

Welcome to **Introduction to O2!**  
We will get started in a few minutes.



**HARVARD**  
MEDICAL SCHOOL

Information Technology

# Intro to O2

## HMS Research Computing

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# Welcome to O2!

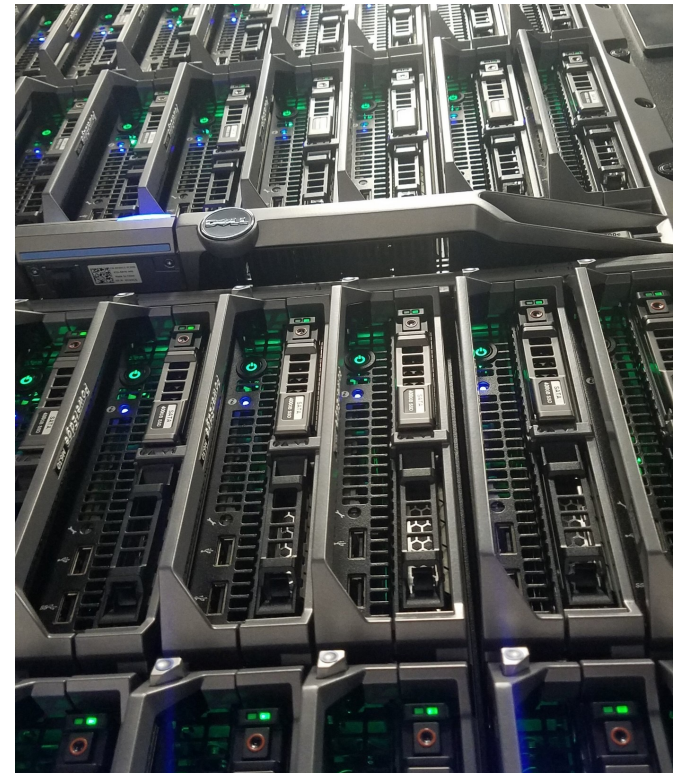
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- Slides available at [github.com/hmsrc/user-training](https://github.com/hmsrc/user-training)
  - **IntroToO2.pdf**
- Register for our other classes [here](#)
- Contact us at [rchelp@hms.harvard.edu](mailto:rchelp@hms.harvard.edu)
- Comments/feedback welcome at course survey (we will have time at the end of the class for this)

# Welcome to O2!



- HMS Research Computing's newest High-Performance Compute cluster 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



# Research Computing Core: Chargeback for Storage & Compute

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- Labs whose PIs do NOT have a primary or secondary appointment with an HMS Quad department (external users) will be charged.
- 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](#)
- Billing is done on a quarterly basis
- 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.

# O2 Tech Specs

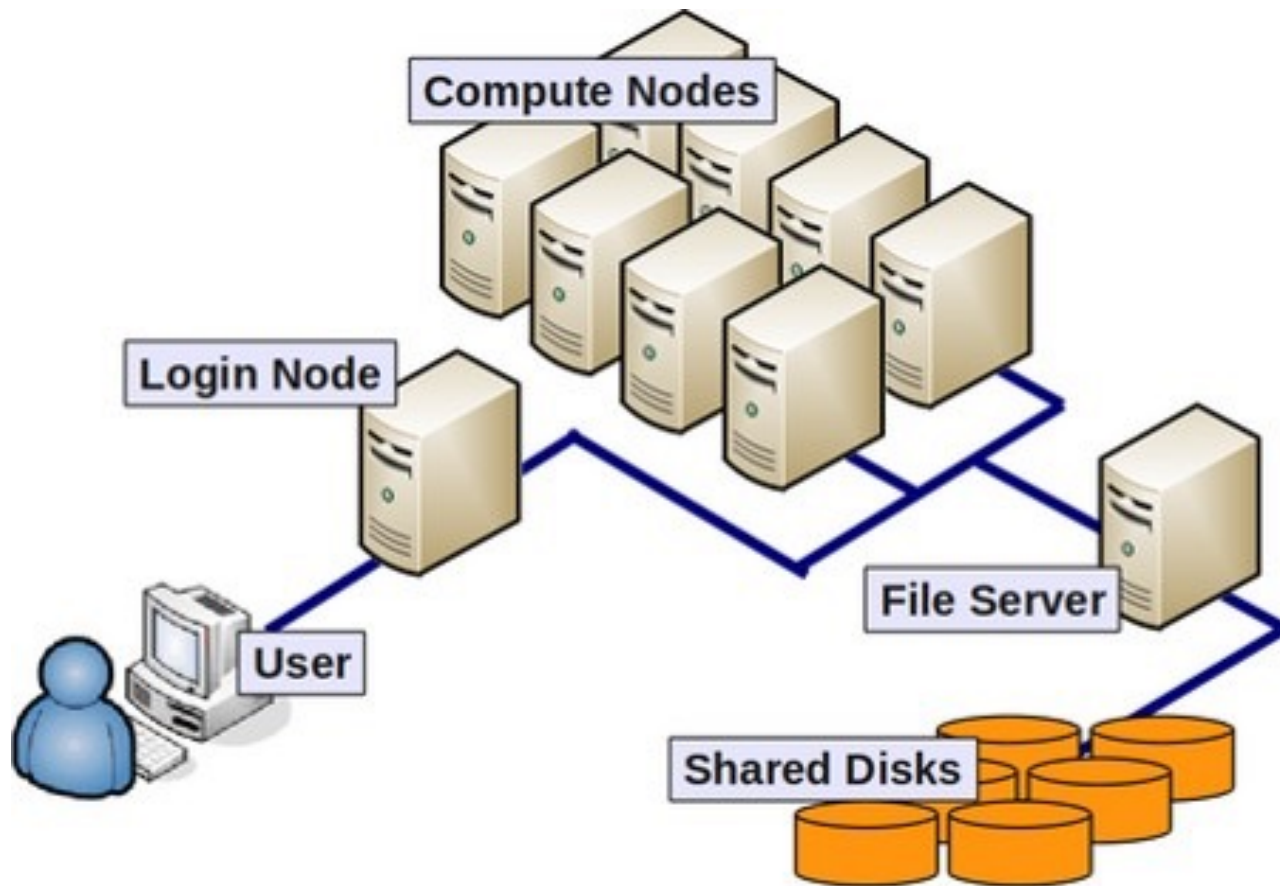
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- 12000+ cores
- 32, 28 or 20 cores per node
- 256-160 GiB RAM per node (8-9GiB/core)
- 9x756 GiB and 1x1TiB highmem nodes
- 147 GPUs
  - 103 GPUs available to Quad-based researchers only
- Login/load balancer 6 VM (8 cores/16GiB memory)
- CentOS 7

