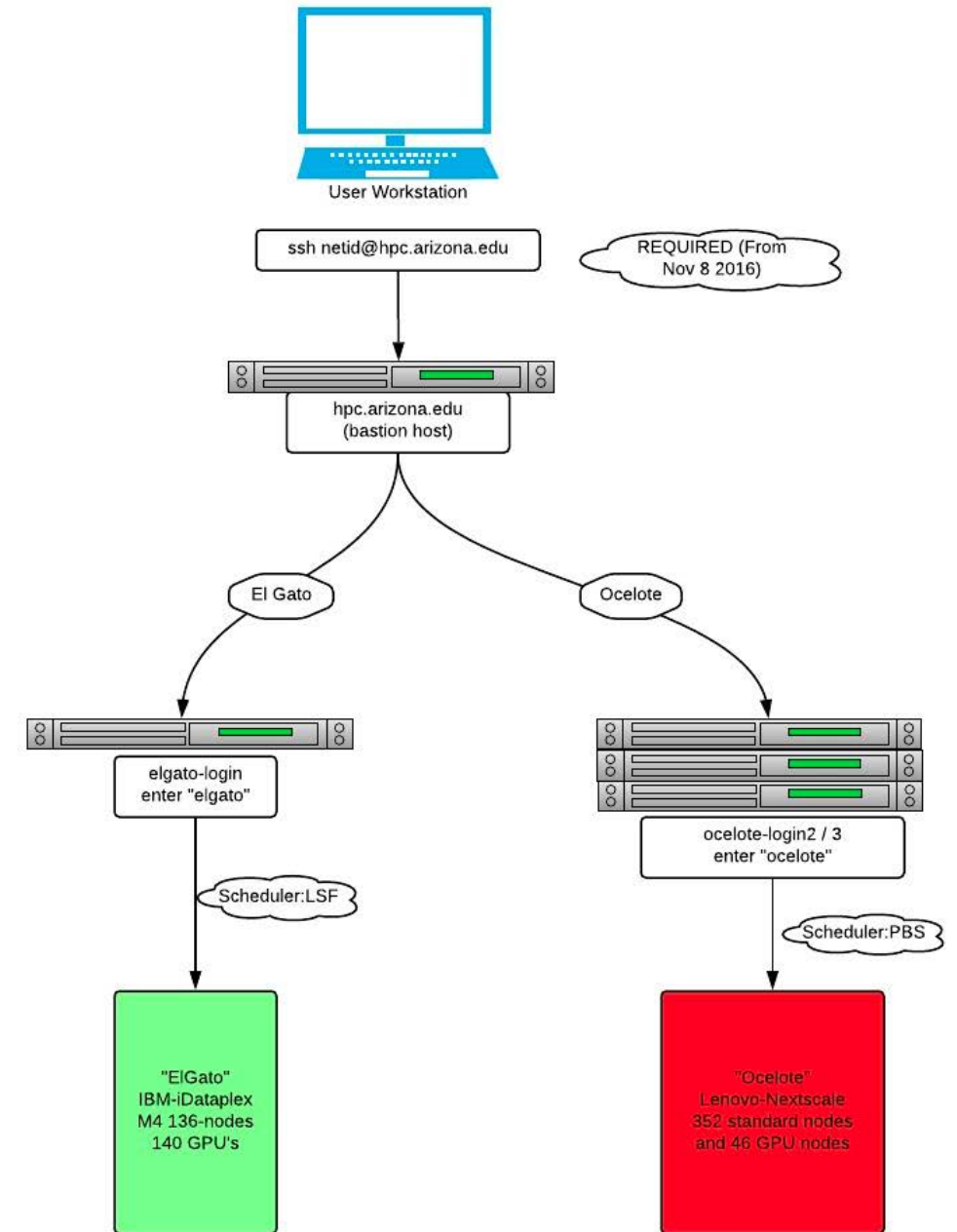
Dima Shyshlov,  
HPC consultant

# 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](https://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:
```

