Introduction to High-Performance Computing (HPC)

Computer components

CPU : Central Processing Unit

cores : individual processing units within a CPU

Storage : Disk drives

HDD : Hard Disk Drive

SSD : Solid State Drive

Memory : small amount of volatile or temporary information storage

Computer components (my Macbook Pro)

Model Name: MacBook Pro

Processor Name: Intel Core i7

Processor Speed: 2.5 GHz

Number of Processors: 1

Total Number of Cores: 4

Memory: 16 GB

Data storage: 512 GB

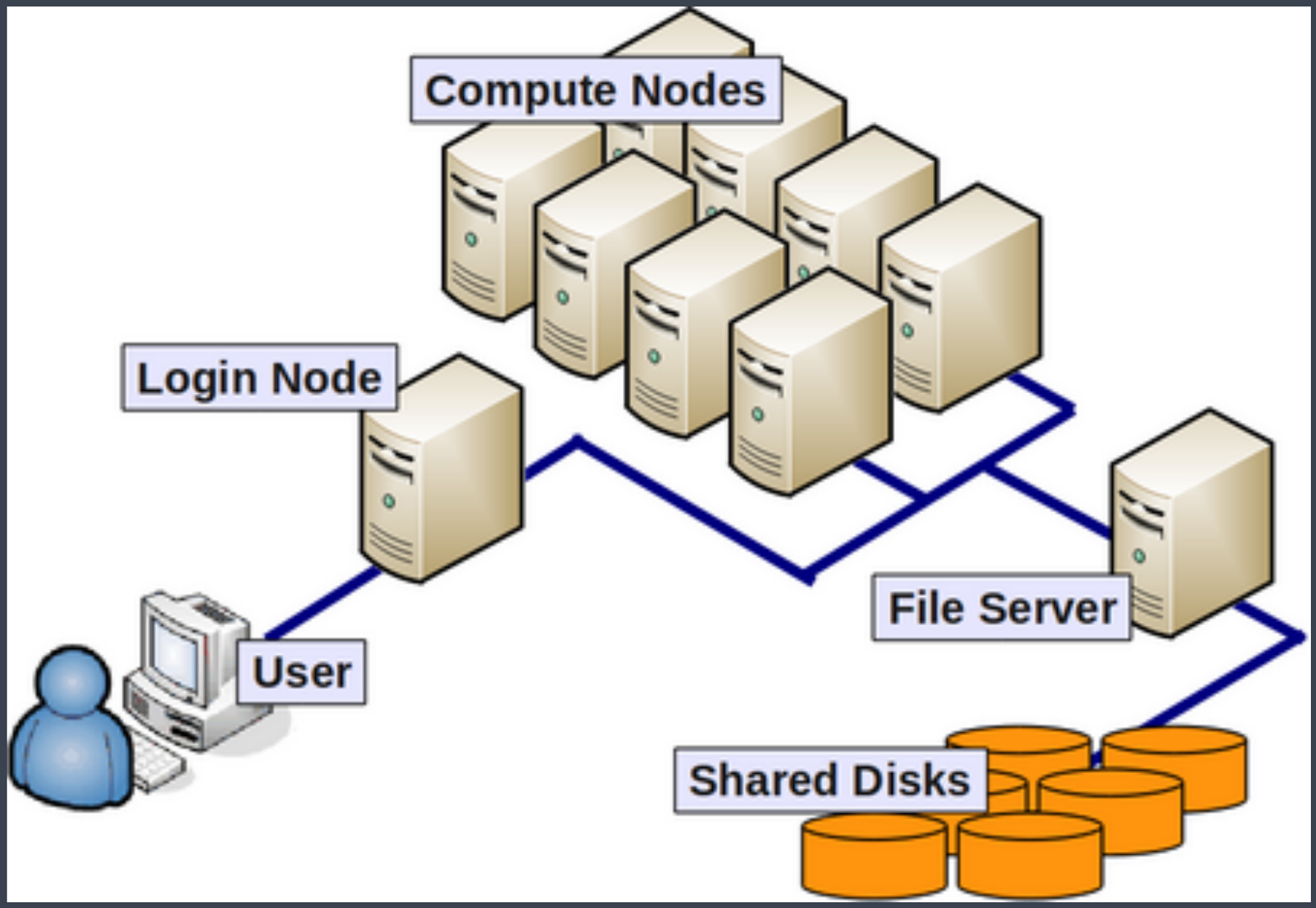
“High Performance Computing most generally refers to the practice of aggregating computing power in a way that delivers much higher performance than one could get out of a typical desktop computer or workstation in order to solve large problems in science, engineering, or business.”

