HPC On-boarding

Sean Cleveland Ph.D, Ron Merrill Ph.D,
David Schanzenbach M.S.

Information Technology Services
Department of Cyberinfrastructure
University of Hawai'i

https://www.hawaii.edu/its/ci/
uh-hpc-help@lists.hawaii.edu

January 18, 2016

Outline

Outline

Parallel Computing

- High Performance Compute
  - Each separate process can send and receive data amongst other processes (MPI & OpenMP)
  - If processes must communicate for the overall program to proceed, high-speed networking is needed (only MPI)
- High Throughput Compute
  - *Pleasantly Parallel* – Processes are independent and no communication is necessary

Outline

Cray CS300 – History

- Brought online Fall 2014 – Spring 2015
- Initial investment of 1.8 Million by the University of Hawai‘i (UH)
- As of October 2015, more than 200 users have been granted access to the cluster

Cray CS300 – Compute Nodes

- 3,800 total cores – **Spring upgrade** $\rightarrow$ 5,400+
- 178 standard nodes – **Spring upgrade** $\rightarrow$ 270
  - Two 10 core Intel® processors (*20 cores total*)
  - Diskless – Some RAM is used for the Operating System
  - $\approx$ 128GB of useable RAM
- 6 large memory nodes
  - Four 10 core Intel® processors (*40 cores total*)
  - Diskless – Some RAM is used for the Operating System
  - $\approx$ 1TB of useable RAM
- CentOS Linux

Cray CS300 – Storage

Two storage options are currently available on the Cray CS300.

1. Lustre®
2. ValueStorage

Cray CS300 – Storage → Lustre®

- Lustre® is a high performance parallel filesystem
- The Cray CS300 has ≈ 582TB of storage space
- Shared between all compute nodes and login nodes
- Primarily used as scratch space for jobs (Input and Output)
- User do not have a usage quota (soft or hard)
- Certain directories are subject to a 90 day purge policy
- **Data is not backed up! Users are responsible for their own data**

Cray CS300 – Storage → ValueStorage

- 500TB of scale out storage
- Currently only available for purchase by cluster users and only accessible via the login nodes
- ValueStorage will eventually be available for purchase by everyone
- ValueStorage owners will eventually be able to mount as a network drive (CIFS) on laptop, workstations, servers
- Purchased in 0.5TB increments

ValueStorage Pricing

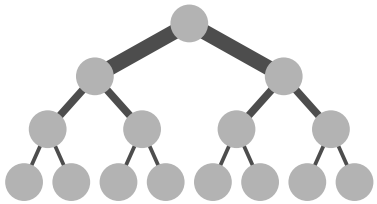
Product	Annual Cost	Product	Annual Cost
0.5TB	$65.00	0.5TB + Replication	$130.00