# Generic Cluster Architecture

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# Storage on O2





# 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

- **Active** – formerly Tier 1
  - 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** – new & improved alternative to Tier 2
  - Infrequently accessed data, that is directly available for reference, retrieval, or analysis.
  - Accessible as /n/standby/institution/dept/lab on transfer cluster
- **Cold** – formerly Tier 3
  - Rarely accessed data requiring long-term retention, for regulatory or historical purposes

# HMS Storage Offerings

- For more detail on all the Storage Offerings, please see [the Research Computing Storage Services Website.](#)
- Please see [the dedicated Standby Storage page](#) for more information on how to access and utilize Standby.
- New/additional Storage can be requested through [the Storage Request Forms through the STAT Service Portal.](#)

# O2 Primary Storage

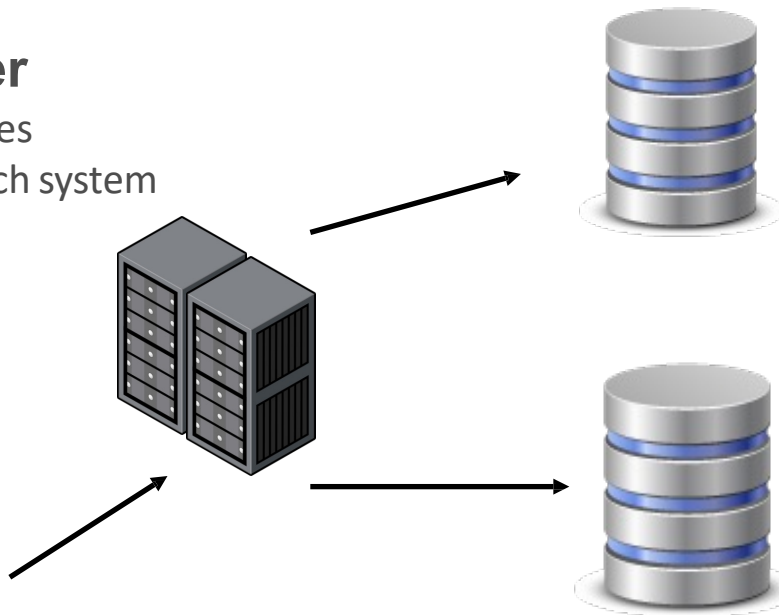


## O2 Cluster

- 11000+ cores
- SLURM batch system



Your computer



## /home

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

# Temporary “Scratch” storage

- 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!**
- Location:  
/n/scratch3/users/<first\_HMS\_account\_char>/<HMS\_account>
- Example
  - `mfk8@login01:~$ cd /n/scratch3/users/m/mfk8`
- For more information: [Scratch3 documentation](#)

# Checking Storage Usage

- To check your storage usage:  
`mfk8@login01:~$ quota-v2`
- /home directory: each user gets 100 GiB, total.
- /n/scratch3 directory: each user gets 10 TiB
- Group directories: space varies, can be increased
  - /n/groups/lab
  - /n/data1/institution/department/lab
  - /n/data2/institution/department/lab

# Storage Policies

- /home: 14 day snapshots + 60 day full backup
- /n/groups, /n/data1, /n/data2: 14 day snapshots + 60 day full backup
- /n/scratch3: 30 day retention, no backups

# Snapshots

Snapshots (frozen) are retained for up to 60 days:  
recover data from a hidden `.snapshot` directory

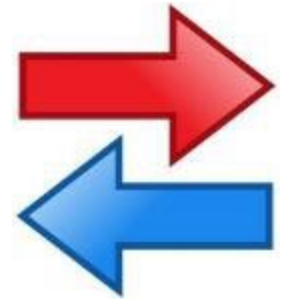


# Snapshots

Snapshots (frozen) are retained for up to 60 days:  
recover data from a hidden `.snapshot` directory

- `mfk8@compute-a:~$ cd .snapshot`
- `mfk8@compute-a:~$ ls`  
O2\_home\_daily\_2015-10-02-02-00  
O2\_home\_daily\_2015-10-01-02-00
- `mfk8@compute-a:~$ cd O2_home_daily_2015-10-02-02-00`
- `mfk8@compute-a:~$ cp MyRetreivedFile ~`

# Research.files O2 access



- Research.files Active filesystem is accessible on select compute nodes via a `transfer` partition and `transfer` cluster
- Access to `transfer` allows `cp/rsync` of files
  - From: Research.files (`/n/files`)
  - To: O2 storage (`/home`, `/n/groups`, `/n/data1`, `/n/data2`, `/n/scratch3`)
  - And reverse direction
- Cannot use O2 to compute against data in Research.files, must be transferred

# O2 Cluster Status

- [Wiki page](#)
- [O2 cluster wiki](#)

## O2 Cluster Status

Created by Bergman, Andrew L., last modified about an hour ago

This page shows all service outages for the O2 cluster, including planned maintenance and unplanned events.

We also post updates on the [HMS RC Twitter page](#).

ONLINE

### July 8: notes after the July OS/Slurm update

- Jupyter Notebooks users should start a new environment and remove any old runtime directories.
- "sbatch" no longer uses the "-x11" option in the new version of Slurm. Just remove it from your script and X forwarding should work by default.
  - "srun" commands still require "-x11" to enable X forwarding, though.
- If you have any custom built software, you may need to recompile or relink it on O2.

# Data and Script Management



# Data Management

1. Planning: Plan ahead
2. Active Research: Document
3. Dissemination: Share confidently

*Note: be sure to ask your PI and your department about standard practices in your field!*



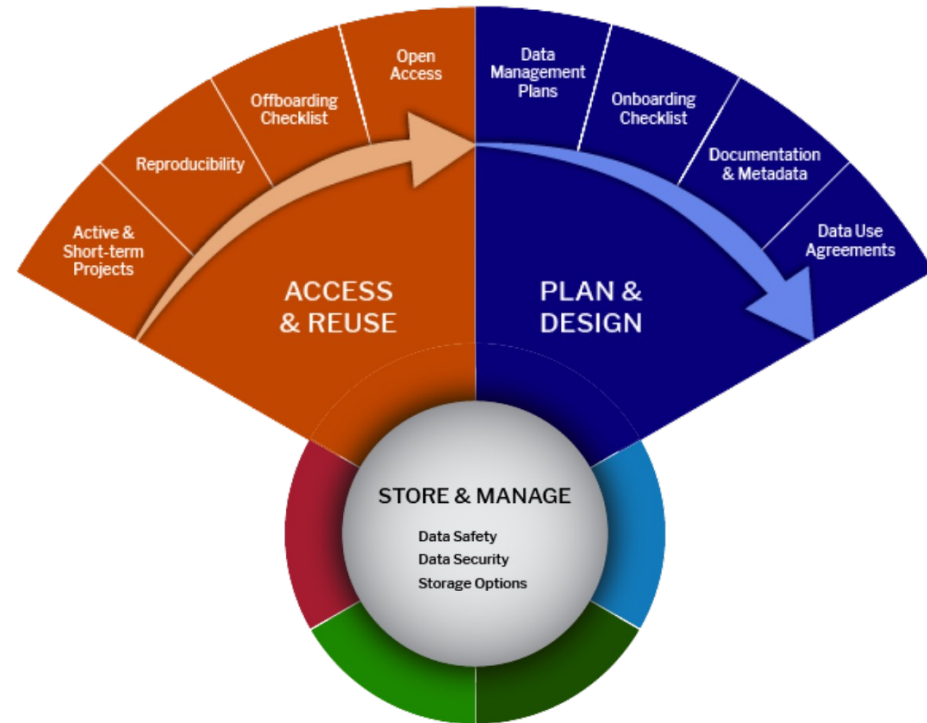
Harvard Biomedical Data Management Website: <https://datamanagement.hms.harvard.edu>