http://insidehpc.com/hpc-basic-training/what-is-hpc/

Need for HPC cluster?

- Resources: Your computer does not have the resources to run the desired NGS analysis
- Speed: You want to produce results faster than your computer
- Software: You need software that is unavailable or unusable on your computer

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.

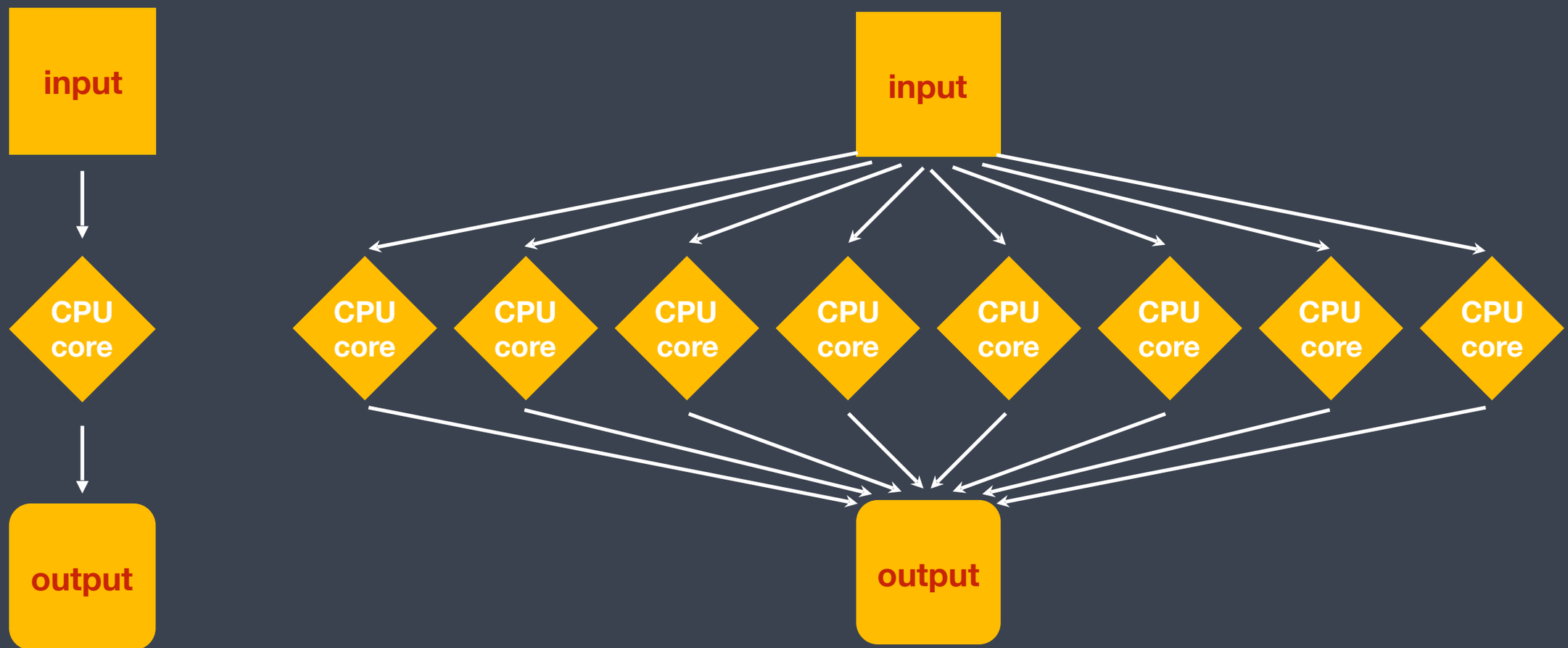
Shared disk: storage that can be shared (and accessed) by all nodes

