

Invitation to chat:

**Have you made a personal O2  
account?**

# Introduction to High-Performance Computing (HPC)

# Introduction to High Performance Computing and O2 for New Users

HMS Research Computing

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

**RESEARCH  
COMPUTING**

<https://rc.hms.harvard.edu/>



**HARVARD**  
MEDICAL SCHOOL

Information Technology

# 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

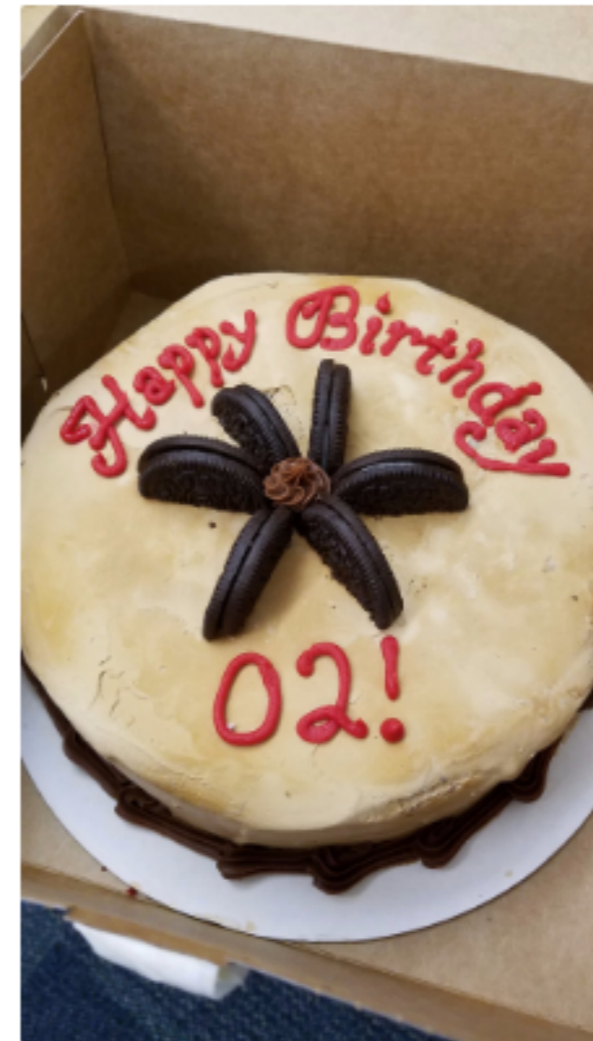
Wiki page:

<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 !!



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](https://hmsrc.me/O2docs)

Sep 12, 2017

# Welcome to O2!

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- One of HMS Research Computing's High-Performance Compute clusters to enhance the compute capacity available to HMS Researchers
- Heterogeneous environment of newer, faster cores with high memory allocation to facilitate multi-core and parallelized workflows
- SLURM scheduler to efficiently dispatch jobs



# O2 Tech Specs

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- 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
- 147 GPU cards
  - (103 GPUs available to Quad researchers only)
- CentOS 7 Linux
  - The OS will be updated this year. Details TBA!
- SLURM job scheduler

# 2-Factor Authentication

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- 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://harvardmed.atlassian.net/wiki/spaces/O2/pages/1605009747/Two+Factor+Authentication+on+O2>



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

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- Open a terminal

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

- If outside of “approved” internet sources (HMS Private/Harvard Secure):  
Type 1/2/3 for DUO push/sms/phone

# Welcome to O2!

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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

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- 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:~$
```

## 2. Using & installing software

# LMOD: Software Modules

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- Most “software” on O2 is installed as an environment module.
- LMOD system adds directory paths of software into \$PATH variable, to make sure the program runs without any issues.
- Allows for clean, easy loading, including most dependencies, and switching versions.

# LMOD: Software Modules

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Most software is compiled against something called “gcc-6.2.0” — so, we need to load that 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

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Check module status (e.g. the alignment tool bowtie2)

```
$ module list
```

```
$ echo $PATH
```

```
$ bowtie2
```

Load the module

```
$ module load bowtie2/2.2.9
```

```
$ bowtie2
```

Which module version is loaded (if at all)?