Resources: <https://datamanagement.hms.harvard.edu/about/what-research-data-management/rdm-resources>



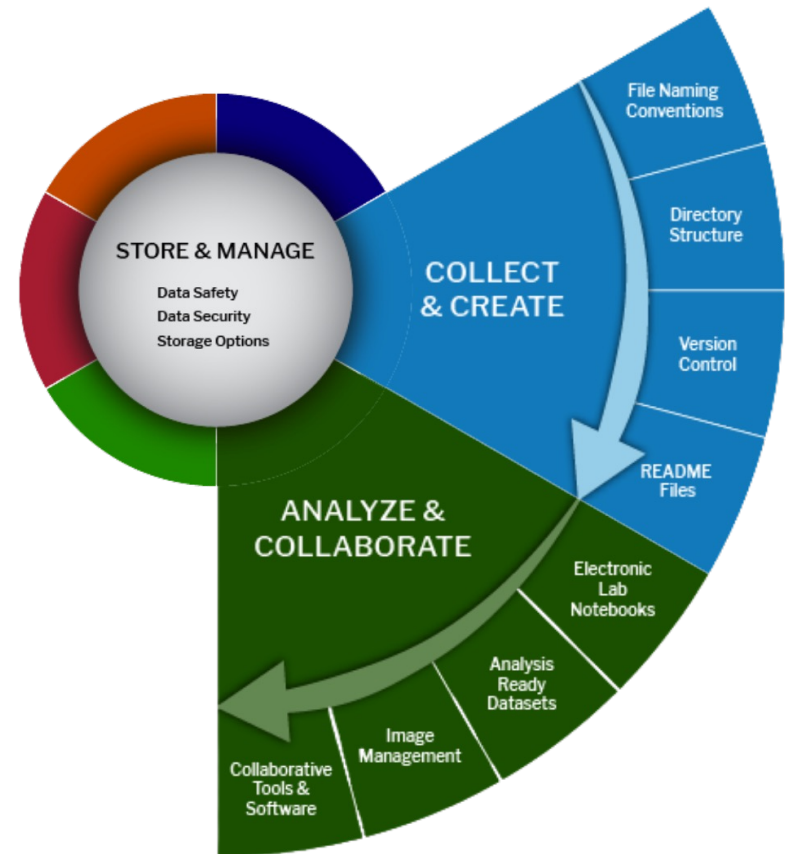
# Planning

- Document the activities for the entire lifecycle in a Data Management Plan
- Determine if you need a Data Use Agreement to acquire or share data
- Adopt a community-based metadata standard if applicable
- Consider how the data will be stored and protected over the duration of the project and beyond
- Assign roles & responsibilities for managing data



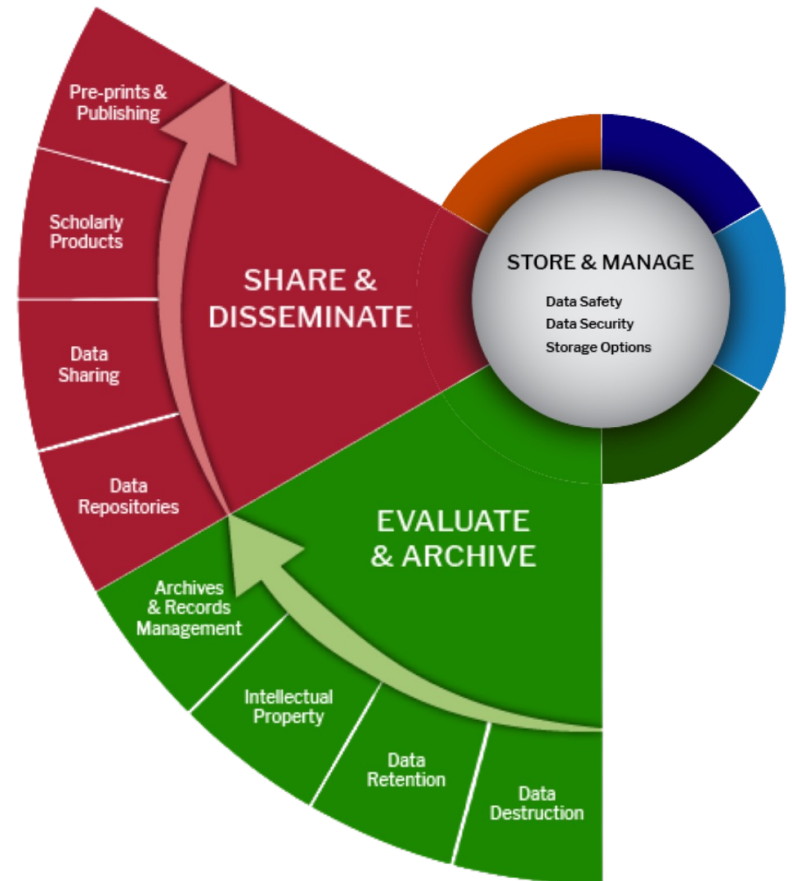
# Active Research

- Determine how the data will be organized including folder structure & file naming
- Consider versioning control for changes for both software and data products
- Create a README file to record the metadata that will be associated with data
- Link related code and algorithms
- Use tools & software to work with collaborators during the project



# Dissemination

- Determine what data will be disseminated, to who, when, and where
- Publish data in an open repository to receive a DOI and citation for your work
- Use standard, nonproprietary approaches and provide accompanying metadata
- Think about your preservation strategy and adhere to your lab's standard practices
- Research records should generally be retained no fewer than seven (7) years after the end of a research project or activity





# Logging into O2



# Create a New O2 Account

- [rc.hms.harvard.edu/o2user](https://rc.hms.harvard.edu/o2user)
- Click the “Get this Service” **red button** and fill out the form!
- Your username will be your HMS Account (formerly known as eCommons ID), with your HMS account password.