Parallel Computing

“Parallel computing is a form of computation in which many calculations are carried out simultaneously, operating on the principle that large problems can often be divided into smaller ones, which are then solved concurrently ("in parallel”)."

http://en.wikipedia.org/wiki/Parallel_computing

Multithreaded

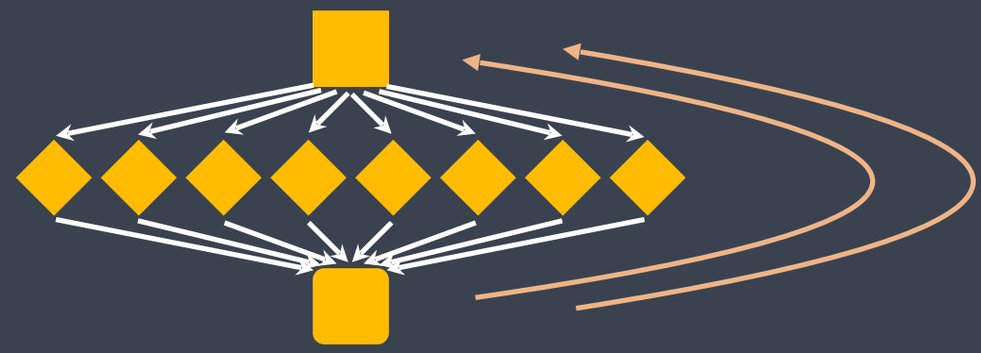


Faster and more efficient

NGS data analysis is very amenable to this strategy

Serial

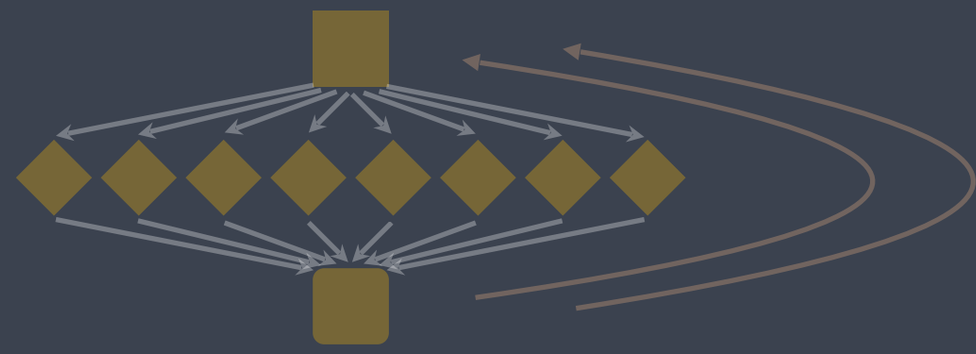
Multithreaded & Serial



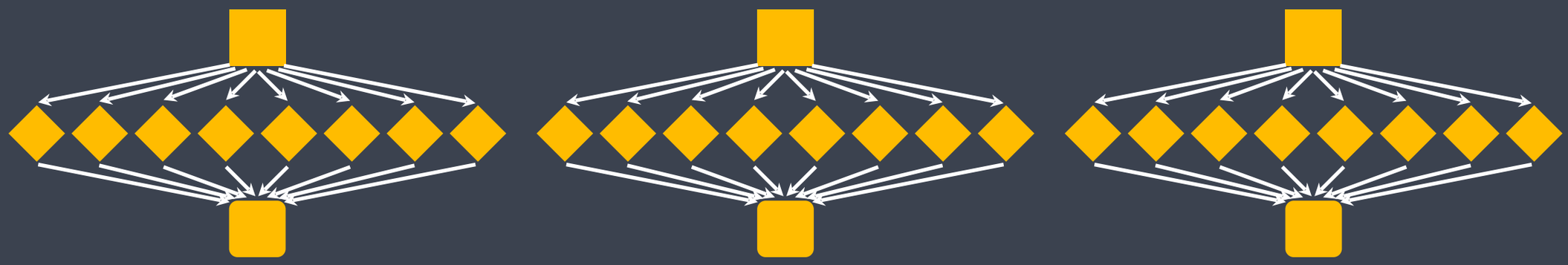
For 3 samples

Serial

Multithreaded & Serial



Multithreaded and “Parallel”



For 3 samples

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.

What is Orchestra?

Please see our Orchestra status page for known issues.

The **Orchestra** platform provides UNIX-based high performance computing, web hosting, and database hosting services at Harvard Medical School.

Orchestra and its associated services are managed by the **Research Computing Group**, part of the HMS Information Technology Department.

Please submit a request via the RC web site for help with Orchestra or feedback. You can also subscribe to the mailing list for Orchestra users.

Wiki page: https://wiki.med.harvard.edu/Orchestra

Introduction to High Performance Computing and Orchestra

HMS Research Computing
