

Introduction to High Performance Computing and O2 for New Users

HMS Research Computing

Presented by Harvard Chan Bioinformatics Core

Meeta Mistry, Ph.D

Will Gammerdinger, Ph.D

(Slides courtesy of Kris Holton & Kathleen Chappell at HMS-RC)



HPC Cluster

- multi-user, shared resource
- lots of nodes = lots of processing capacity + lots of memory
- a system like this requires constant maintenance and upkeep, and there is an associated cost

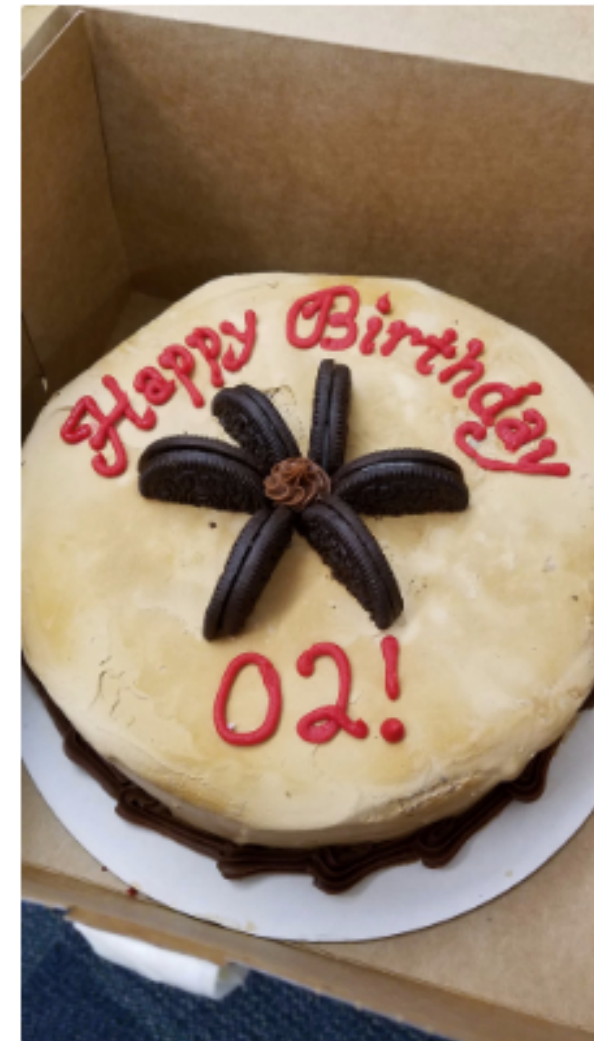
Wiki page:

<https://harvardmed.atlassian.net/wiki/spaces/O2/overview>



Tweets by @hms_rc

HMSResearchComputing @hms_rc
It's cake time for RC -- happy birthday to O2 !!



♡ [replies]

Sep 12, 2017

HMSResearchComputing @hms_rc
O2 is officially being launched today as the new RC production HPC cluster!! (thnx beta testers!) Get started at: hmsrc.me/O2docs

♡ [replies]

