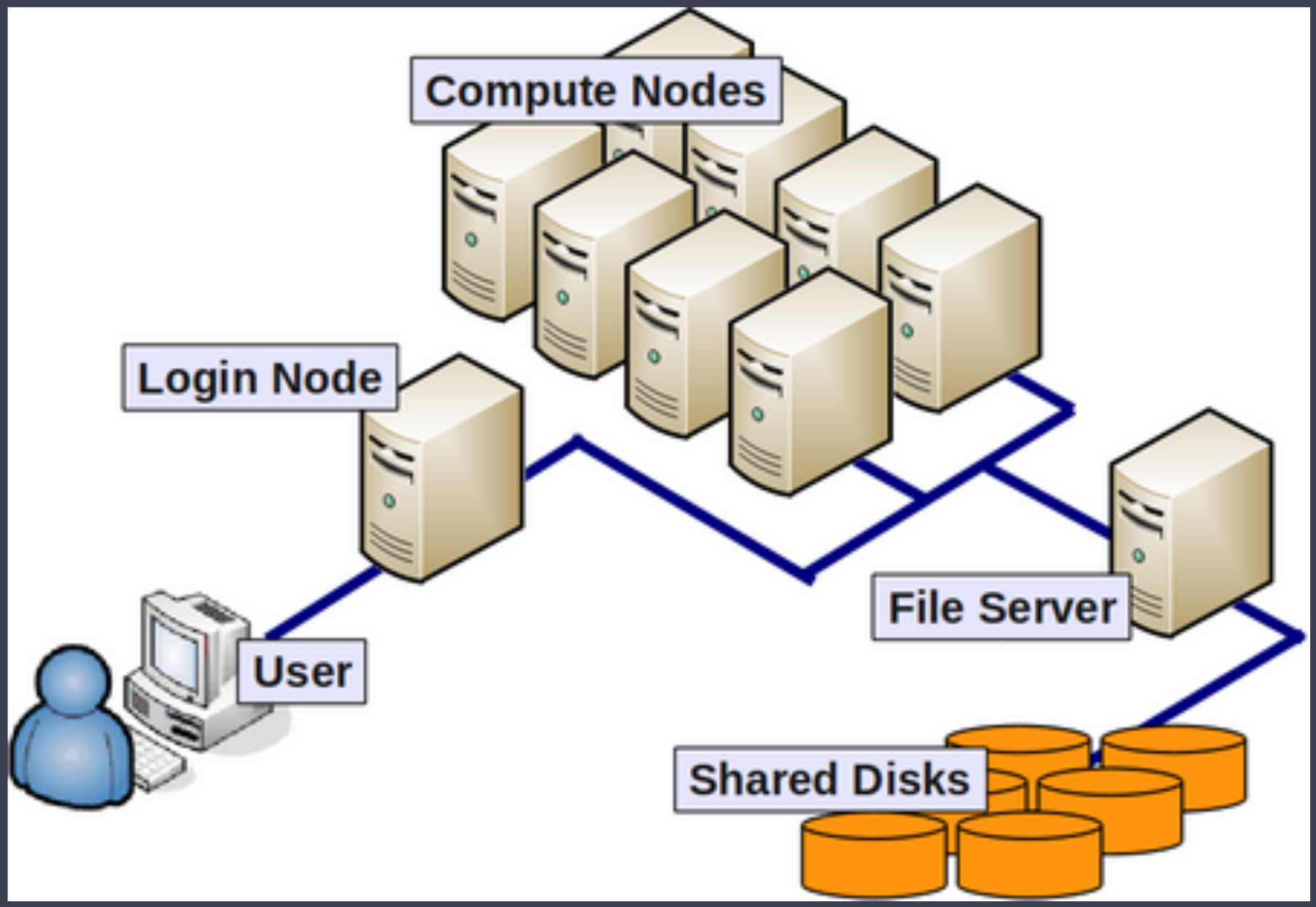
(Re)Introduction to High-Performance Computing (HPC)