Spring 2017

What is Orchestra?

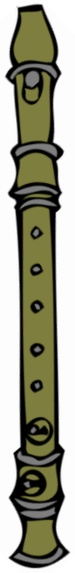
- Tech specs:
  - Over 550 compute nodes
  - Over 7,500 cores
  - 10GigE interconnection
  - Over 42TB RAM
- CentOS 6 Linux
- LSF scheduler
- Total 28+PB storage

Orchestra Compute Nodes

Clarinet
4500 cores
12 x 96GB

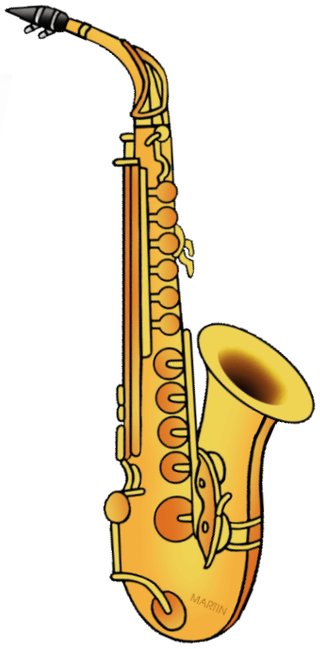
Piccolo
800 cores
20 x 120GB

Ocarina
256 cores
32 x 512GB



Fife
400 cores
20 x 160GB

Ottavino
2000 cores
28 x 224GB



Saxophone
24 cores
12 X 1TB

Using Orchestra!

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**

2. Using tools/software

Using Software Environment Modules

- Most “software” on Orchestra is installed as an environment module.
- An environment module makes the necessary modifications in $PATH to make sure the program runs without any issues.
- Allows for clean, easy loading, including most dependencies, and switching versions.

Using Software Environment Modules

- Most “software” on Orchestra is installed as an environment module.
- An environment module makes the necessary modifications in $PATH to make sure the program runs without any issues.
- Allows for clean, easy loading, including most dependencies, and switching versions.

```
$ module avail
$ module avail seq/
$ module avail stats/
$ module avail seq/bowtie/
```

What software environment modules are available on Orchestra?