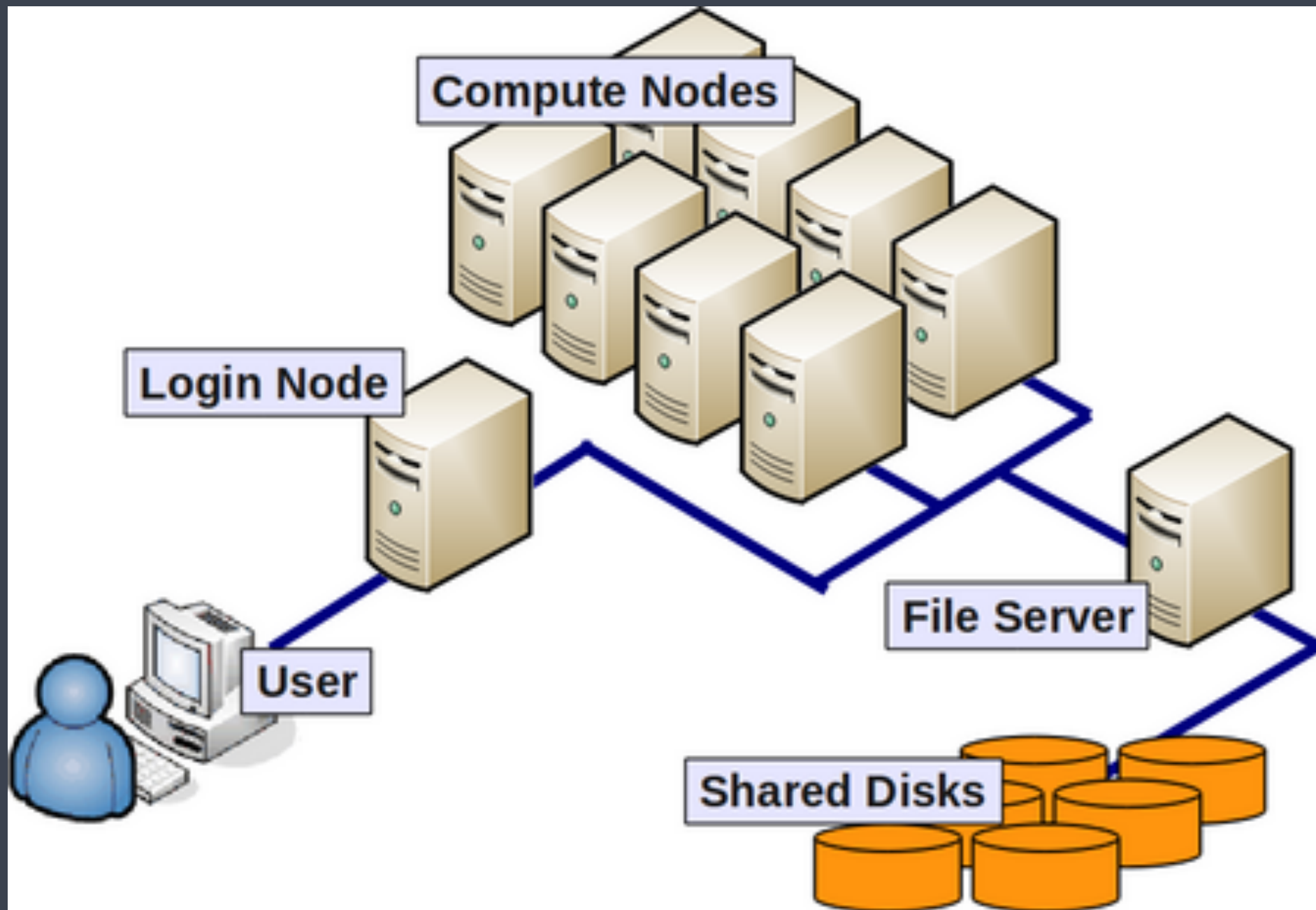
Sep 12, 2017

O2 Tech Specs



- 12200+ cores
- 32, 28, or 20 cores per node
- 256-160GiB RAM (memory) per node (8-9GiB/core)
- 9 756GiB RAM and 1 1TiB highmem nodes
- 133 GPU cards
 - (103 GPUs available to Quad researchers only)
- CentOS 7 Linux
- SLURM job scheduler

HPC



Using O2!

1. Logging in to remote machines (securely)

- When logging in we used the “ssh” command,
ssh stands for Secure Shell
- **ssh** is a protocol for data transfer that is secure, i.e the data is encrypted as it travels between your computer and the cluster (remote computer)
- Commonly used commands that use the **ssh** protocol for data transfer are, **scp** and **sftp**

Logging Into O2

- Open a terminal

```
ssh yourHMSaccount@o2.hms.harvard.edu
```

- If logging in from outside of “approved” internet/WiFi sources (HMS Private/Harvard Secure), 2-factor authentication is required using DUO

Welcome to O2!

