

Intro to O2

HMS Research Computing

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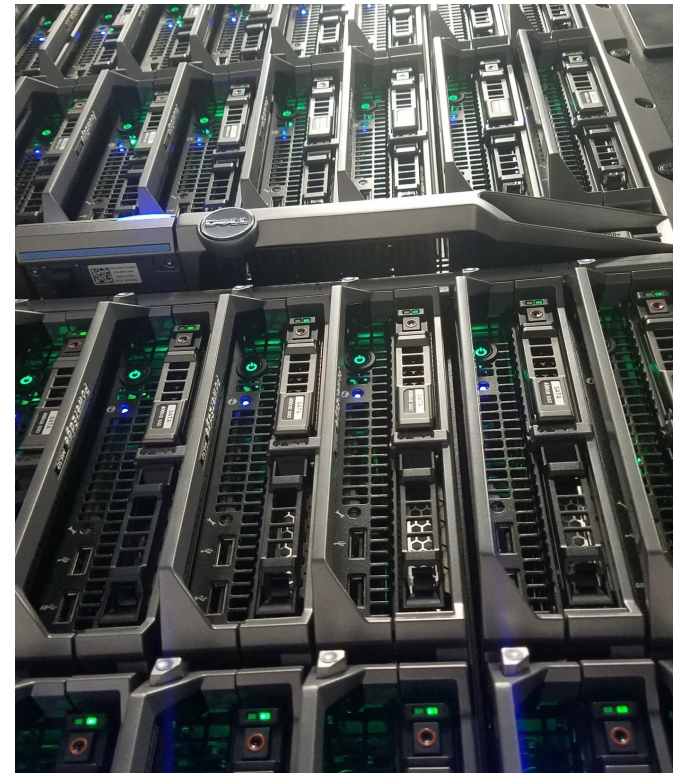
Welcome to O2!

- Slides available at github.com/hmsrc/user-training
 - **IntroToO2.pdf**
- Register for our other classes [here](#)
- Contact us at rchelp@hms.harvard.edu
- Comments/feedback welcome at course survey in the Harvard Training Portal

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

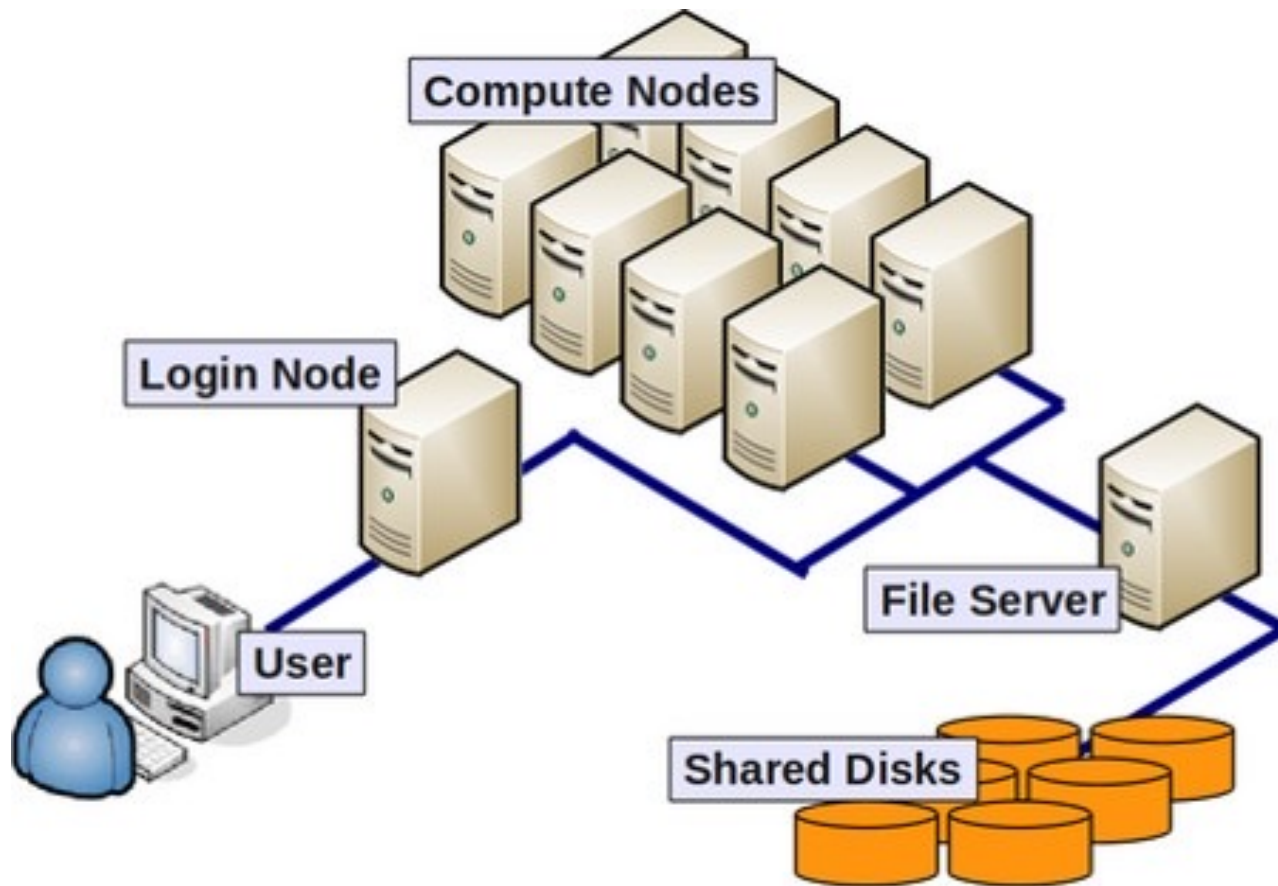
- Labs whose PIs do NOT have a primary or secondary appointment with an HMS Quad department (external users) will be charged.
- External users and PIs must register with the [RC Core in the PPMS system](#) prior to obtaining an O2 account.
 - [Details on the O2 Account Request Process for Off Quad Labs](#)
- 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 with any questions.