**Get this service**

# 2-Factor Authentication



- More secure: thing you know, and thing you have
- Easiest: download Duo app to phone
- [Setup details detailed here](#)
- If you believe an email to be a phishing scheme, please forward to:  
[phishing@harvard.edu](mailto:phishing@harvard.edu)

# Logging Into O2: Mac or Linux



- Open a terminal (search “terminal”)  
`ssh yourHMSaccount@o2.hms.harvard.edu`
- 2-Factor (when necessary): Choose 1/2/3  
(push/phone/sms)



# Logging Into O2: Windows



- Install MobaXterm (google it)  
`ssh yourHMSaccount@o2.hms.harvard.edu`
- 2-Factor (when necessary): Choose 1/2/3 (push/phone/sms)

# Logging Into O2: X11

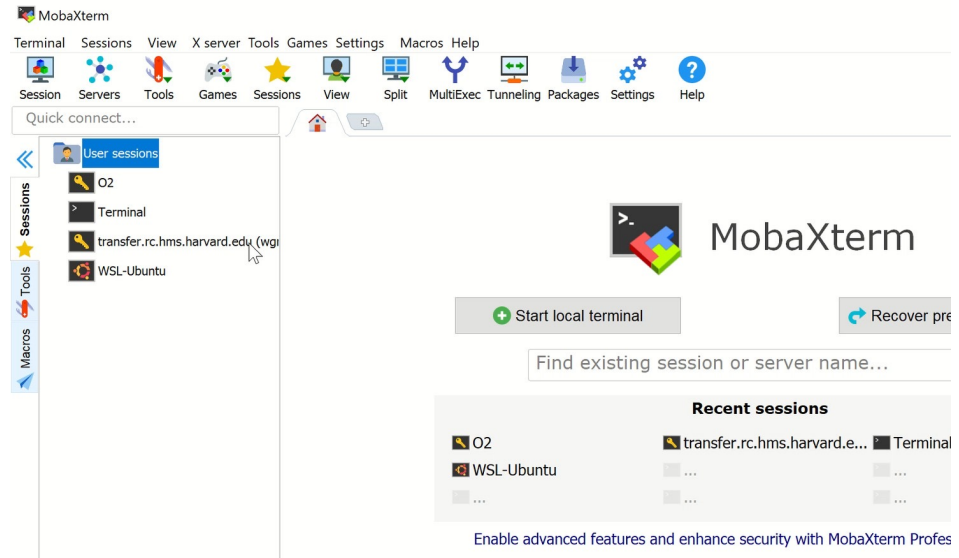
- You can display graphics (that a program on O2 is generating) back to your desktop using X11 forwarding.
- We won't be doing this for today's class.
- If you need to do this in the future, login with the -XY options:  
`ssh -XY yourHMSaccount@o2.hms.harvard.edu`
- If you're on Mac, open XQuartz before connecting to O2.
- If you're on Windows, use MobaXterm (X11 server is built-in)

# Connecting to O2...

## MAC/Linux: Terminal



## Windows: MobaXterm



***If you do not have an O2 account, use a training account!***  
***Please see your instructor for training account information during class.***

# Welcome to O2!

```

 02

You've landed on login04 which is a
8 core system with 15.51 GiB memory
running kernel 3.10.0 born on 2018-12-04

==== O2 =====

News (Mar 15 2019)

+-----+
| * With a recent expansion, O2 now contains over 11,000 shared cpu cores!
|
| * O2 requires 2-factor authentication for all logins originating from outside
|   of the HMS network. Please see:
|   https://wiki.rc.hms.harvard.edu/display/O2/Two+Factor+Authentication+on+O2
|
|
| * Resource intensive jobs should not be run on O2's login servers.
|   Any programs (Python, R, samtools, gzip, etc.) that run for more
|   than ten minutes or use too much CPU on O2's login servers will be
|   automatically killed.
|
| * Learn more about O2 at: http://hmsrc.me/O2docs
|
| * Status updates and upcoming service outages are posted at:
|   https://wiki.rc.hms.harvard.edu/display/O2/O2+Cluster+Status
|
+-----+

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Contact HMS Research Computing:

E-mail      rchelp@hms.harvard.edu
Web         https://rc.hms.harvard.edu
Twitter     @hms_rc

=====

[wgr4@login04 ~]$
```





# Welcome to O2!

```
02

You've landed on login04 which is a
8 core system with 15.51 GiB memory
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=====

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=====

contains over 11,000 shared cpu cores!

on for all logins originating from outside

display/O2/Two+Factor+Authentication+on+O2

it be run on O2's login servers.
, gzip, etc.) that run for more
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Contact HMS Research Computing:

E-mail      rchelp@hms.harvard.edu
Web         https://rc.hms.harvard.edu
Twitter     @hms_rc

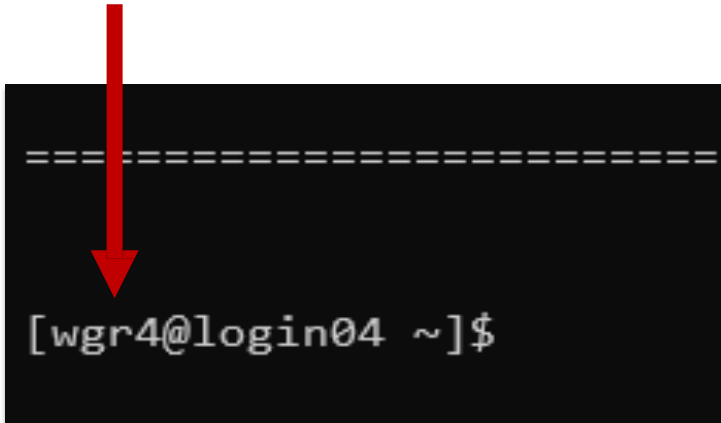
=====

[wgr4@login04 ~]$
```



# Welcome to O2!

Your HMS Account



# Welcome to O2!

```
=====
[wgr4@login04 ~]$
```

You are logged into a “shell login server”  
These are **not** meant for heavy lifting!

# Welcome to O2!

```
=====
[wgr4@login04 ~]$
```

You're in your HOME directory.  
/home/<HMS\_Account>

# Welcome to O2!

```
=====
[wgr4@login04 ~]$
```

Ready to receive commands!

# Getting Data Onto O2



- Use an FTP client of your choice
- Mac/Windows/Linux: Filezilla (google it)
- Connect to:

**Host:** transfer.rc.hms.harvard.edu

**Username:** <HMS\_Account> (lowercase username)

**Password:** <your\_password>

**Port:** 22

- Two-factor: will use default option setup in  
~/.bashrc as

```
export DUO_PASSCODE=push/phone
```

# Getting Data Onto O2



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# 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!”