Where are you in O2?

```
mfk8@login01:~$
```

You are logged into a “**shell login server**”,
login01-05. These are not meant for heavy lifting!

```
mfk8@login01:~$ pwd
```

You are in your home directory.

Interactive Sessions

- The login servers are not designed to handle intensive processes, and CPU usage is throttled.
- Start by entering your first job! This will (usually) log you into a “**compute** node!”

```
mfk8@login01:~$ srun --pty -p interactive -t 0-12:00  
--mem 1G bash
```

“srun --pty” is how interactives are started

“-p interactive” is the partition

“-t 0-12:00” is the time limit (12 hours)

“--mem 1G” is the memory requested

```
mfk8@compute-a:~$
```

Using & installing software

LMOD: Software Modules

- Most “software” on O2 is installed as an **environment module** using the LMOD system.
- LMOD adds (or removed) the paths of software executables and their dependencies into your path, i.e. into the \$PATH variable
- Allows for clean, easy loading, including most dependencies, and switching versions.

LMOD: Software Modules

- The primary command for LMOD is “module” which has lots of different subcommands
- Most software is compiled against something called “gcc-6.2.0” or “gcc-9.2.0” - so, we need to load one of those before loading other programs that depend on it.

```
$ module load gcc/6.2.0
```

```
$ module avail #to see software now available to load
```

```
$ module spider #verbose list of all software available
```

Loading/Unloading Modules

Check module status (e.g. the statistical software R)

```
$ module list
```

```
$ echo $PATH
```

```
$ R
```

Loading/Unloading Modules

Check module status (e.g. the statistical software R)

```
$ module list
```

```
$ echo $PATH
```

```
$ R
```

Load the module

```
$ module load R/4.1.1
```

```
$ R
```

Loading/Unloading Modules

Check module status (e.g. the statistical software R)

```
$ module list
```

```
$ echo $PATH
```

```
$ R
```

Load the module

```
$ module load R/4.1.1
```

```
$ R
```

Which module version is loaded (if at all)?

```
$ which R
```

```
$ module list
```

```
$ echo $PATH
```

Loading/Unloading Modules

Need help with the module?

```
$ module help R/4.1.1
```

Unloading modules

```
$ module unload R/4.1.1
```

Dump all modules

```
$ module purge
```


The Job Scheduler, SLURM

Simple Linux Utility for Resource Management (SLURM)

- Fairly **allocates** access to resources (computer nodes) to users for some duration of time so they can perform work
- Provides a **framework** for starting, executing, and monitoring batch jobs
- **Manages** a queue of pending jobs; ensures that no single user or core monopolizes the cluster

Submitting Jobs

srun starts an interactive session

```
mfk8@login05:~$ srun -pty -p interactive -t 0-3:00  
-c 4 --mem 8G bash
```

In an “interactive session”, programs can be run directly, however your computer will have to remain connected to the cluster for the duration of this run.

```
mfk8@compute-a:~$ module load gcc/9.2.0 R/4.1.1
```

```
mfk8@compute-a:~$ Rscript sqrt_input.R 60
```

Submitting Jobs

What if you wanted to run the program, close your computer and come back later to check on it?

*A **script** with the required commands can be submitted to O2 (SLURM) using the **sbatch** command.*

```
mfk8@login05:~$ sbatch myRscript.slurm
```

Creating a job submission script

```
#!/bin/sh

#SBATCH -p short
#SBATCH -t 0-03:00
#SBATCH -c 4
#SBATCH --mem=8G
#SBATCH -o %j.out
#SBATCH -e %j.err
#SBATCH -J Rscript_sqrt
#SBATCH --mail-type=ALL
#SBATCH --mail-user=mfk8@med.harvard.edu

module load gcc/9.2.0 R/4.1.1

Rscript sqrt_input.R 60
```

Save script as myRscript.slurm and run it as follows:

```
$ sbatch myRscript.slurm
```