More Information

All prices are subject to change

Cray CS300 – Network

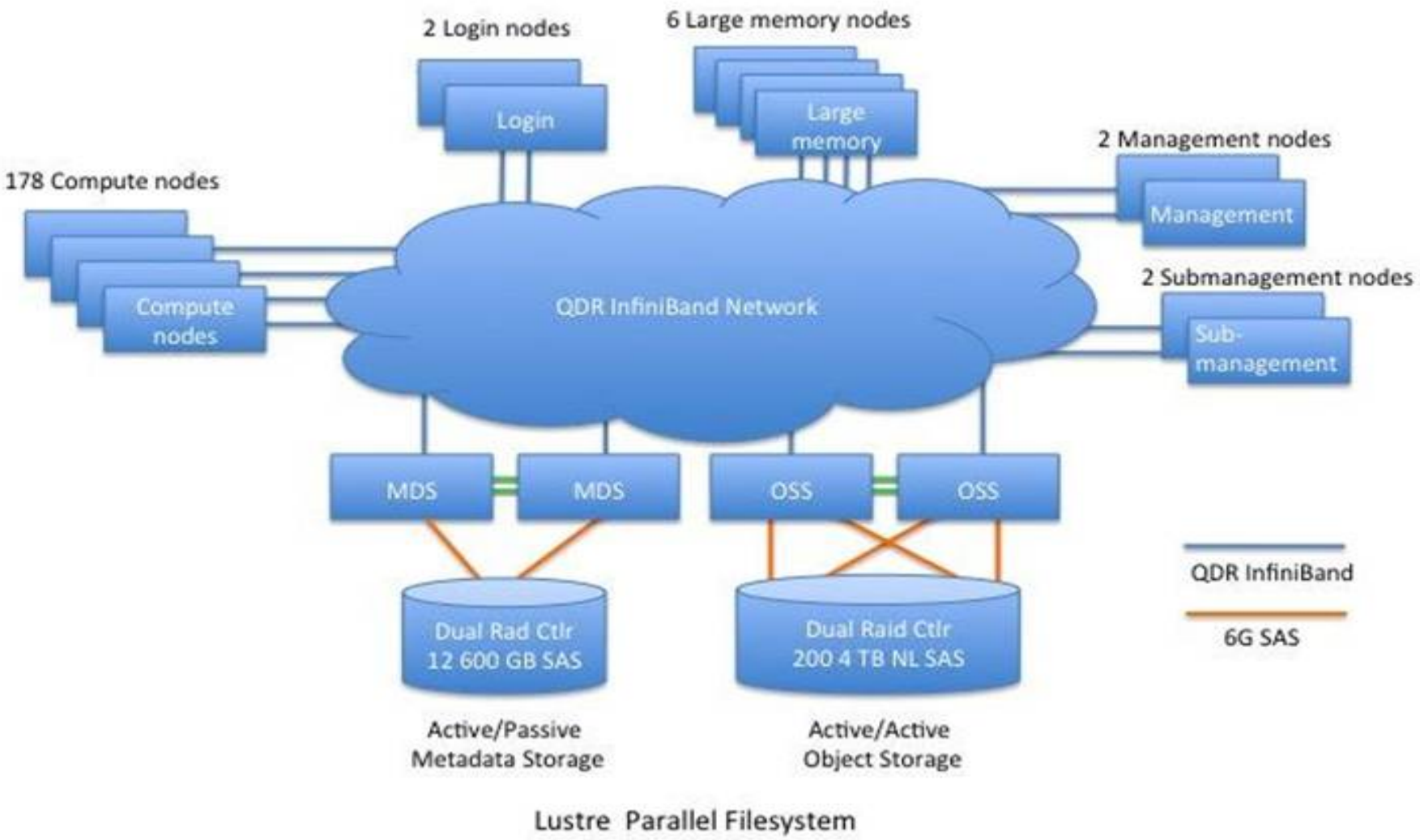
- 40Gb Infiniband inter-connects (QDR)
  - High speed inter-connect between compute nodes, Lustre® storage and Login nodes
  - Utilizes the *fat tree network topology*



Source: https://en.wikipedia.org/wiki/Fat_tree

- 10Gb login node internet connectivity
  - Speed test from UH to CERN clocked transfer speeds up to 2+ Gb/s

Cray CS300 – Layout



Outline

Community Resources

- The initial investment in the cluster provides resources for all Faculty, Staff, and Students affiliate with the University of Hawai'i
- All users can run on the publicly accessible partitions: *community.q, lm.q, sb.q, kill.q, htc.q*
- For some users, the publicly available resources may not be enough . . .

Condo Model

- The Condo model allows users to buy nodes (*condos*) to incorporate into the cluster
- Node owners are provided with priority access to their purchased hardware
- All nodes have a *5 year warranty*
  - Once a nodes warranty has expired, it will be removed from the cluster
- Condo owners are given early access to purchased nodes
  - Access is granted as soon as the funds land in our accounts
  - The 5 year warranty will not begin until newly ordered nodes are installed
- Condo owners are also given the option to purchase 1TB of Lustre® storage per node purchased

Service Units

- In some cases, users will not require owning a node, but still need priority access
- An alternative to purchasing a node, is to purchase service units (SU)
- SUs come in two variates:
  - Standard node units
    - 20 core hours, with access to 128GB of ram on a standard node
  - Large memory node units
    - 40 core hours, with access to 1TB of ram on a large memory node
- A minimum order totaling $500 is required

Price Card

Condo Price Card

Product	Cost	Product	Cost
Standard	$6,600.00	Standard + 2 GPUs (Nvidia® K40)	$13,600.00
Large Memory	$33,900.00	1 TB Lustre® Storage for 5 years	$600.00