O2 Tech Specs



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

Generic Cluster Architecture



Storage on O2



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.

HMS Storage Offerings

- Renamed HMS storage spaces to:
 - Better align with how researchers think about and use data
 - Better manage data within the research data lifecycle
- Storage offerings:
 - *Active*
 - *Active Compute*
 - *Active Collaboration*
 - *Standby*
 - *Cold*

HMS Storage Offerings

- **Active** – available now, 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** – available now, 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** – future offering, 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

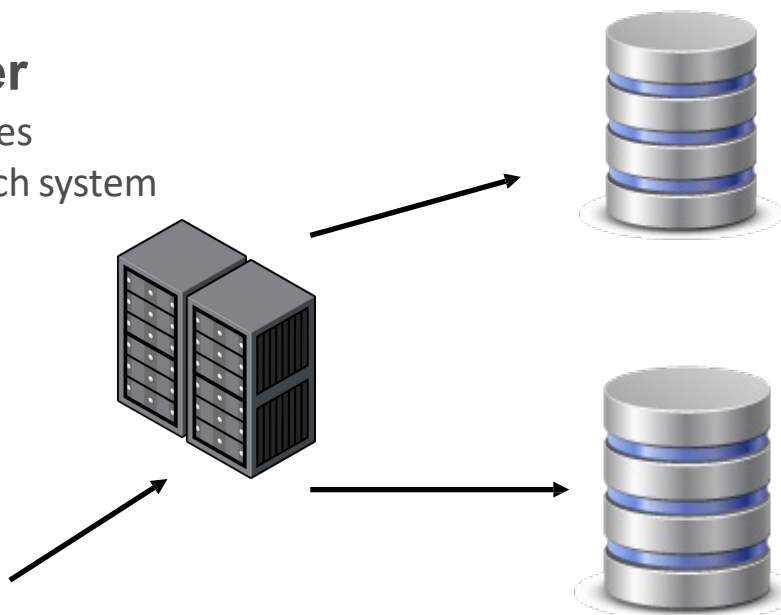


O2 Cluster

- 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`
- /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

Deleting files from O2 storage when hitting the Storage limit

- Currently, there is an interaction between O2 filesystems and vendor software which prevents deleting files/directories when you hit one of your storage quotas.
- Affects the following filesystems:
 - /home
 - group directories under /n/data1, /n/data2, or /n/groups
 - /n/scratch3
- Workaround: empty files using echo to go below quota, then remove using the rm command
- [See more details on this wiki page](#)