HPC cluster structure



HPC cluster components

Nodes: Individual computers in the cluster

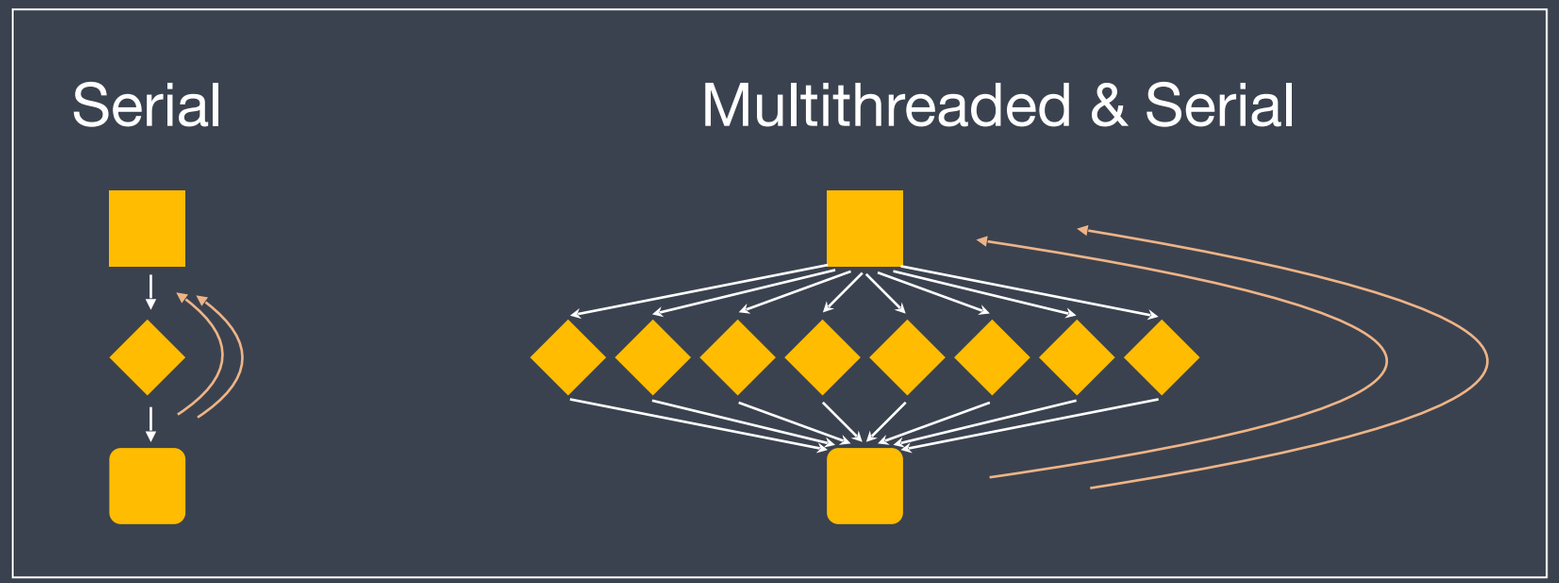
Cores (threads): individual processing units available within each CPU of each Node

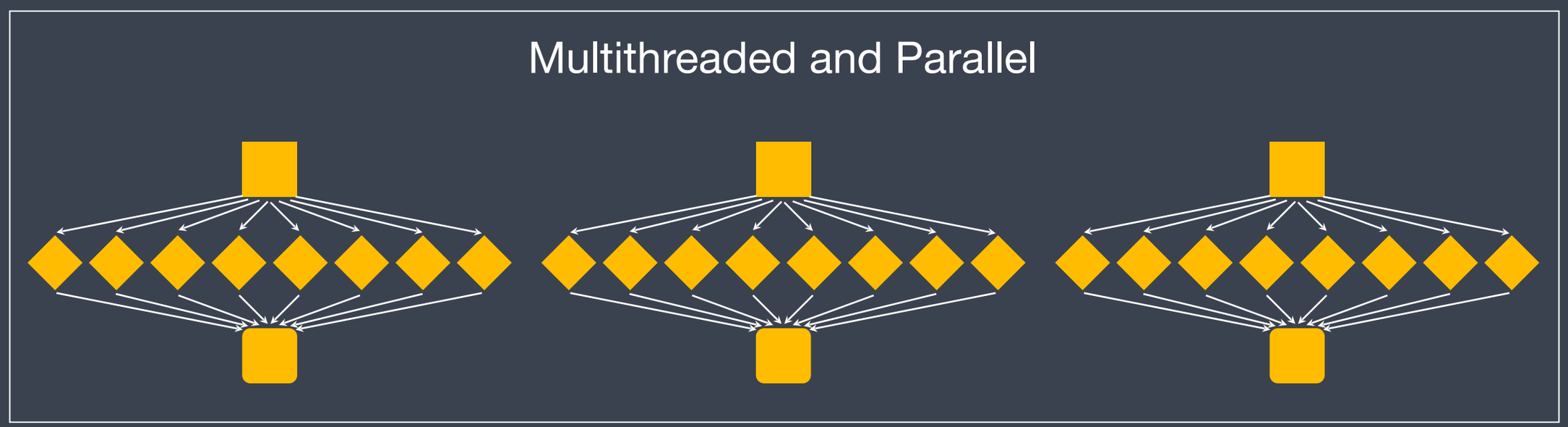
e.g. a “Node” with eight “quad”-core CPUs = 32 cores for that node.