Service Unit Price Card

Product	Cost	Minimum Order
Standard node	$0.50 per SU	1,000 SU ($500.00)
Large memory node	$2.00 per SU	250 SU ($500.00)

All prices are subject to change

Outline

Overview – Cluster Interaction

- Connecting to a cluster @ UH
  - Login to the cluster
  - Verify user permissions
- User directories
- Transferring files
  - Globus
- Software
  - Modules
  - Acquiring software
  - Compiliers
- Managing user jobs
  - Job scheduler
  - Using SLURM
  - Partition layout
  - Submitting jobs (Examples)

Connecting to a cluster @ UH

- To connect to the cluster, we utilize a client which communicates using the Secure Shell (*SSH*) protocol
- Linux and MacOSX, typically have a SSH client already installed
- Windows typically does not come with an SSH client installed
- Windows 10 may come pre-installed with a SSH client, but it might not be stable
- Suggested SSH clients for Windows include:
  - SSH Secure Shell (SSH 3.2.9)
  - Putty

- The Cray CS300 has two login nodes:
  - uhhpc1.its.hawaii.edu
  - uhhpc2.its.hawaii.edu

Let's attempt to login!

Login to the Cray CS300

Windows

- If SSH 3.2.9 installed (Lab PCs have it installed)
- Open the start menu, and type "SSH" and you should see a program called "SSH Secure File Terminal Client"
- Click "Quick Connect" and enter the following information:

  Host Name: uhhpc1.its.hawaii.edu –OR– uhhpc2.its.hawaii.edu
  User Name: Your UH User name e.g., user99
  Port: 22

- Press "Connect"
- Enter your UH user password when prompted and press the return key

Login to the Cray CS300

Mac & Linux

- Open a terminal window
- Enter one of the following:
  - ssh <UH User name>@uhhpc1.its.hawaii.edu
  - ssh <UH User name>@uhhpc2.its.hawaii.edu
  - **Example:** ssh user99@uhhpc1.its.hawaii.edu
- Enter your UH user password when prompted and press the return key

On Initial Login . . .

Validate that all system permissions are correct for your user

1. Test that you can list files in your home: '`ls -la`'
2. Test making a file in your home: '`touch test.txt`'
3. Go into ~/lus: '`cd ~/lus/`'
4. Test making a file in your lus directory: '`touch test.txt`'
5. Go into ~/apps: '`cd ~/apps/`'
6. Test making a file in your apps directory: '`touch test.txt`'

Result

Did you get any errors? Let us know if you did

Notes:

- On login you are placed in /home/<username>/
- By default, ~ is equivalent to /home/<username>/

Overview – Cluster Interaction

- Connecting to a cluster @ UH
  - Login to the cluster
  - Verify user permissions
- User directories
- Transferring files
  - Globus
- Software
  - Modules
  - Acquiring software
  - Compilers
- Managing user jobs
  - Job scheduler
  - Using SLURM
  - Partition layout
  - Submitting jobs (Examples)

User Directories

Home

```
[user99@login ~]$ ls -l
total 0
lrwxrwxrwx 1 user99 user99 23 Jan 15 20:38 apps -> /lus/scratch/usr/user99
lrwxrwxrwx 1 user99 user99 19 Jan 15 20:38 lus -> /lus/scratch/user99
lrwxrwxrwx 1 root   root   37 Jan 15 20:41 purge -> /lus/scratch/log/purge/current/user99
```

- ~/ is not on the Lustre® filesystem and **should not be used for job data!**
- ~/lus/ is a symlink to the Lustre® scratch
  - This is where all your job data files should live
  - Items in this directory ***are*** subject to our 90 day purge policy
- ~/apps/ is a symlink to where programs should be stored
  - Items in this directory ***are not*** subject to our 90 day purge policy
  - Directory is monitored for abuse
- ~/purge/ is typically a dead symlink
  - Symlink becomes active if the user has files that are part of the next automatic purge
  - When ~/purge/ is active, the directory containing two files – *purge_list.txt* & *totals.txt*
  - An email is sent to users if they have files that will be purged
  - Email notification is sent out 14 days before the purge takes place