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

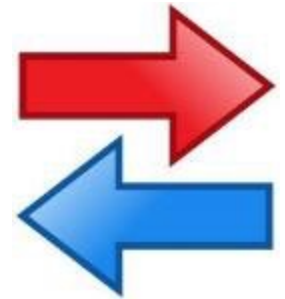
Snapshots (frozen) are retained for up to 60 days:
recover data from a hidden `.snapshot` directory

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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 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>



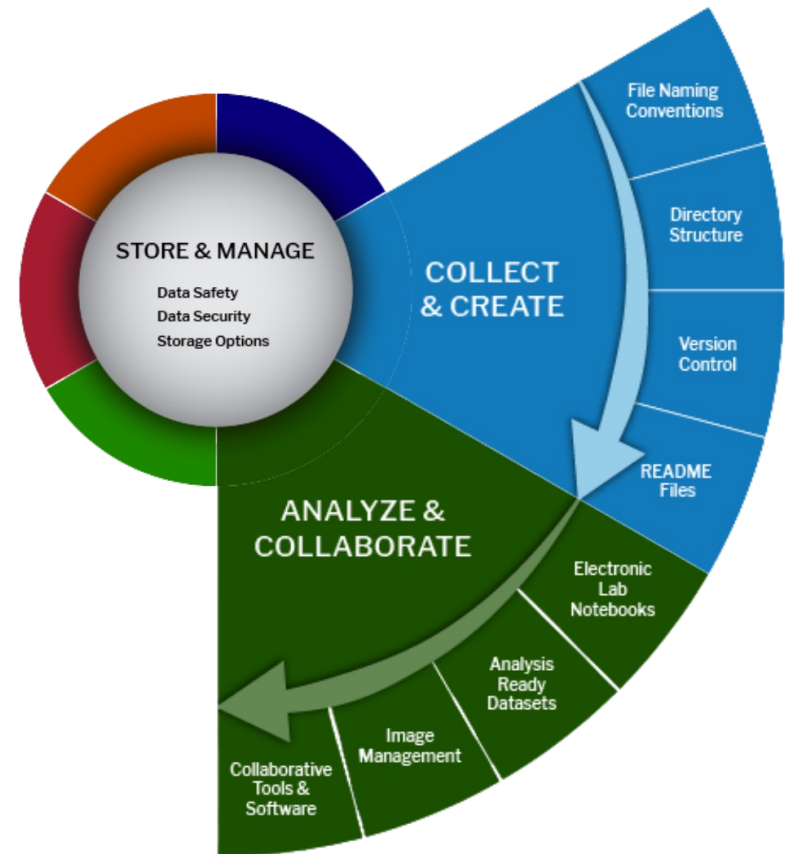
Planning

- 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



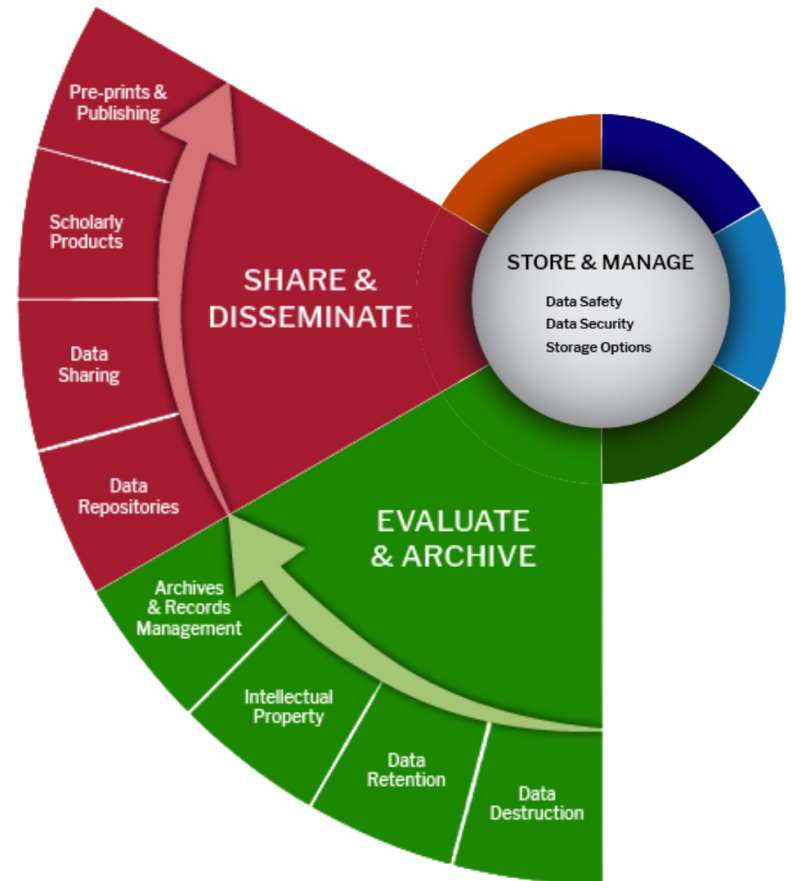
Active Research

- 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
- 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

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