***O2 will notify you when the job is done, or if there is an error*

Choosing the proper resources for your job with
the appropriate options

Partitions -p

Partition	Priority	Max Runtime	Max Cores	Limits
short	12	12 hours	20	
medium	6	5 days	20	
long	4	30 days	20	
interactive	14	12 hours	20	2 job limit
priority	14	30 days	20	2 job limit
mpi	12	5 days	640	20 core min
highmem	12	5 days	20	
gpu, gpu_quad, gpu_requeue	12	160 GPU hours	34 (total)	420GiB (total)
transfer	1	5 days	4	

Runtime: -t

- -t days-hours:minutes
- -t hours:minutes:seconds
- Need to specify how long you estimate your job will run for
- Aim for 125%
- Subject to maximum per partition
- Excessive runlimits (like partition max) take longer to dispatch, and affect fairshare

Cores: -c

- -c X to designate cores: max 20 per job
- -N X to constrain all cores to X nodes
- CPU time: wall time (-t) * (-c) cores used
- Unable to use cores not requested (no overefficient jobs): cgroups constraint
- Adding more cores does not mean jobs will scale linearly with time, and causes longer pend times

Memory: --mem

- Only 1GiB is allocated by default
- `--mem xG` #total memory over all cores
- `--mem-per-cpu xG` #total memory per CPU requested, use for MPI
- No unit request (G) defaults to Mebibytes (MiB)
 - 8G ~= 8000

Managing jobs and getting information about
submitted/running jobs

Job Monitoring: Current jobs

- `$ O2squeue`
 - JOBID, PARTITION, STATE, TIME_LIMIT, TIME, NODELIST(REASON), ELIGIBLE_TIME, START_TIME, TRES
 - [O2squeue documentation](#)
- *Other options:*
 - `$ squeue -u eCommons -t RUNNING/PENDING`
 - `$ squeue -u eCommons -p Partition`
 - `$ squeue -u eCommons -start`
- *Detailed job info:*
 - `$ scontrol show jobid <jobid>`