User Directories

Filesystems

```
[user99@login ~]$ df -h
Filesystem                                  Size  Used Avail Use% Mounted on
10.10.0.3:/ha_cluster/home                  1.8T  888G  851G  52% /home
10.12.0.51@o2ib:10.12.0.52@o2ib:/scratch    582T  429T  125T  78% /lus/scratch
```

- /home/<username> exists on a NFS mounted filesystem
  - Only has 1.8TB of useable space
  - Using all this space may cause problems for the entire cluster
  - Not a high performance filesystem and small in size
- /lus/scratch/ is the Lustre® filesystem
  - Has 582TB of useable space
  - ~/apps/, ~/lus/, and ~/purge/ all point to directories on this filesystem
  - High performance and a lot more space for users to use
  - No hard or soft quotas are in place
  - Utilization is managed through the 90 day purge policy

Overview – Cluster Interaction

- Connecting to a cluster @ UH
  - Login to the cluster
  - Verify user permissions
- User directories
- Transferring files
  - Globus
- Software
  - Modules
  - Acquiring software
  - Compilers
- Managing user jobs
  - Job scheduler
  - Using SLURM
  - Partition layout
  - Submitting jobs (Examples)

Available File Transfer Protocols

- The cluster has the following options for transferring files:
  - scp (RCP+SSH protocol)
  - rsync (rsync protocol with SSH transport)
  - SFTP (SSH FTP protocol)
  - Globus (Grid FTP protocol)
- All options are widely used, and have clients that can be found for on most major operating systems

SFTP, scp, and rsync are fairly common on Linux systems,
but Globus is not as common . . .

Globus

What is Globus?

The Globus transfer service provides high-performance, secure, file transfer and synchronization between endpoints.

Globus handles all the difficult aspects of data transfer, allowing application users to easily start and manage transfers between endpoints, while automatically tuning parameters to maximize bandwidth usage, managing security configurations, providing automatic fault recovery, and notifying users of completion and problems.

Definition

An ***endpoint*** is one of the two file transfer locations – either the source or the destination – between which files can move. Once a resource (such as a server, cluster, storage system, laptop, or other system) is defined as an endpoint, it will be available to authorized users who can transfer files to or from this endpoint.

---

https://www.globus.org/file-transfer

Globus

If you already use Globus, the endpoints for the Cray CS300 are:

- hawaii#UHHPC1
- hawaii#UHHPC1

For those that have not used Globus, and wish to try it out, you can learn how to use Globus by visiting the Cyberinfrastructure website for more information:
http://www.hawaii.edu/its/ci/hpc-resources/hpc-tutorials/globus-quick-start-guide/

Overview – Cluster Interaction

- Connecting to a cluster @ UH
  - Login to the cluster
  - Verify user permissions
- User directories
- Transferring files
  - Globus
- Software
  - Modules
  - Acquiring software
  - Compilers
- Managing user jobs
  - Job scheduler
  - Using SLURM
  - Partition layout
  - Submitting jobs (Examples)

Modules

A tool to help users manage their Unix or Linux shell environment, by allowing groups of related environment-variable settings to be made or removed dynamically.[1]

- We globally install popular/frequently requested software packages and create modules for all users to access
- Access to modules is via the **module** command
  - 'module avail' – list installed modules
  - 'module load <module name>' – Loads the named module
  - 'module unload <module name>' – Remove named module
  - 'module purge' – Unload all loaded modules
- Installing software in your ~/apps directory is suggested to prevent us from being a bottleneck
  - Two ways to install software on the cluster
    - Download compatible binaries
    - Compile software from source

[1] https://en.wikipedia.org/wiki/Environment_Modules_(software)

Acquiring Software – Binaries and/or Source

- You can transfer software source, binaries or scripts into your ~/apps directory on the Cray CS300
  - Binaries compiled as x86_64 (64-bit) for CentOS 6.5 or RHEL6.5 should work
- You may also download tar or zipped software/source code directly from the login nodes using tools like **wget** & **curl**
- You may also clone source repositories using the correct software revision tool: **git**, **svn**, **hg**, **cvs**, etc.