```
$ which bowtie2
```

```
$ module list
```

```
$ echo $PATH
```



# Loading/Unloading Modules

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Need help with the module?

```
$ module help bowtie2/2.2.9
```

Unloading modules

```
$ module unload bowtie2/2.2.9
```

Dump all modules

```
$ module purge
```

## 3. 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

Choosing the proper resources for your job with  
the appropriate `SBATCH` options

# Submitting Jobs

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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:~$ bowtie2 -c 4 hg19 file1_1.fq
```

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

# Creating a job submission script

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```
#!/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 bowtie2_run1
#SBATCH --mail-type=ALL
#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:

```
$ sbatch myJobScript.run
```

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

# 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	200 GPU hours	34 (total)	420GiB (total)
transfer	1	5 days	4	

# Runtime: -t

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- -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

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- -c X to designate cores: max 20 per job
- -N X to constrain all cores to X nodes
  - Only relevant for MPI partitions
- 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

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- 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  $\approx$  8000

# Job Priority

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- Dynamically assigned
- Factors contributing: Age, Fairshare, Partition, QOS, Nice
- Fairshare: 0-1 scale
- Check your fairshare:
  - `$ sshare -Uu $USER`
- Check job priority values for your pending jobs:
  - `$ sprio -u $USER`



Managing jobs and getting information about  
submitted/running jobs

# Job Monitoring: Current jobs

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- `$ O2squeue`
  - JOBID, PARTITION, STATE, TIME\_LIMIT, TIME, NODELIST(REASON), ELIGIBLE\_TIME, START\_TIME, TRES\_ALLOC
  - [O2squeue documentation](#)
- *Detailed job info:*
  - `$ scontrol show jobid <jobid>`
  - Output has the command/script you ran & the location your stdout and stderr messages are being written to
- *Another option is the Slurm command `squeue`, but it is less user friendly.*

# Job Information: Past Jobs

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- \$ [O2\\_jobs\\_report](#)
  - JobID, User, Account, Partition, State, Starttime, Walltime (hr), nCPU, RAM(GB), nGPU, PENDINGTIME(hr), CPU\_EFF(%), RAM\_EFF(%), WALLTIME\_EFF(%)
  - Can specify job ID, job status, and/or timeframe to report accounting info
  - Can get a summary report instead of per-job information
  - [O2\\_jobs\\_report documentation](#)
- *Another option is the Slurm command `sacct`, but it is less user friendly.*

# Cancelling/Pausing Jobs

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- `$ 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`