Cancelling/Pausing Jobs

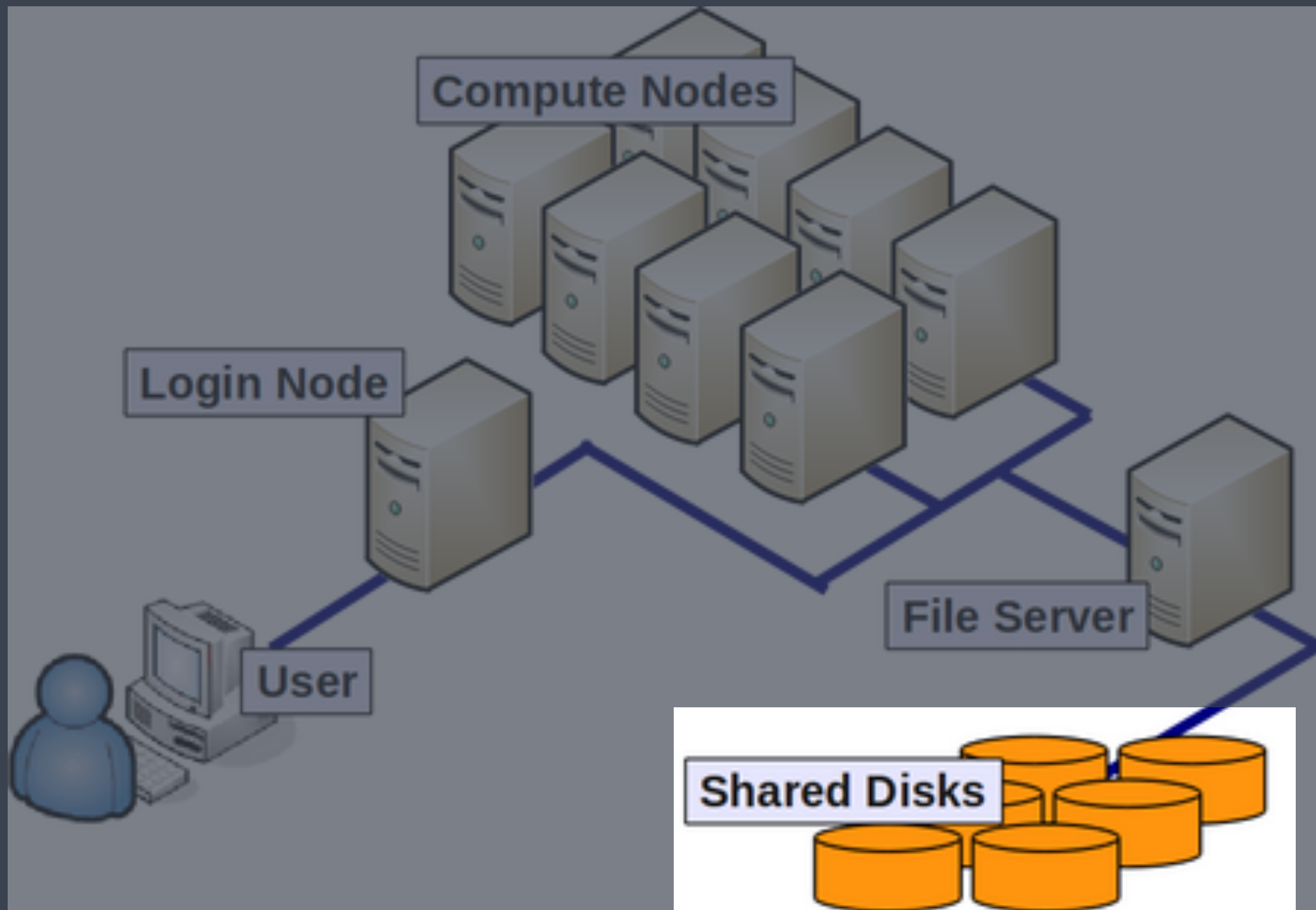
- `$ scancel <jobid> #Cancels specific job`
- `$ scancel -t PENDING #Cancels pending job`
- `$ scancel --name JOBNAME #Cancels job by name`
- `$ scancel jobid_[indices] #array indices`
- `$ scontrol hold <jobid> #pause pending jobs`
- `$ scontrol release <jobid> #resume`

Exercise!