Loading/Unloading Modules

- Loading modules

```
$ echo $PATH
$ module load seq/bowtie/2.0.6
$ echo $PATH
```

- Which module version is loaded (if at all)?

```
$ which bowtie
```

- See all modules that have been loaded

```
$ module list
```

- Unloading modules

```
$ module unload seq/bowtie/2.0.6
```

- Dump all modules

```
$ module purge
```

3. The Job Scheduler, LSF

LSF: Fair Sharing

- **L**oad **S**haring **F**acility: distributes jobs across Orchestra fairly
- Ensures that no single user or core monopolizes Orchestra
- Users are assigned dynamic priorities
- Queues also have priorities
- Submitting lots of jobs reduces your fairshare priority
- Even if many jobs are pending, your jobs will start quickly provided you have not submitted many jobs

3a. Running and submitting jobs with the LSF scheduler

Submitting Jobs

- In an “interactive session”, programs can be called directly.

```
mfk8@clarinet001:~$ bowtie –p 4 hg19 file1_1.fq file1_2.fq
```

You will have to wait until the job finishes to do more work in this terminal.

- Or jobs can be submitted with a shell script

```
mfk8@balcony:~$ bsub -q mcore -W 12:00 -n 4 -e %J.err -o
%J.out -N sh myshellscript.sh
```

With this type of a submission, you can exit the cluster, or work on other things, Orchestra will notify you when the job is done, or if there is an error.

3b. Choosing the proper resources for your job with the appropriate **bsub** options

The “bsub”

```
mfk8@clarinet001:~$ bsub –q queue –W hr:min job
```

- Necessary to specify:
  - -q (queue)
  - -W (runtime in hr:min)

Shared Queues

- ***mpi*** queue if you have an MPI parallel job
- ***priority*** queue if you have just one or two jobs to run
- ***mcore*** queue if you have multi-core jobs to run.
- ***short*** queue if your jobs will take less than 12 hours to run.
- Else: ***long*** queue.

Runtime Limit

- -W in hours:minutes
- Runtimes are subject to the maximum time permitted per queue (see table)
- If your job exceeds your runtime, your job will be killed ☹
- Running many jobs that finish quickly (less than a few minutes) is suboptimal and may result in job suspension, contact RC to learn how to batch jobs

bsub options

```
-n 4                (number of cores requested)
-R “rusage[mem=8000]”    (memory requested in MB)
-J jobname
-a openmpi          (type of mpi run)
-Is                 (interactive shell)
-e %J.err           (send  errors to file)
-o %J.out           (send screen output to file)
-N                   (notify when job completes)
```

CPU Limit

- Amount of seconds the cluster works on your job (calculated by LSF)
- Ncores * Runlimit (-n * -W)
- Common error:

bsub –q short –W 8:00 tophat –p 8

tophat program asks for 8 cores (-p 8) but only 1 core requested from bsub (no -n), job killed in 1 hour (8/8)

Reserving Memory

- Most nodes have 90GB memory available over all cores, some have more
- Make a resource request with

  -R “rusage[mem=8000]” (memory requested in MB)
- Memory multiplies by cores requested, so

  -n 4 –R “rusage[mem=16000]” reserves 64GB memory
- Asking for more memory may cause jobs to pend longer
- TERM_MEMLIMIT errors indicate that not enough memory was reserved

Multithreading

- A single CPU can execute multiple processes (threads) concurrently
- -n indicates how many cores are requested
- Jobs that are overefficient (use more cores than reserved) jeopardize the health of a node
- Reserve the same amount of cores in your job and your bsub!