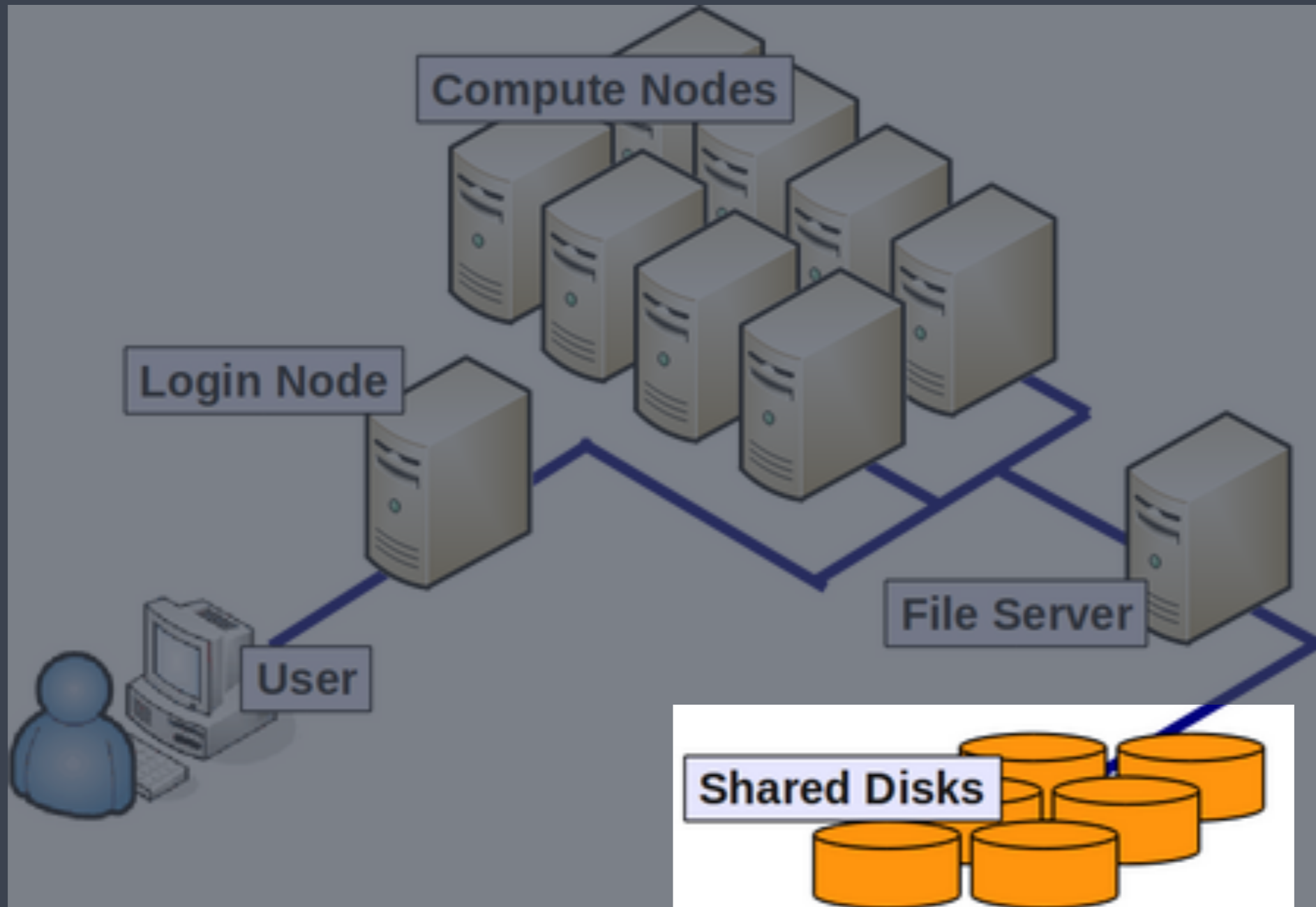
# Exercise!