Compilers

- We have the Intel®, GNU (gcc, g++), Cray® & PGI® compilers
- Compiling must take place on a compute node
  - Interactive sessions are useful for compiling software
  - Sandbox nodes mirror the environment the compute nodes provide and are ideal for compilation
  - Login nodes **do not** load all the software and libraries found on the compute nodes
- Intel® compilers are recommended for best performance
  - Intel® 2013 compilers:
    - module load intel/ics – Loads Intel® compilers: **icc**, **ifort**, **icpc**
    - module load intel/impi – Loads Intel® MPI wrapper: **mpiicc**, **mpiifort**, **mpiicpc**
  - Intel® 2016 compilers:
    - We have 2 floating seats for Intel® 2016 compiler
    - intel_2016/ics
    - intel_2016/impi

Overview – Cluster Interaction

- Connecting to a cluster @ UH
  - Login to the cluster
  - Verify user permissions
- User directories
- Transferring files
  - Globus
- Software
  - Modules
  - Acquiring software
  - Compilers
- Managing user jobs
  - Job scheduler
  - Using SLURM
  - Partition layout
  - Submitting jobs (Examples)

Managing User Jobs

User jobs all come in different shapes and sizes:

- Require multiple nodes working in concert towards a common goal (MPI)
- Require a single node, in which they use multiple threads work together (OpenMP, pthreads, TBB)
- Require a lot of cores to process a lot of data in an identical manner, yet none of the inputs have dependencies on another (HTC)

The Cray CS300 is capable of handle many different types of jobs, but in a multi-user environment with so many users, how do we turn chaos into organized chaos?

This looks like a job for a ***job scheduler***!

What is a Job Scheduler?

Definition

A job scheduler is a computer application for controlling unattended background program execution (commonly called batch processing).

Basic features expected of a job scheduler include:

- Interfaces which help to define workflows and/or job dependencies
- Automatic submission of executions
- Interfaces to monitor the executions
- Priorities and/or queues to control the execution order of unrelated jobs

For the Cray CS300, we utilize the **S**imple **L**inux **U**tility **R**esource **M**anager or simply known as the *SLURM scheduler*.

---

https://en.wikipedia.org/wiki/Job_scheduler

https://en.wikipedia.org/wiki/Slurm_Workload_Manager

http://slurm.schedmd.com/slurm.html

How to use SLURM

SLURM has a series of commands, each of which allow users to interact with the job scheduler

- sbatch –
- srun –
- srun.x11 –
- sacct –
- scontrol –
- scancel –

Let us look at how the nodes are partitioned, as well as some examples of submitting jobs and create job scripts

Partition layout

Interactive Job with SLURM

Interactive session (no X11)

```
[login ~]$ srun --immediate --partition sb.q --nodes 1 --cpus-per-task 5 --tasks-per-node 1 --time 0-01:00 --pty /bin/bash
```

Interactive session (with X11)

1. Connect via SSH using the -Y option, X11 forwarding enabled
2. run srun.x11 to start a session on a node

```
[local ~]$ ssh -Y user99@uhhpc1.its.hawaii.edu
[login ~]$ srun.x11 --immediate --partition sb.q --nodes 1 --cpus-per-task 5 --tasks-per-node 1 --time 0-01:00
[compute-0001 ~]$ xterm
```

SLURM Submission Script File (MPI Job)

```
[login lus]$ cat mpi.slurm

#!/bin/sh
#SBATCH --job-name=MPI_example
#SBATCH --partition=exclusive.q
## 3 day max run time for community.q, kill.q, exclusive.q, and htc.q.  1 Hour max run time for sb.q
#SBATCH --time=3-00:00:00
## task-per-node x cpus-per-task should not typically exceed core count on an individual node
#SBATCH --nodes=4
#SBATCH --tasks-per-node=20
#SBATCH --cpus-per-task=1
#SBATCH --mem-per-cpu=6400 ## max of 6400 for standard nodes, max of 26214 for large memory nodes
#SBATCH --error=hello-%A_%a.err ## %A - filled with jobid. %a - filled with job arrayid
#SBATCH --output=hello-%A_%a.out ## %A - filled with jobid. %a - filled with job arrayid
## Useful for remote notification
#SBATCH --mail-type=BEGIN,END,FAIL,REQUEUE,TIME_LIMIT_80
#SBATCH --mail-user=user@test.org

## All options and environment variables found on schedMD site: http://slurm.schedmd.com/sbatch.html
## Intel MPI manual: https://software.intel.com/en-us/mpi-refman-lin-html
export OMP_NUM_THREADS=${SLURM_CPUS_PER_TASK}
export I_MPI_FABRICS=tmi
export I_MPI_PMI_LIBRARY=/opt/local/slurm/default/lib64/libpmi.so

cd $SLURM_SUBMIT_DIR
srun  -n ${SLURM_NTASKS}  ./hello_mpi.intel
```