Shared disk: storage that can be shared (and accessed) by all nodes

High-Performance Computing

For 3 samples





Introduction to High Performance Computing and O2 for New Users

HMS Research Computing

(Slides courtesy of Kris Holton at HMS-RC)

O2 Tech Specs

- 11000 cores
- 32, 28, or 20 cores per node
- 256-160GB RAM (memory) per node (8-9GB/core)
- 756GB RAM (high memory nodes)
- 40 GPUs (V100, K80, M40)
- CentOS 7 Linux
- SLURM job scheduler

2-Factor Authentication

- For logins using WiFi networks other than HMS Private/ Harvard Secure
- Easiest: download Duo app to phone
- Similar to the setup for Harvard Key logins
- Setup details at: https://wiki.rc.hms.harvard.edu:8443/display/O2/Two+Factor+Authentication+on+O2

The Job Scheduler, SLURM

Choosing the proper resources for your job with the appropriate `Slurm` arguments

Submitting Jobs

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@login-1:~$ srun --pty -p interactive -t 0-8:00
—mem 6G /bin/bash

mfk8@compute-a:~$ bowtie2 -c 4 hg19 file1_1.fq
```

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@login-1:~$ sbatch mybowtiejob.sh
```

OR

```
mfk8@compute-a:~$ sbatch mybowtiejob.sh
```

Creating a job submission script

```
#! /bin/sh

#SBATCH -p short
#SBATCH –t 0-03:00    #aim for 125% over
#SBATCH –c 4          #number of cores/threads, match with what is used in script
#SBATCH --mem=8G
#SBATCH –o %j.out
#SBATCH –e %j.err
#SBATCH -J bowtie2_run1    #job name
#SBATCH –mail-type=ALL     #notify about job completion or errors
#SBATCH ––mail-user=mfk8@med.harvard.edu

module load gcc/6.2.0
module load bowtie2/2.2.9

bowtie -c 4 hg19 file1_1.fq
```

Save script as myJobScript.run and run it as follows from login or compute node:

```
$ sbatch myJobScript.run
```

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	8	750G
gpu		120 GPU hours	20 cpu	
transfer		5 days	4	

Job Priority

- Dynamically assigned
- Factors contributing: Age, Fairshare, Partition, QOS, Nice
- Fairshare: 0-1 scale

Managing jobs and getting information about submitted/running jobs

Job Monitoring

- `$ O2squeue #HMS wrapper`
- `$ squeue –u eCommons`

Detailed job info:

- `$ scontrol show jobid <jobid>`

Completed job statistics:

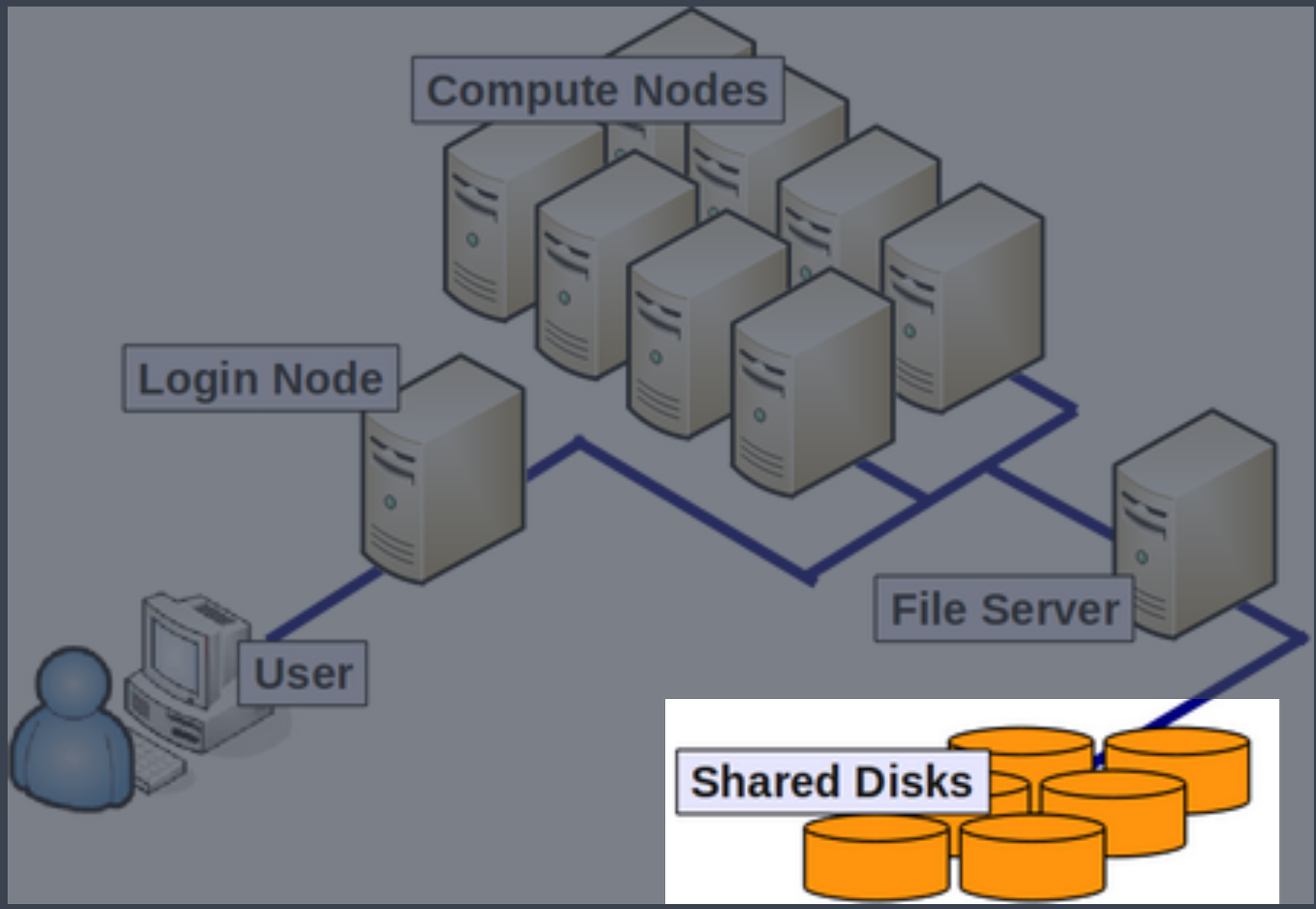
- `$ O2sacct #HMS wrapper`

Cancelling Jobs

- `$ scancel <jobid>`
- `$ scancel --name JOBNAME`

Filesystems and storage

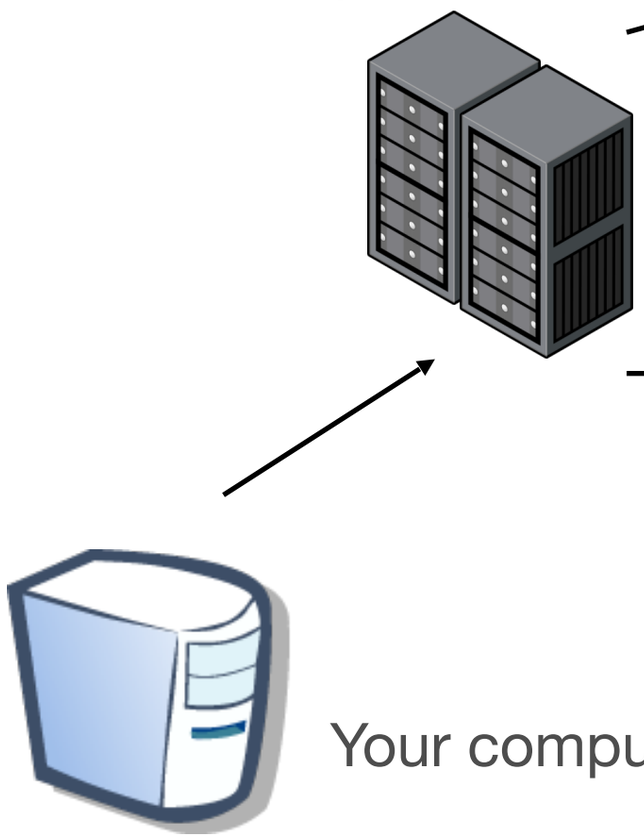
Filesystems and storage



O2 Primary Storage

O2 Cluster

- 11000+ cores
- SLURM batch system



Your computer

/home

- /home/user_id
- quota: 100GB 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/scratch2**
- **For data only needed temporarily during analyses.**
- **Each account can use up to 10 TB and 1 million files/directories**
  - **Lustre** --> a high-performance parallel file system running on DDN Storage.
  - More than 1 PB of total shared disk space.
  - No backups! Files are automatically deleted after unaccessed for 30 days, to save space.
  - More info at: http://hmsrc.me/O2docs

Checking storage usage

- For `/n/data1, /n/data2, /n/groups`
  - `$ quota`
  - Breaks down per user, directory
- For `/n/scratch2`
  - `$ lfs quota -h /n/scratch2`
  - 1 million files/folders, 10TB limit

For more direction

- http://hmsrc.me/O2docs
- http://rc.hms.harvard.edu
- RC Office Hours: Wed 1-3p Gordon Hall 500
- rchelp@hms.harvard.edu