```
$ ocelote
```

```
El Gato:
```

```
$ elgato
```

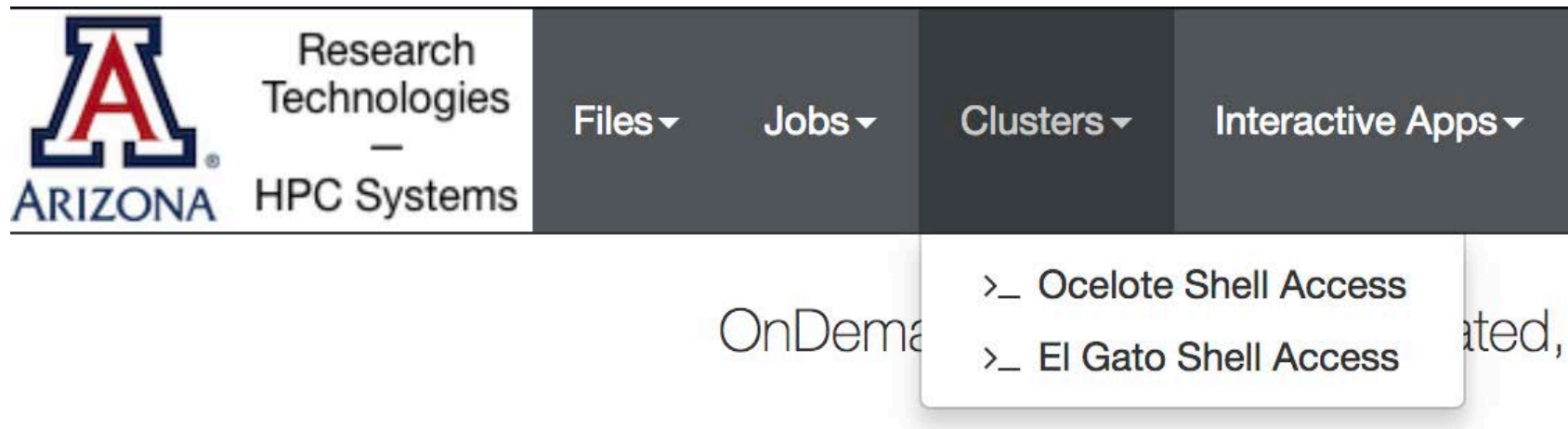
```
[dshyshlov@gatekeeper ~]$ ocelote
```