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```
mfk8@login0~$ srun --pty -p interactive -t 0-2:00 --mem 2G bash
```

“srun --pty” is how interactive jobs are started

“-p interactive” is the partition

“-t 0-2:00” is the time limit (2 hours)

“--mem 2G” is the memory requested, 2GiB

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

# Interactive Sessions

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“srun --pty” is how interactive jobs are started

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mfk8@compute-a:~\$

# Class Practical

---

- Copy the class files and scripts to your /home

```
mfk8@compute-a:~$ cp -r /n/groups/rc-training/o2 ~
```



# Class Practical

---

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mfk8@compute-a:~$ cp -r /n/groups/rc-training/o2 ~
```

**o2**

```
|— date_parallel.sh  
|— fastqc_job_array.sh  
|— sample_1_R1.fastq  
|— sample_2_R1.fastq  
|— sample_3_R1.fastq  
|— sample_4_R1.fastq  
|— submit.slurm
```

# Listing a Folder's Contents

- To see the contents of the current folder you are in (~ means “/home/username/”), type **list** (**ls**):

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

- To get the details of a folder's contents, add “-l”

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

- You don't have to be in a directory to see its contents

```
mfk8@compute-a:~$ ls /n/groups/rc-training/introthpc
```

# Viewing File Contents

- “less” to view file contents
- Navigate up/down, search
- “q” to quit

```
mfk8@compute-a:~$ less ~/.bashrc
```

# Making a Folder (Directory)

- “mkdir” stands for “**make directory.**”
- Create a new directory for this exercise
- Spaces are discouraged. (Underscores are fine!)  
Case counts in Linux.

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

# Moving Around: Change Directory

- “cd” stands for “**c**hange **d**irectory”
- 1 period “.” means “current directory”
- 2 periods “..” means “the directory above”

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

*Notice how the prompt tells you where you are!*

```
mfk8@compute-a:~/MyTestDir$ cd ..
```

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



# Creating a Simple Text File

- “Nano,” “vi,” “emacs” are simple command-line editors available.
- To create a new file, type the editor you want, then the name of the new file. To edit an existing file, do the same.

```
mfk8@compute-a:~$ nano myfile.txt
```

```
This is my new file text.
```

*(Control-X to save (yes) and exit.)*

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

```
mfk8@compute-a:~$ ls  
myfile.txt
```

# Copying Files

- “cp” to **copy** a file from a destination to a new destination. “cp” “from” “to”
- `cp -r` to copy folders (recursively)

```
mfk8@compute-a:~$ cp myfile.txt MyTestDir/
```

- You can copy a file to the current folder or to a new folder with a different name by specifying a different name (rename)

```
mfk8@compute-a:~$ cp myfile.txt mycopy2.txt
```

#copying and renaming

# Moving Data

- “move” “from” “to”

```
mfk8@compute-a~:$ mv MyTestDir/myfile.txt ~
```

#this rewrites myfile.txt, since it already exists!

```
mfk8@compute-a~:$ mv MyTestDir/ MyTestDir2/
```

#in-place move and rename

# Removing Files/Folders

- “rm” to remove a file

```
mfk8@compute-a:~$ rm myfile.txt
```

- “rm -r” to remove a folder recursively

```
mfk8@compute-a:~$ rm -r MyTestDir2
```

# Wildcard \* Pattern Matching

- Useful for copying/removing/etc all files matching a certain pattern

- Example Case:

To copy “all” files ending in “.fastq”:

```
$ cp *.fastq NewFastqFolder/
```

# Software on O2



# LMOD: Software Modules

---

- LMOD system adds directory paths of software into \$PATH variable, and resolves software dependencies and conflicts
- Most software compiled against gcc-6.2.0: load first
- `$ module load gcc/6.2.0`
- `$ module avail` #to see software now available
- `$ module spider` #verbose list of software available on O2
- `$ module load software/version` #load software
- `$ module unload software/version` #unload
- `$ module purge` #dump all modules
- `$ module help <software>` #displays run info

# Loading/Unloading Modules

---

- Load modules  
`$ module load gcc/6.2.0 bowtie2/2.2.9`
- Which module version is loaded (if at all)?  
`$ which bowtie2`
- See all modules you have loaded  
`$ module list`
- Unload a specific module  
`$ module unload bowtie2/2.2.9`
- Dump all modules  
`$ module purge`



# Public Databases on O2

---

## **/n/shared\_db**

- More recently updated
- Folder structure: Genome/Software/Version/Database
- Example: /n/shared\_db/hg19/uk/bowtie2

## **/n/groups/shared\_databases**

- Older databases – this directory is no longer updated
- Folder structure: Software/GenomeVersion/Database
- Example: /n/groups/shared\_databases/star\_reference/grch37

For more information, [please see this wiki page](#)


# Compiling your own software

---

- Users can compile software in their /home or group directories, where they have permission
- Binaries just require “unzipping”, for example:
  - `tar -zxvf *.tgz`

# Installing Software: Binary Example

---

- `mfk8@login01:~$ srun --pty -p interactive -t 0-12:00 --mem 8G bash`
- `mfk8@compute-a:~$ wget http://path/to/binary/mysoftware.tar.gz`
- `mfk8@compute-a:~$  -zxvf mysoftware.tar.gz`
- `mfk8@compute-a:~$ ls mysoftware/bin`

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# Programming Languages

- [Python](#): load module (2.7.12, conda2, 3.6.0, 3.7.4, 3.8.12, 3.9.14, 3.10.11)  
Use virtualenv to maintain packages (pip/easy install)
- [R](#): load module (4.0.1, 4.1.1, 4.1.2, 4.2.1, 4.3.1)  
Setup O2-specific personal R library
- [Perl](#): load module (5.24.0, 5.30.0)  
Setup O2-specific local::lib (cpan/cpanm) in .bashrc
- [MATLAB](#): load module (2022a, 2022b, 2023a)  
Setup cluster profile specific to O2



# MPI on O2

---

- Message Passing Interface
- Distribute work over multiple nodes, allowing for the utilization of more cores
- openMPI-4.1.2 compiled against GCC 6.2.0
- MATLAB, Python, R, Perl, Java, C++, Fortran implementations
- Needs wrapper function “mpirun” to dispatch to compute nodes with SLURM
- Run in “mpi” partition -p mpi after obtaining access to partition
- Core cap: **640 processors, 5-day runtime**

# Constructing Jobs





# Submitting Jobs

---

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

```
mfk8@compute-a:~$ bowtie -c 4 hg19 file1_1.fq file1_2.fq
```

- From the login shell (and also interactive or any compute nodes), a program is submitted to O2 via a job (sbatch)

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

# Submitting Jobs

---

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

# Jobs: sbatch

---

- All in one line: `--wrap="command here"`

- This approach is not recommended!

```
mfk8@login01:~$ sbatch -p partition -t 0-1:00 --wrap="command_here"
```

- Using a complete shell script is recommended!

```
mfk8@login01:~$ sbatch completeSlurmJob.run
```

# Jobs: sbatch

---

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- Using a complete shell script is recommended!

```
mfk8@login01:~$ sbatch completeSlurmJob.run
```