<https://tinyurl.com/sbatch-Rexercise>

Filesystems and storage

Filesystems and storage



Filesystems and storage

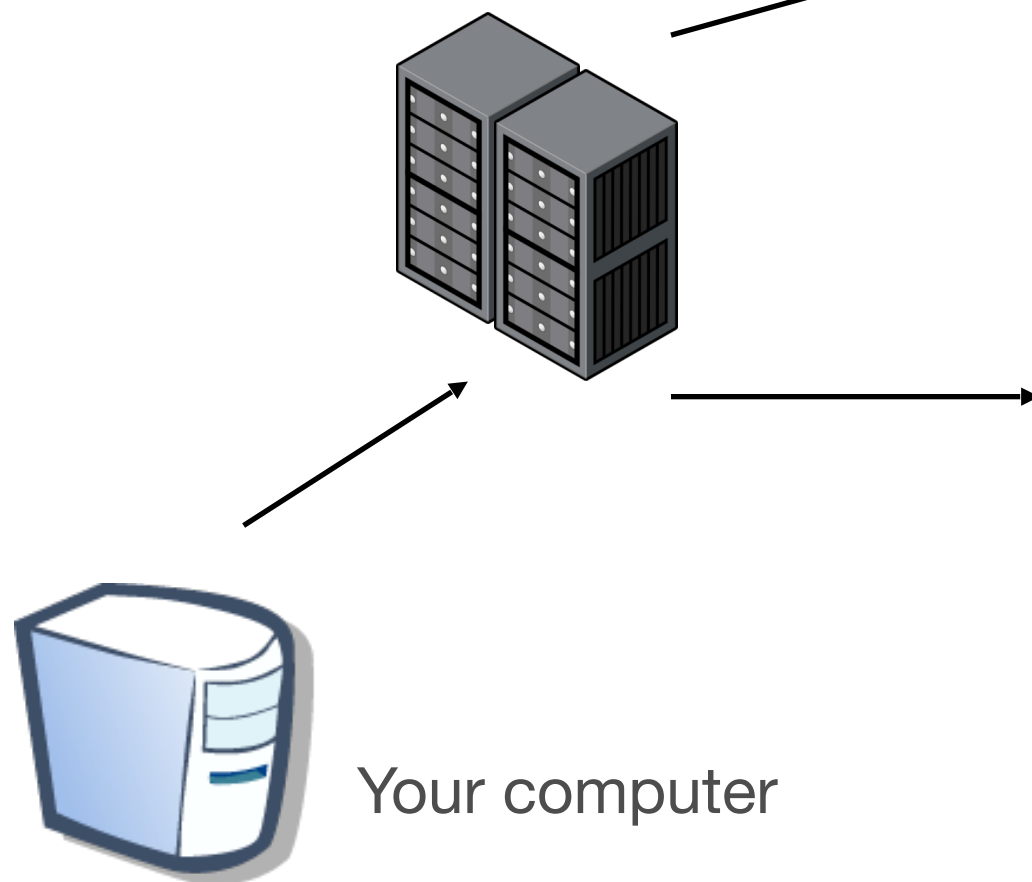
- Storage on HPC systems is organized differently than on your personal machine
- Physical disks are bundled together into a virtual volume; this volume may represent a single filesystem, or may be divided up, or partitioned, into multiple filesystems
- Filesystems are accessed over the internal network

O2 Primary Storage



O2 Cluster

- 11000+ cores
- SLURM batch system



/home

- [/home/HMS_account](#)
- quota: 100GiB per user
- Backup: extra copy & snapshots:
- daily to 14 days, weekly up to 60 days

/n/data1, /n/data2, /n/groups

- [/n/data1/institution/dept/lab/your_dir](#)
- quota: expandable
- Backup: extra copy & snapshots:
- daily to 14 days, weekly up to 60 days

Temporary “Scratch” storage

- `/n/scratch3/users/<first_HMS_account_char>/<HMS_account>`
e.g. /n/scratch3/users/m/mfk8
- For data only needed temporarily during analyses
- Each user can use up to 10 TiB and 1 million files/directories
- Files not accessed for 30 days are automatically purged
- No backups!
- Create your folder:
 - `$ /n/cluster/bin/scratch3_create.sh`
- [Scratch3 documentation](#)

Important Note about O2 Storage

- O2 can only be used to store data of [Harvard Security Level 3](#) and below.
- None of the standard filesystems are automatically encrypted, and **cannot** be used for HIPAA-protected or other secure data (Harvard's data security above level 3) unless those data have been de-identified.


Chargeback for Storage & Compute

- Charges apply to labs whose PIs do NOT have a primary or secondary appointment with an HMS Quad department (*external users*)
- External users and PIs must register with the [RC Core in the PPMS system](#) prior to obtaining an O2 account.
- [Details on the O2 Account Request Process for Off Quad Labs](#)
- Bills are sent out quarterly
 - Charged: O2 jobs, O2 group folders, research.files
 - Free: Scratch and Home folders
- More details (including billing rates) are on the [Research Computing Core website](#).
- Reach out to rccore@hms.harvard.edu with any questions.

For more direction


 **Email:** rchelp@hms.harvard.edu

 **Website:** <https://it.hms.harvard.edu/our-services/research-computing>

 **Phone:** 617-432-2000 (HMS IT Service Desk, 8a-5p)

 **Twitter:** http://twitter.com/hms_rc

 **Location:** 1635 Tremont Street

 **Office hours:** Wednesdays 1:00-3:00 pm (Currently via Zoom - <https://rc.hms.harvard.edu/office-hours>)

[Click on image above for a link to the O2 wiki page](#)