```
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`

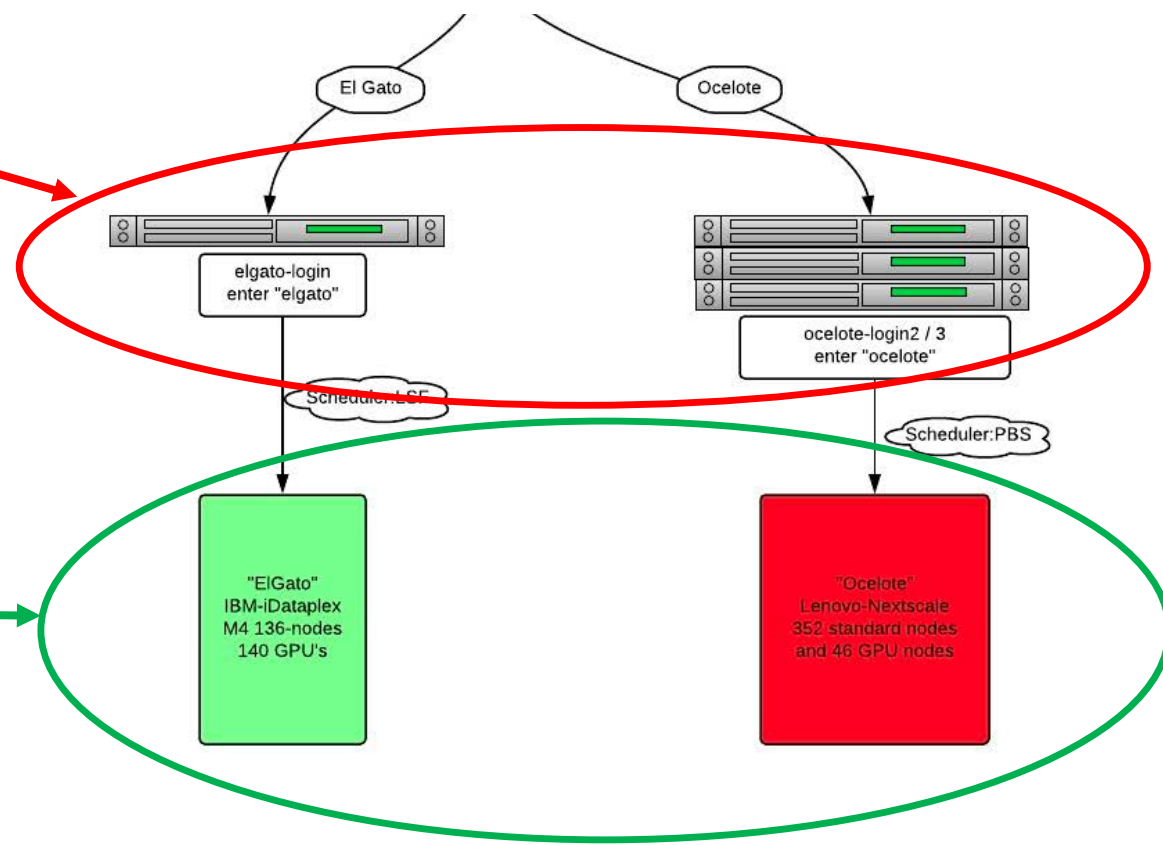




# Login nodes VS Compute nodes

- 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

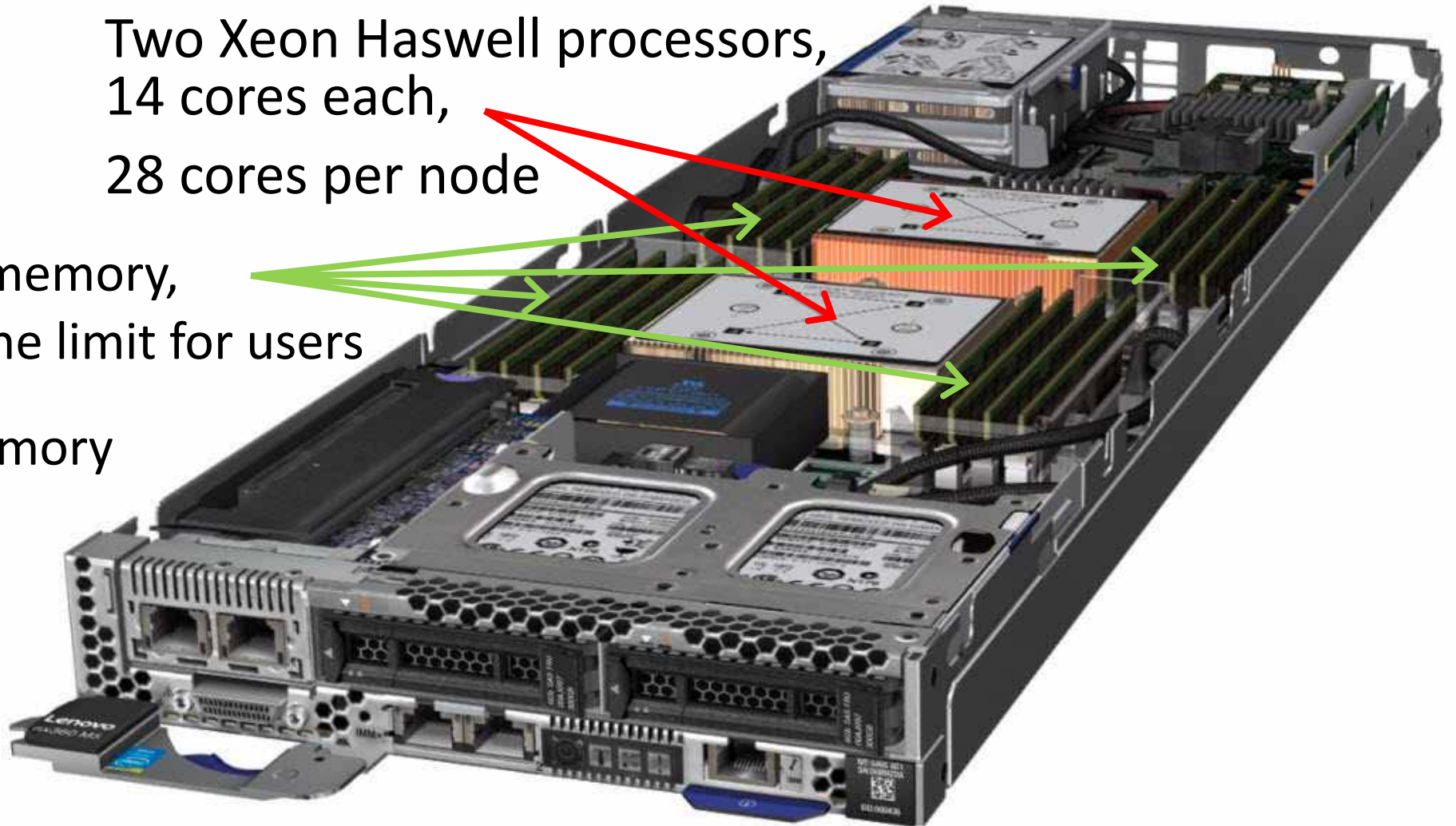


# Anatomy of a node

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
  - /rsgroups – 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

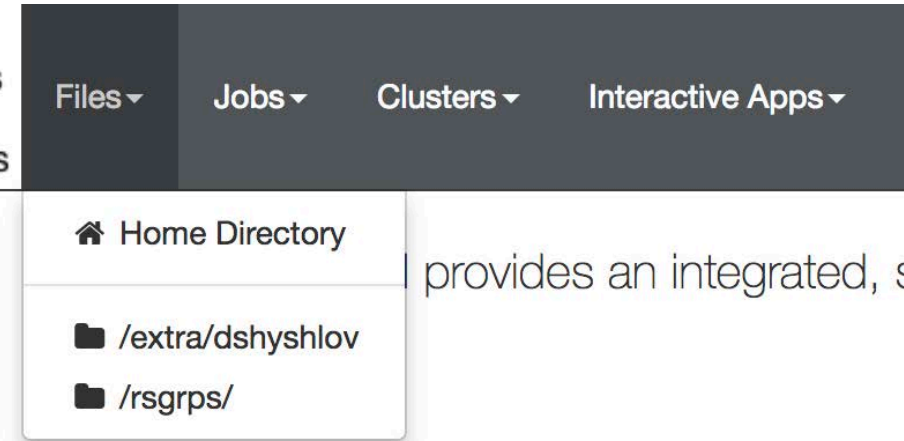


# File transfer

- 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

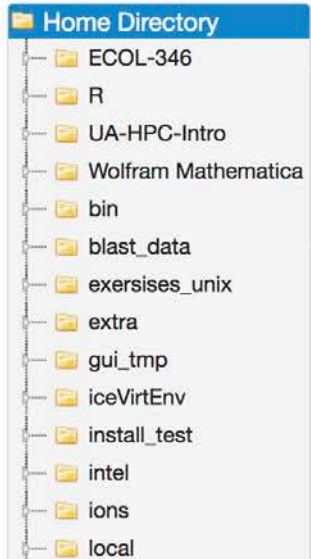
- Display and manage your files
- Drag and drop files to/from the file explorer



provides an integrated, s

File Explorer v1.3.6

Go To... Open in Terminal New File New Dir Upload Show Dotfiles Show Owner/Mode



/home/u1/dshyshlov/

View Edit A-Z Rename Download Copy Paste (Un)Select All

Delete

name	size	modified date
..	<dir>	
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
exersises_unix	<dir>	06/13/2018
extra	<dir>	08/22/2018
...	..	.....