**Line 1:** `#!/bin/bash`

**Line 2:** `#SBATCH -p short`

**Line 3:** `#SBATCH -t 0-1:00`

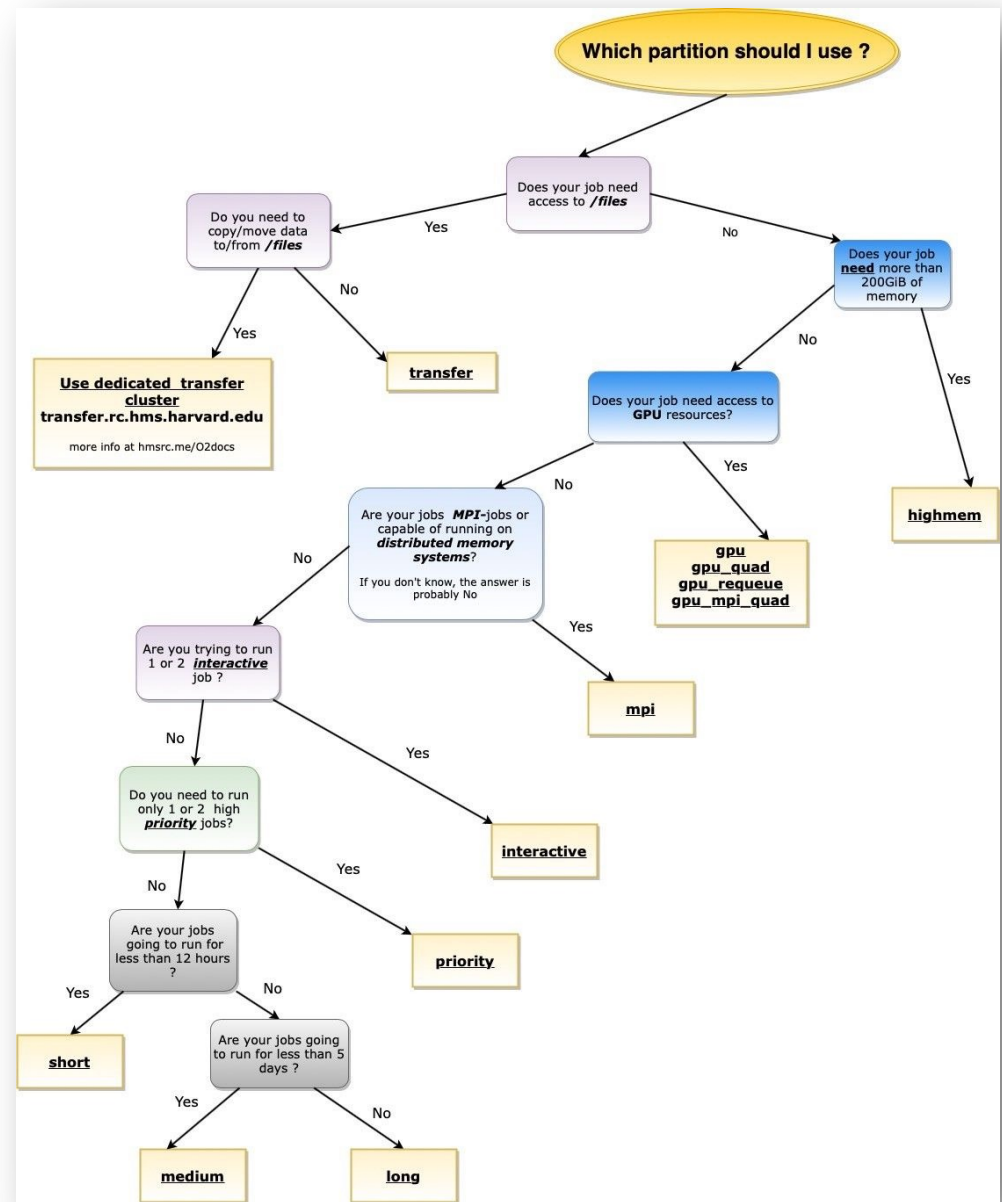
**Line 4:** `command_here ..`

# Partitions (queues): -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		5 days	20	
gpu, gpu_quad, gpu_requeue		160 GPU hours	34 (total)	420GiB (total)
transfer		5 days	4	

# Confused about which partition to use for your jobs?

[Reference the “How to choose a partition” wiki page](https://rc.hms.harvard.edu/)



# Wall-Time: -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 wall-time (like partition max) takes longer to dispatch, and affect fair-share

# CPU: -c

---

- -c X to designate CPU: max 20
- -N X to constrain all cores to X nodes
  - (only relevant for MPI partitions)
- CPU time: wall time  $(-t) * (-c)$  CPUs used
- Unable to use CPU 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
  - On interactive jobs you get 4GiB by default
- --mem XG #total memory over all cores
- --mem-per-cpu XG #total memory per CPU requested, use for MPI
- If you don't include a unit request (like G), it defaults to Mebibytes (MiB)

# Job Construction

---

```
#!/bin/bash
#SBATCH -p short #partition
#SBATCH -t 0-01:00 #time days-hr:min
#SBATCH -c X #number of cores
#SBATCH --mem=XG #memory per job (all cores), GiB
#SBATCH -o %j.out #out file
#SBATCH -e %j.err #error file
#SBATCH --mail-type=BEGIN,END,FAIL,ALL
#SBATCH --mail-user=mfk8@med.harvard.edu
# put any module load commands here
# put any analysis commands you want to run here
```

# Job Construction

---

**Line 1:** `#!/bin/bash`

**Line 2:** `#SBATCH -p short #partition`

**Line 3:** `#SBATCH -t 0-01:00 #time days-hr:min`

**Line 4:** `#SBATCH -c X #number of cores`

**Line 5:** `#SBATCH --mem=XG #memory per job (all cores), GiB`

**Line 6:** `#SBATCH -o %j.out #out file`

**Line 7:** `#SBATCH -e %j.err #error file`

**Line 8:** `#SBATCH --mail-type=BEGIN,END,FAIL,ALL`

**Line 9:** `#SBATCH --mail-user=mfk8@med.harvard.edu`

**Line 10:** `# put any module load commands here`

**Line 11:** `# put any analysis commands you want to run here`

# Output/Error Files

---

- Can add jobid to filename with %j
- Sample:
  - e %j.err
  - o %j.out
- SLURM by default creates this outfile: slurm-<jobid>.out
- Additional Flags
  - %a job array id
  - %A master array job id
  - %N node name
  - %u user id

# Output/Error Files

---

- Can add jobid to filename with %j
- Sample:
  - e %j.err
  - o %j.out
- SLURM by default creates this outfile: slurm-<jobid>.out
- Additional Flags
- %a job array id
- %A master array job id
- %N node name
- %u user id

**“Intermediate O2” class covers  
job arrays:**

[Slides available here](#)

# Mail

---

- Mail is not auto-generated upon completion/failure
- `#SBATCH --mail-type= NONE, BEGIN, END, FAIL, REQUEUE, ALL`
- `#SBATCH --mail-user=mfk8@med.harvard.edu`
- Not recommended, not a verbose output
- Use `02_jobs_report` or `sacct` commands instead

# Account

---

- If you are associated with more than one SLURM Account (i.e. Lab or Group), you need to specify which account a job will be run with.
- Check if you are associated with multiple SLURM accounts:
  - `sshare -u $USER -U`
- Use the `--account=` flag in your `sbatch` or `srun` job submission.
- More details are located on [Understanding O2 Slurm Accounts/Associations and Unix Accounts/Groups](#) wiki page.