SLURM Submission Script File (Non-MPI Job)

```
[login lus]$ cat hello_world.slurm

#!/bin/sh
#SBATCH --job-name=example
#SBATCH --partition=community.q
## 3 day max run time for community.q, kill.q, exclusive.q, and htc.q.  1 Hour max run time for sb.q
#SBATCH --time=3-00:00:00
## task-per-node x cpus-per-task should not typically exceed core count on an individual node
#SBATCH --nodes=1
#SBATCH --tasks-per-node=1
#SBATCH --cpus-per-task=5
#SBATCH --mem-per-cpu=6400 ## max of 6400 for standard nodes, max of 26214 for large memory nodes
#SBATCH --error=hello-%A_%a.err ## %A - filled with jobid. %a - filled with job arrayid
#SBATCH --output=hello-%A_%a.out ## %A - filled with jobid. %a - filled with job arrayid
## Useful for remote notification
#SBATCH --mail-type=BEGIN,END,FAIL,REQUEUE,TIME_LIMIT_80
#SBATCH --mail-user=user@test.org

## All options and environment variables found on schedMD site: http://slurm.schedmd.com/sbatch.html

export OMP_NUM_THREADS=${SLURM_CPUS_PER_TASK}

cd $SLURM_SUBMIT_DIR
./hello_world
```

SLURM Submission Script File (Job Array)

```
[login lus]$ cat job_array.slurm

#!/bin/sh
#SBATCH --job-name=example
#SBATCH --partition=community.q
## 3 day max run time for community.q, kill.q, exclusive.q, and htc.q.  1 Hour max run time for sb.q
#SBATCH --time=3-00:00:00
## task-per-node x cpus-per-task should not typically exceed core count on an individual node
#SBATCH --nodes=1
#SBATCH --tasks-per-node=1
#SBATCH --cpus-per-task=5
#SBATCH --mem-per-cpu=6400 ## max of 6400 for standard nodes, max of 26214 for large memory nodes
#SBATCH --error=buzz-%A_%a.err ## %A - filled with jobid. %a - filled with job arrayid
#SBATCH --output=buzz-%A_%a.out ## %A - filled with jobid. %a - filled with job arrayid
## Useful for remote notification
#SBATCH --mail-type=BEGIN,END,FAIL,REQUEUE,TIME_LIMIT_80
#SBATCH --mail-user=user@test.org

## All options and environment variables found on schedMD site: http://slurm.schedmd.com/sbatch.html

export OMP_NUM_THREADS=${SLURM_CPUS_PER_TASK}

cd $SLURM_SUBMIT_DIR
./worker_bee -i input_${SLURM_ARRAY_TASK_ID}.flower -o output_${SLURM_ARRAY_TASK_ID}.honey
```

Outline

Cluster Etiquette

Outline

Overview

- Login node usage policy
- Scratch filesystem purge policy

Login Node Usage Policy

Login node usage policy is subject to change
Users will be notified via email prior to changes taking effect

Lustre® Filesystem Purge Policies

Due to users not having any quotas on the Lustre® filesystem, we need some policy in place which removes older files from the system. To accomplish this, we have currently implemented a purge policy, for any file that is older than 90 days.

- Which of my directories are subject to the purge policy?
  - **Answer:** All files and folders found in ~/lus/ are subject to the 90 day purge policy. Symlinks are excluded from the purge, and are not followed by the purge bot.
- How frequently are files for purging identified?
  - **Answer:** Current frequency is every other month, but the frequency many increase or decrease based on the fill rate of the Lustre® filesystem

Purge policy is subject to change
Users will be notified via email prior to changes taking effect

Outline

FAQ

- Are files on the cluster backed up?
  - **Answer: NO!** User files on the cluster ***are not backed up***. It is up to you as the user to validate and maintain your own backups. The Cyberinfrastructure team takes no responsibility for any data that is lost due to human or mechanical error.

Questions?