# 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](http://www.globus.org/app/transfer)

The screenshot displays the Globus web interface for file transfer. At the top, there is a navigation bar with the Globus logo and links for Manage Data, Publish, Groups, Support, and Account. Below this, a secondary navigation bar includes links for Transfer Files, Activity, Endpoints, Bookmarks, and Console. The main section is titled "Transfer Files" and features a "RECENT ACTIVITY" section with three circular icons and the number 0. The interface is divided into two panels for selecting endpoints and paths. The left panel shows the "Work Laptop" endpoint with a path of "/~/", displaying a list of folders (Applications, CUDA, Desktop, Documents, Downloads, Dropbox (Personal), Dropbox (UA HPC), KeplerData, Movies, Music, Pictures, Public, PycharmProjects, VirtualBox VMs, singularity-vm) and a file "htc2.pbs" (2.02 KB). The right panel shows the "arizona#sdmz-dtn" endpoint with a path of "/~/", displaying a list of folders (ECOL-346, R, UA-HPC-Intro, Wolfram Mathematica, bin, blast\_data, exersises\_unix, extra, gui\_tmp, iceVirtEnv, install\_test, intel, ions, local, matlab, modules, mpi\_hello\_world, ondemand, p27\_virtenv, permtest). Both panels include controls for "select none/all", "up one folder", "refresh list", and "share".

globus

Manage Data Publish Groups Support Account

Transfer Files | Activity | Endpoints | Bookmarks | Console

## Transfer Files

RECENT ACTIVITY 0 0 0

Endpoint: Work Laptop Path: /~/ Go

Endpoint: arizona#sdmz-dtn Path: /~/ Go

select none up one folder refresh list share

- Applications Folder
- CUDA Folder
- Desktop Folder
- Documents Folder
- Downloads Folder
- Dropbox (Personal) Folder
- Dropbox (UA HPC) Folder
- KeplerData Folder
- Movies Folder
- Music Folder
- Pictures Folder
- Public Folder
- PycharmProjects Folder
- VirtualBox VMs Folder
- singularity-vm Folder
- htc2.pbs 2.02 KB

select all up one folder refresh list share

- ECOL-346 Folder
- R Folder
- UA-HPC-Intro Folder
- Wolfram Mathematica Folder
- bin Folder
- blast\_data Folder
- exersises\_unix Folder
- extra Folder
- gui\_tmp Folder
- iceVirtEnv Folder
- install\_test Folder
- intel Folder
- ions Folder
- local Folder
- matlab Folder
- modules Folder
- mpi\_hello\_world Folder
- ondemand Folder
- p27\_virtenv Folder
- permtest Folder

# Software

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



# Singularity containers

- Custom environment – OS, software, libraries, workflows, data...
- Where to get containers:
  - UA HPC provides pre-built containers from Nvidia
  - Container registries
    - Singularity Hub
    - Docker Hub
  - Build your own containers
    - Locally, need a Linux machine with root privileges (or virtual box)
    - In cloud, using Singularity Hub
- module load singularity
  - singularity shell container\_name.simg
  - singularity exec container\_name.simg list\_of\_commands

# Exercise

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

# PBS Script

- Parameters for scheduler
  - use *va* to find group name
  - GPU nodes use all 28 cores
  - $\text{cput} = \text{walltime} * \text{ncpus}$
- Loading necessary software
- Navigating to the working directory
- Run the program

```
#!/bin/bash
#PBS -N JobName
#PBS -W group_list=
#PBS -q standard
#PBS -l select=1:ncpus=28:mem=168gb:pcmem=6gb:ngpus=1
#PBS -l walltime=0:1:0
#PBS -l cput=0:28:0

module load singularity

cd ~/UA-HPC-Intro-Pytorch

CONTAINER=/unsupported/singularity/nvidia/nvidia-
pytorch.18.06-py3.simg

singularity exec --nv $CONTAINER python helloworld.py
```

# 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](https://docs.hpc.arizona.edu)
- HPC consulting – [hpc-consult@list.arizona.edu](mailto:hpc-consult@list.arizona.edu)
- Visualization consulting – [vislab-consult@list.arizona.edu](mailto:vislab-consult@list.arizona.edu)
- Statistics consulting – [stat-consult@list.arizona.edu](mailto:stat-consult@list.arizona.edu)