# Practical: simple sbatch script

---

- From your ~/o2 directory,  
**\$ sbatch submit.slurm**

#!/bin/bash

#SBATCH -p short

#SBATCH -t 0-00:01

#SBATCH -c 1

#SBATCH --mem=1G

#SBATCH -o hostname.%j.out

#SBATCH -e hostname.%j.err

hostname

# Partition to submit to

# Time in minutes

# Number of cores requested

# Memory total in GiB

# Standard out goes to this file

# Standard err goes to this file

#command



# Command Line Arguments

---

- slurm scripts can take command line arguments  
Reference as \$1, \$2 etc. within the script
- sbatch submit.run 25 output.txt

```
#!/bin/bash  
#SBATCH -p short  
#SBATCH -t 0-1:00  
python3 myscript.py $1 $2
```

The above runs as

python3 myscript.py 25 output.txt

# Job Priority

---

- 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`

# X11 on O2

---

- To visualize or initiate plot devices, an X11 device must be active
- Mac: XQuartz installed and running
- Windows: MobaXterm download software
- Login: `ssh -XY`
- To interactives, `srun` add: `--x11`
  - No extra parameter required for batch jobs
- For more detail, [see this wiki page](#)



# Job Management



# Job Monitoring: Current jobs

---

- `$ O2queue`
  - JOBID, PARTITION, STATE, TIME\_LIMIT, TIME, NODELIST(REASON), ELIGIBLE\_TIME, START\_TIME, TRES
  - [O2queue 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

---

- `$ 02_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 detail accounting info for
  - Can get a summary report instead of per-job info
  - [02\\_jobs\\_report documentation](#)
- *Another option is the Slurm command `sacct`, but it is less user friendly.*

# Slurm Job States

---

- BF BOOT\_FAIL
- CA CANCELLED
- CD COMPLETED
- CF CONFIGURING
- CG COMPLETING
- DL DEADLINE
- F FAILED
- NF NODE\_FAIL
- OOM OUT\_OF\_MEMORY
- PD PENDING
- PR PREEMPTED
- R RUNNING
- RS RESIZING
- S SUSPENDED
- TO TIMEOUT

# Cancelling/Pausing Jobs

---

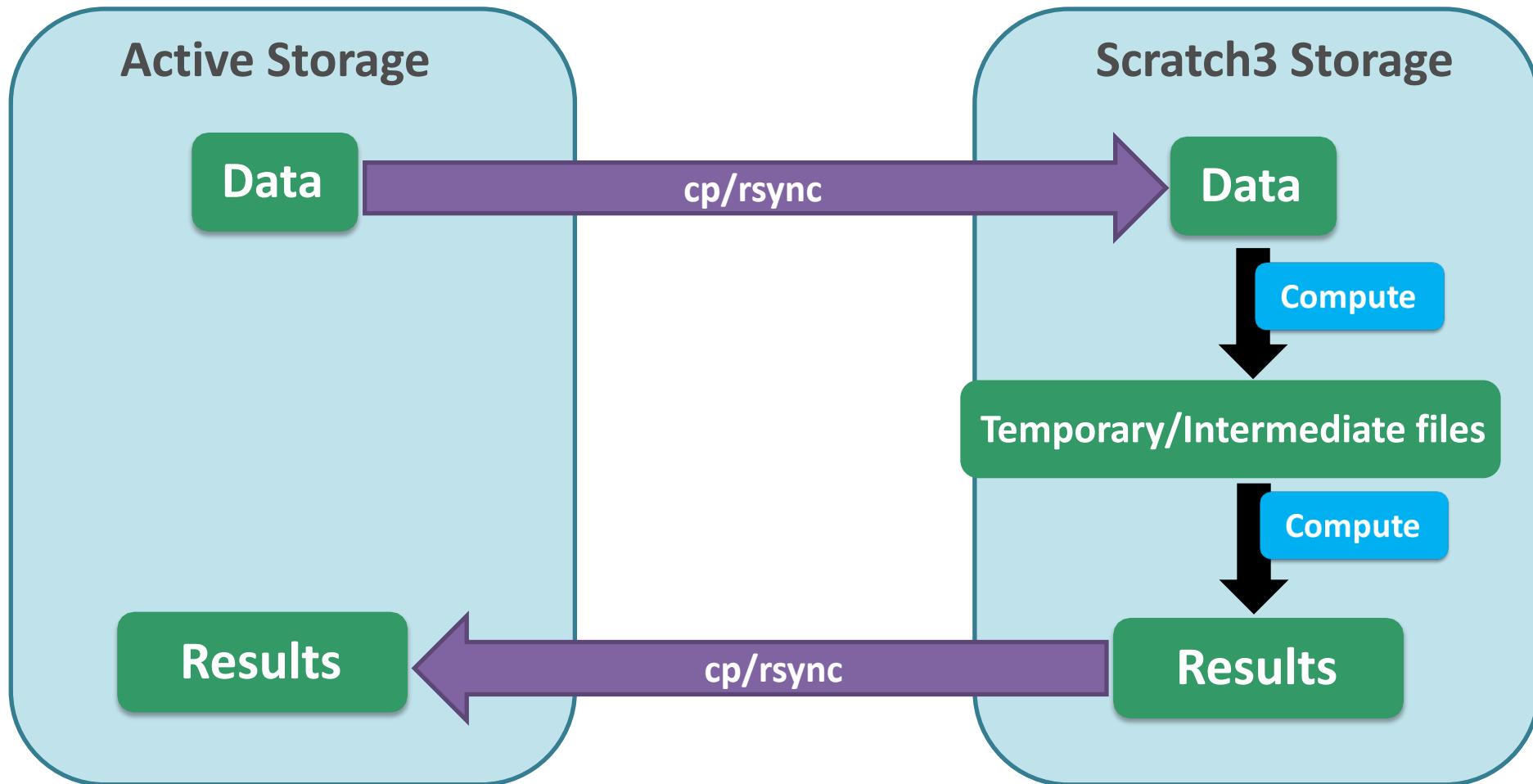
- `$ scancel <jobid> #Cancels specific job`
- `$ scancel -t PENDING #Cancels pending job`
- `$ scancel --name JOBNAME #Cancels job by name`
- `$ scancel jobid_[indices] #array indices`
- `$ scontrol hold <jobid> #pause pending jobs`
- `$ scontrol release <jobid> #resume`