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



## 4. Filesystems and storage

# Filesystems and storage



# Filesystems and storage

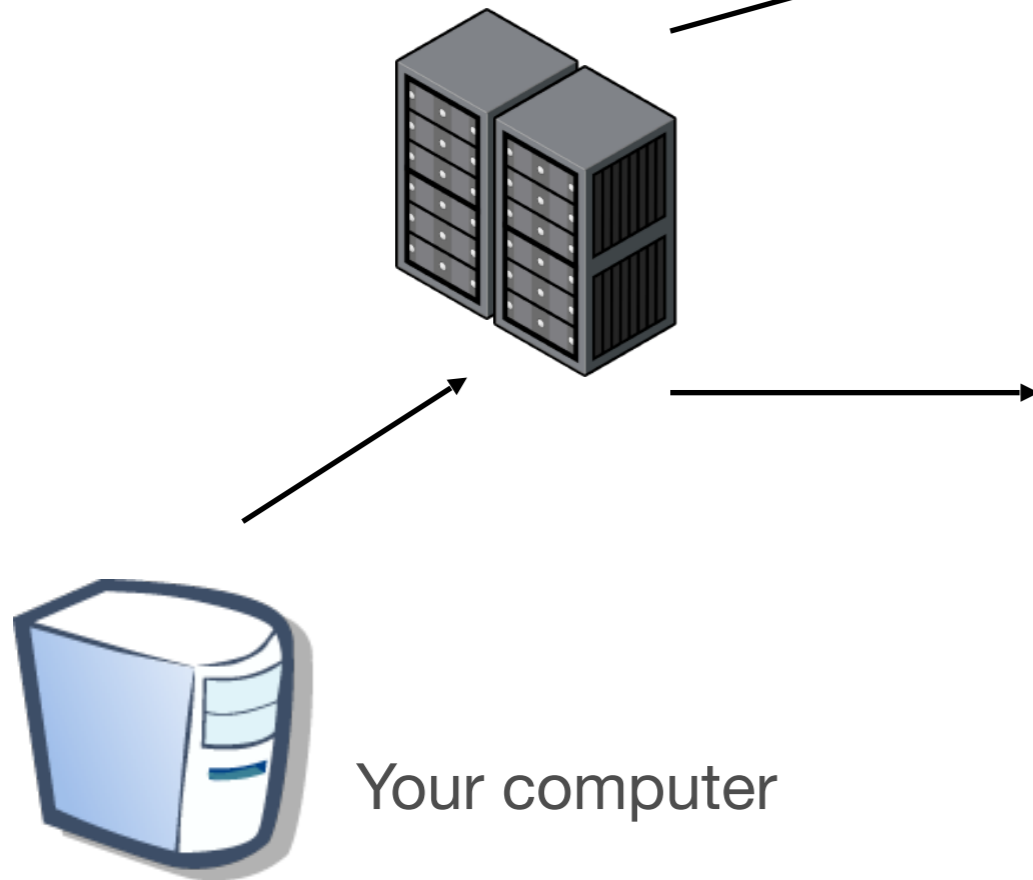
- Storage on HPC systems is organized differently than on your personal machine
- Physical disks are bundled together into a virtual volume; this volume may represent a single filesystem, or may be divided up, or partitioned, into multiple filesystems
- Filesystems are accessed over the internal network

# 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

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- `/n/scratch/users/<first_HMS_account_char>/<HMS_account>`  
*e.g.* `/n/scratch/users/m/mfk8`
- For data only needed temporarily during analyses
- Each user can use up to 25 TiB and 2.5 million files/directories
- Files not **changed** for 45 days are automatically purged!
  - What is “**change time**” or “**ctime**”? The timestamp that reflects when the file metadata or file contents were last updated. Simply accessing a file (without changing the file content or properties) will not update ctime.
- No backups!
- Create your folder:
  - `$ /n/cluster/bin/scratch3_create.sh`
- [Scratch documentation](#)

# Important Note about O2 Storage

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- 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.



# HMS Storage Offerings

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- **Active**

- Active Compute: O2 group folders, /n/data1, /n/data2, /n/groups
  - e.g., /n/data1/institution/dept/lab
- Active Collaboration: research.files, /n/files on transfer cluster
- Research data that is frequently accessed, modified, or computed against.

- **Standby**

- Infrequently accessed data, that is directly available for reference, retrieval, or analysis.
- Accessible as /n/standby/institution/dept/lab on transfer cluster

- **Cold**

- Rarely accessed data requiring long-term retention, for regulatory or historical purposes

# HMS Storage Offerings

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- For more detail on all the Storage Offerings, please see [the Research Computing Storage Services Website](#).
- New/additional Storage can be requested through [the Storage Request Forms through the STAT Service Portal](#).



# Chargeback for Storage & Compute

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- 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](mailto:rccore@hms.harvard.edu) with any questions.

# For more direction

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**Email:** [rchelp@hms.harvard.edu](mailto:rchelp@hms.harvard.edu)

**Website:** <https://it.hms.harvard.edu/rc>

## Office hours:

Wednesdays, 1:00-3:00 pm

Zoom: <https://rc.hms.harvard.edu/office-hours>

## O2 documentation:

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