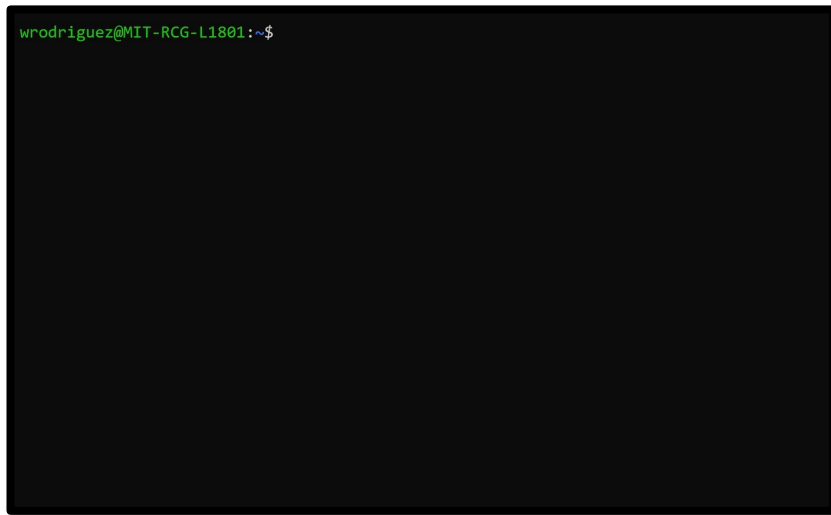
- Install MobaXterm (google it)
`ssh yourHMSaccount@o2.hms.harvard.edu`
- 2-Factor (when necessary): Choose 1/2/3 (push/phone/sms)

Logging Into O2: X11

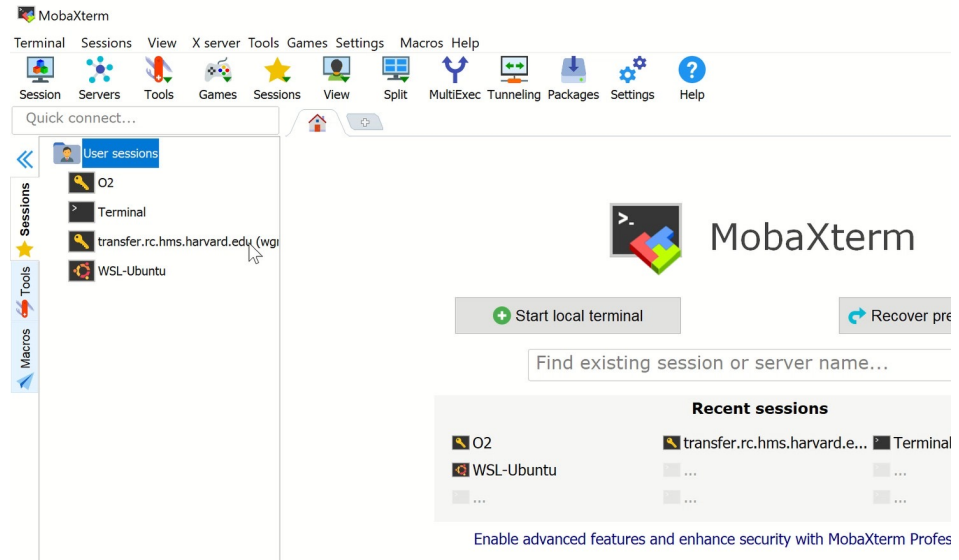
- You can display graphics (that a program on O2 is generating) back to your desktop using X11 forwarding.
- We won't be doing this for today's class.
- If you need to do this in the future, login with the -XY options:
`ssh -XY yourHMSaccount@o2.hms.harvard.edu`
- If you're on Mac, open XQuartz before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

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!