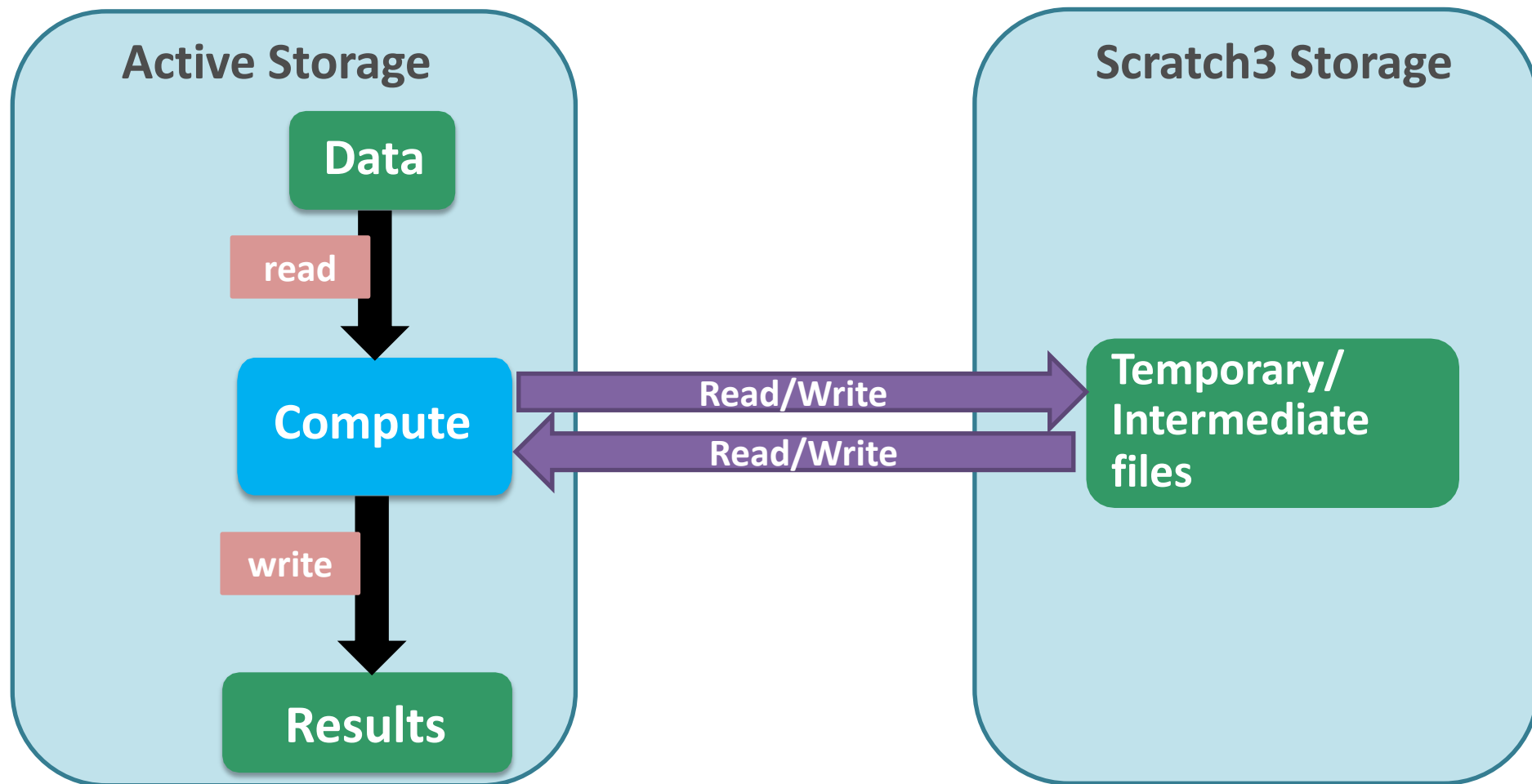
# Utilizing /n/scratch3



# /n/scratch3 Workflow: Redundancy



# /n/scratch3 Workflow: Best Practice



# Utilizing /n/scratch3

---

- Designed for writing a large number of small temporary files
- Use cases:
  - Keep original files in /n/groups (/n/data\*) or /home, write intermediate files to /n/scratch3, write final files to /n/groups (/n/data\*) or /home
  - Change working directory to /n/scratch3, read files from /n/groups (/n/data\*) or /home, write temp files to working directory, write or copy output back to /n/groups (/n/data\*) or /home
  - Copy input files to /n/scratch3, compute against, copy output files to /n/groups (/n/data\*) or /home

# File Properties



- “chmod” to change who can read/write/execute files/directories
- chmod options file/directory
  - Who? **u**ser **g**roup **o**thers **a**ll (u/g/o/a)
  - What? **r**ead **w**rite **x**ecute (r/w/x)
  - Do? +/-
- For example:
  - To make the file called “myfile” an executable  

```
$ chmod u+x myfile
```
  - To take away permission from others to read/write/execute for the same file  

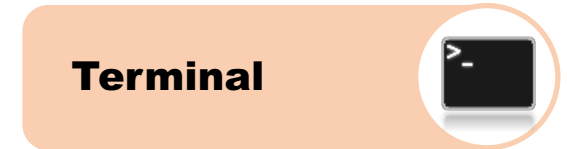
```
$ chmod o-rwx myfile
```

# O2 Portal: another way to access O2

---



 **Portal**



<https://o2portal.rc.hms.harvard.edu/>

# O2 Portal applications

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## **O2 Portal documentation**



# O2 Portal applications

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**Upcoming class on O2 Portal:**

Wednesday, Aug 2, 2023

[Registration details here](#)

[Slides available here](#)



**[O2 Portal documentation](#)**



**HARVARD**  
MEDICAL SCHOOL



# OMERO



## Overview:

OMERO is a visualization platform for the management of microscope images and metadata, available for use across the HMS research community.

## Eligibility:

Available to HMS Quad-based faculty, staff, postdocs, and graduate students. External sponsored collaborators who are working with HMS Labs or Cores.

## Requirements:

The user must have an HMS ID/account.

## Cost:

No Cost for HMS Quad-based faculty, staff, postdocs, and graduate students.  
No Cost for external sponsored collaborators who are working with HMS Labs or Cores.

# OMERO



## Features:

- Microscopy image and metadata management service of the Image Management Core
- Java Application or web interface
- Browse and filter through dimensions, z-sections and timepoints
- Analyze through Java, Python, C++ or MATLAB, Fiji/ImageJ using API/plugins to interface with OMERO server
- O2: CLI environment module, Java desktop client, or web interface
- Upload data from research.files, /home, /n/groups, /n/data1, /n/data2

Any questions please email us at: [rchelp@hms.harvard.edu](mailto:rchelp@hms.harvard.edu)

# For more direction

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



# Please fill out the survey

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- *Please see the instructor during your class for the class survey information.*
- We appreciate any feedback or comments!