Creating a Complete Shell Script

```
#! /bin/sh
#BSUB -q mcore
#BSUB -W 12:00
#BSUB -o %J.out
#BSUB -e %J.err
#BSUB –N
#BSUB -n 4
#BSUB –R “rusage[mem=12000]”

module load seq/tophat2.1.1 seq/bowtie/2.2.1 seq/samtools/1.2

tophat -p 4 -o ./mytophatdir1 hg19 file1_1.fastq file1_2.fastq

#save as myshellscript2.lsf
```

Calling a Complete Shell Script

```
mfk8@balcony:~$ bsub < myshellscript2.lsf
```

3c. Managing jobs and getting information about submitted/running jobs

Monitoring Jobs

- List info about jobs/their status:

```
mfk8$loge:~$ bjobs
```

-r (running jobs)

-p (pending jobs)

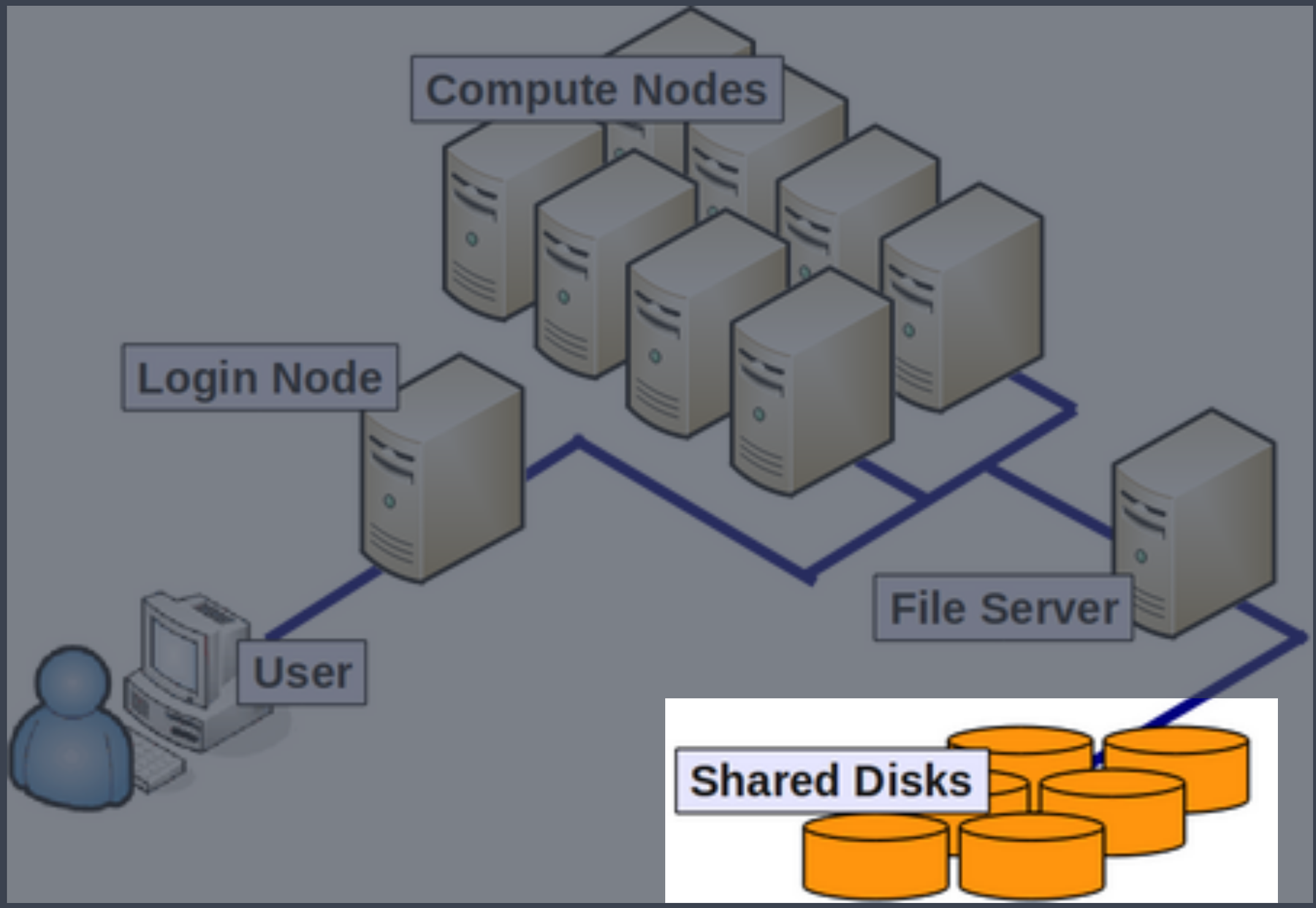
-l (command entered, long form)