A terminal window showing the O2 login process. At the top, a green 'O2' logo is displayed. Below it, a message states: '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'. A large black rectangular box is overlaid on the left side of the terminal, containing the text '[wgr4@login04 ~]\$'. To the right of this box, the terminal text continues with a dashed line separator, followed by 'contains over 11,000 shared cpu cores!', 'on for all logins originating from outside', 'isplay/O2/Two+Factor+Authentication+on+O2', 't be run on O2's login servers.', 'g, gzip, etc.) that run for more', and 'than ten minutes or use too much CPU on O2's login servers will be automatically killed.'. Below this, there are two bullet points: '* Learn more about O2 at: <http://hmsrc.me/O2docs>' and '* Status updates and upcoming service outages are posted at: <https://wiki.rc.hms.harvard.edu/display/O2/O2+Cluster+Status>'. This is followed by another dashed line separator and the text 'Contact HMS Research Computing:'. Below this, contact information is listed: 'E-mail rchelp@hms.harvard.edu', 'Web <https://rc.hms.harvard.edu>', and 'Twitter @hms_rc'. At the bottom of the terminal, another instance of '[wgr4@login04 ~]\$' is shown, enclosed in a red rectangular box. A line connects this box to the black box above it.

```
O2

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

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E-mail      rchelp@hms.harvard.edu
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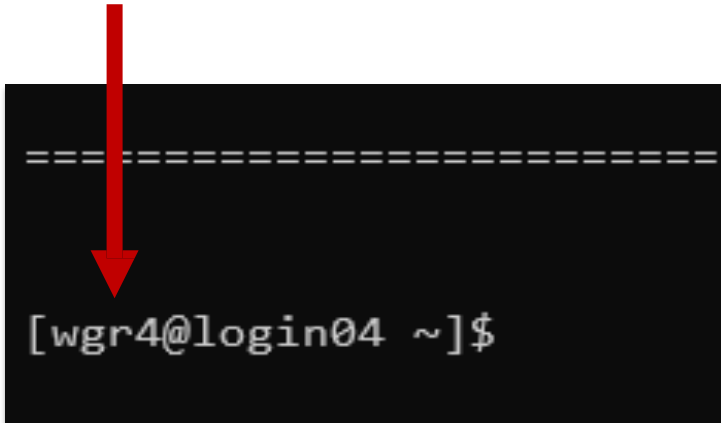
=====

[wgr4@login04 ~]$
```



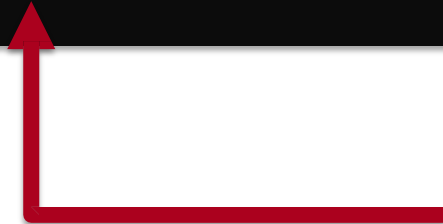
Welcome to O2!

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:~$
```

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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 ~
```



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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`

Installing Software: Binary Example

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- `mfk8@compute-a:~$ ls mysoftware/bin`

Programming Languages

- Python: load module (2.7.12, conda2, 3.6.0, 3.7.4, 3.8.12)
Use virtualenv to maintain packages (pip/easy install)
- R: load module (3.6.1, 4.0.1, 4.1.1, 4.1.2, 4.2.1)
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 (2021a, 2021b, 2022a)
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
```

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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

- 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
```

Line 1: `#!/bin/bash`

Line 2: `#SBATCH -p short`

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

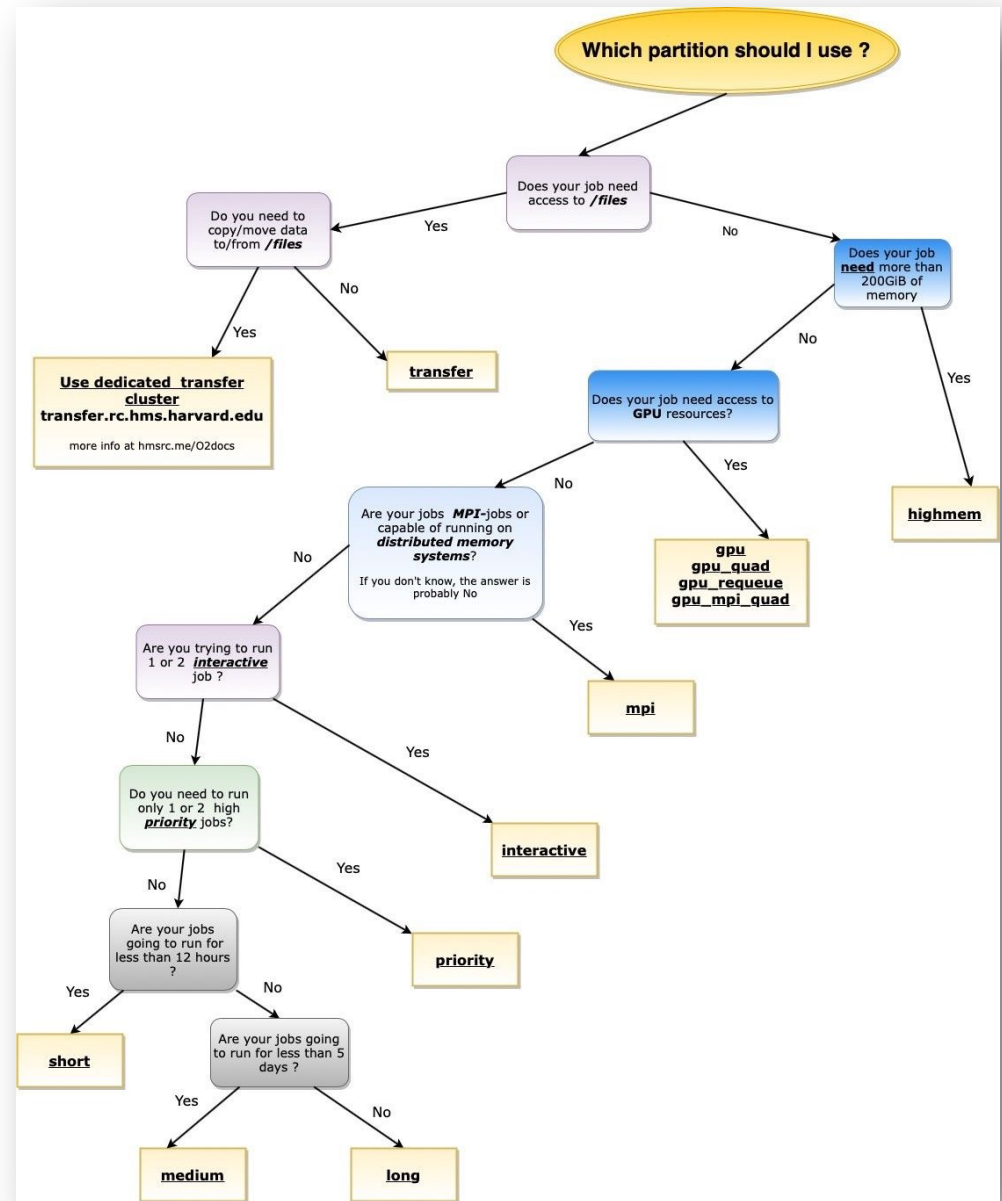
Line 4: `command_here ..`

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

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- %N node name
- %u user id

**Upcoming Intermediate O2 class,
which covers job arrays:**

October 26, 2022

[Registration details 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 `02sacct` 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](#)
- *Other options:*
 - `$ queue -u HMS_Account -t RUNNING/PENDING`
 - `$ queue -u HMS_Account s -p Partition`
 - `$ queue -u HMS_Account -start`
- *Detailed job info:*
 - `$ scontrol show jobid <jobid>`