- List historical job information

```
mfk8$loge:~$ bhist jobid
```

4. Filesystems and storage

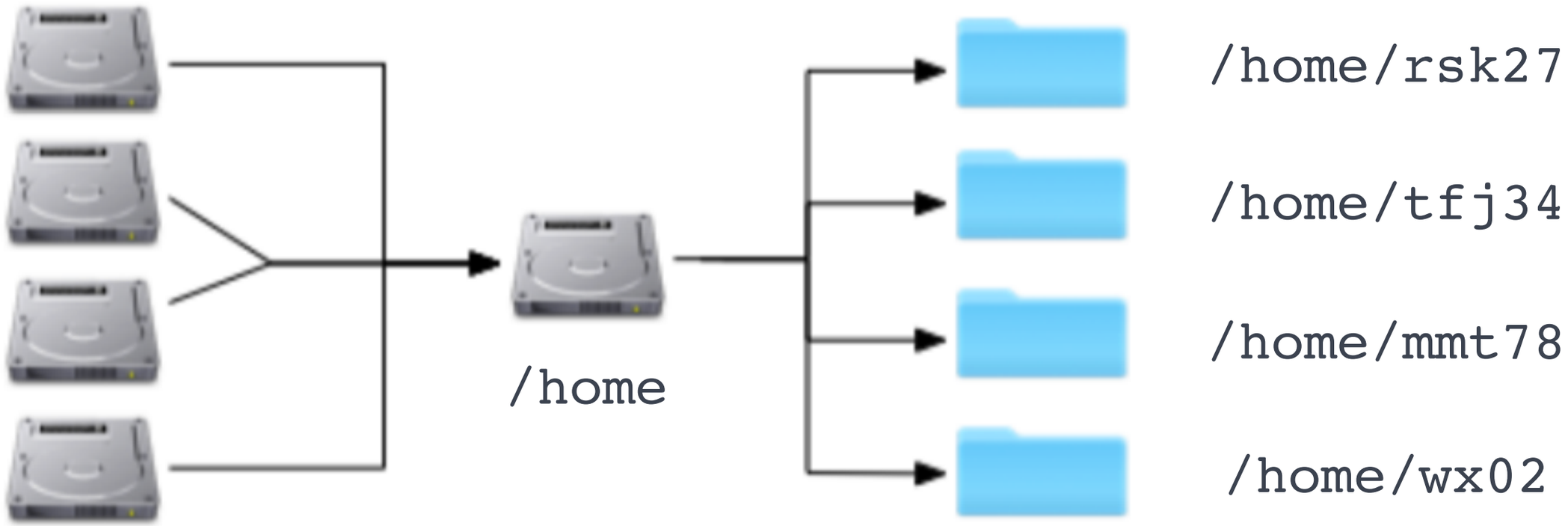
Filesystems and storage



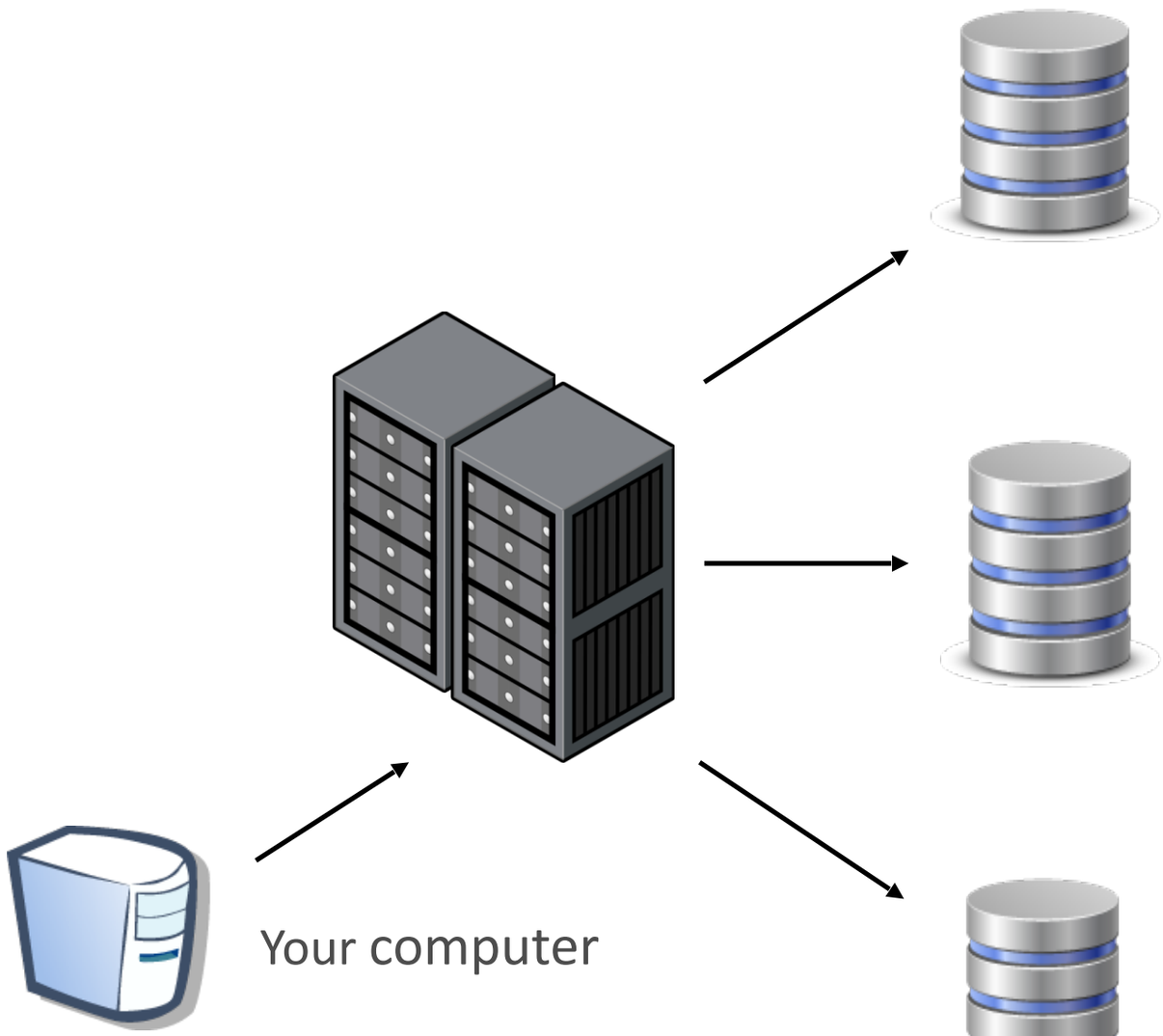
Filesystems and storage

- 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

Filesystems and storage



Storage on Orchestra



/home

- /home/user_id
- quota: 100GB per user
- Backup: 14-day snapshots + 60 day weekly snapshots

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

- /groups/your_lab/your_dir
- quota: expandable
- Backup: 14-day snapshots + 60-day weekly snapshots

/n/scratch2

- /n/scratch2/user_id
- quota: 10TB per user
- Backups: none
- Run workflows here

For more direction:

- https://wiki.med.harvard.edu/Orchestra/NewUserGuide
- http://rc.hms.harvard.edu
- rchelp@hms.harvard.edu
- Office Hours: Wednesdays **1-3p Gordon Hall 500**