Job Information: Past Jobs

- `$ 02sacct`
 - JobID, Partition, State , NodeList, Start, Timelimit, Elapsed, CPUTime , TotalCPU, AllocTRES, MaxRSS
 - Can specify job ID, job status, and/or timeframe to report accounting info for
 - [02sacct documentation](#)
- *Other options:*
 - `$ sacct -j jobid`
 - `$ sacct -r partition`
 - `$ squeue -s state`
 - `$ sacct --helpformat #get available fields you can specify`

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

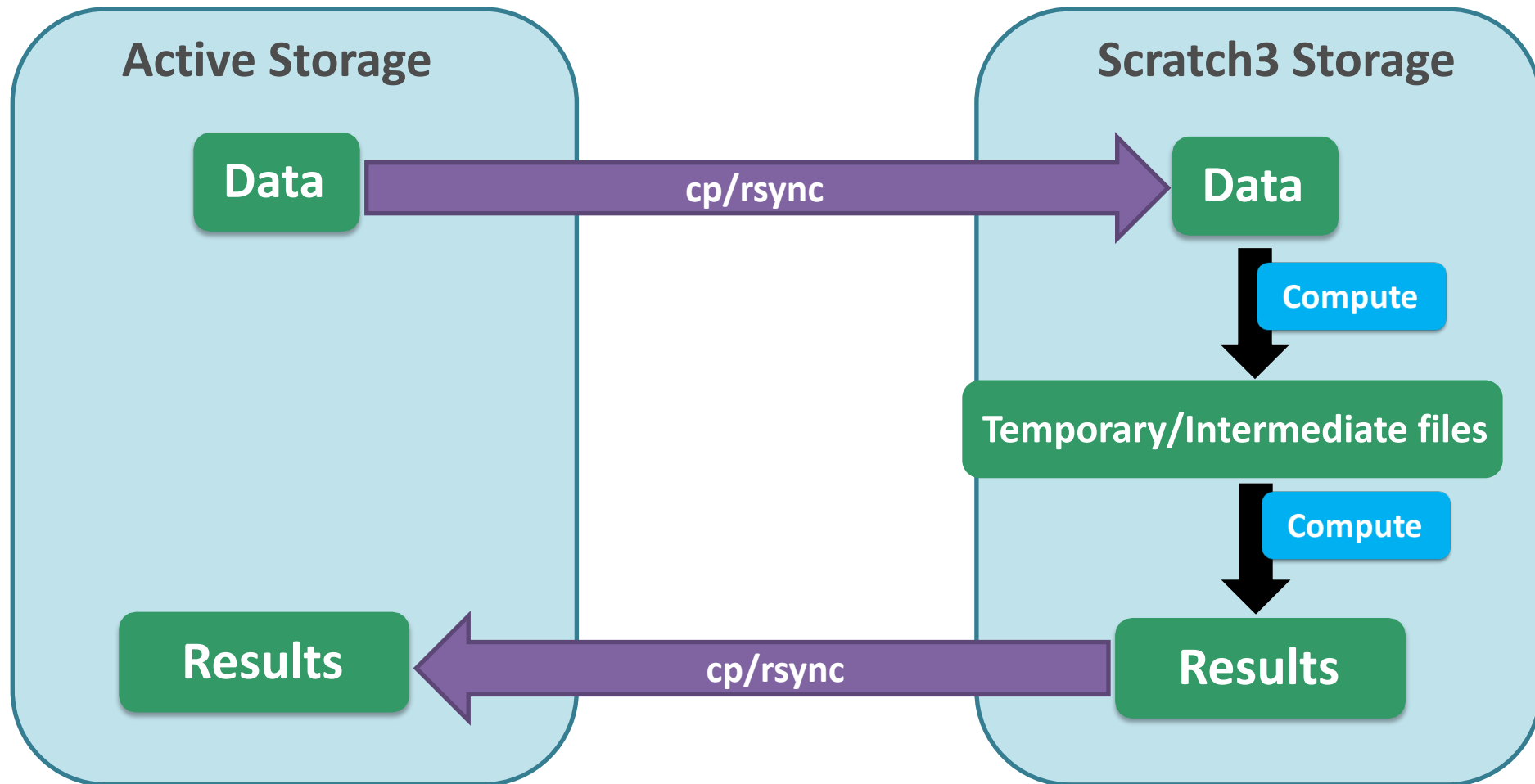
Cancelling/Pausing Jobs

- `$ 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`

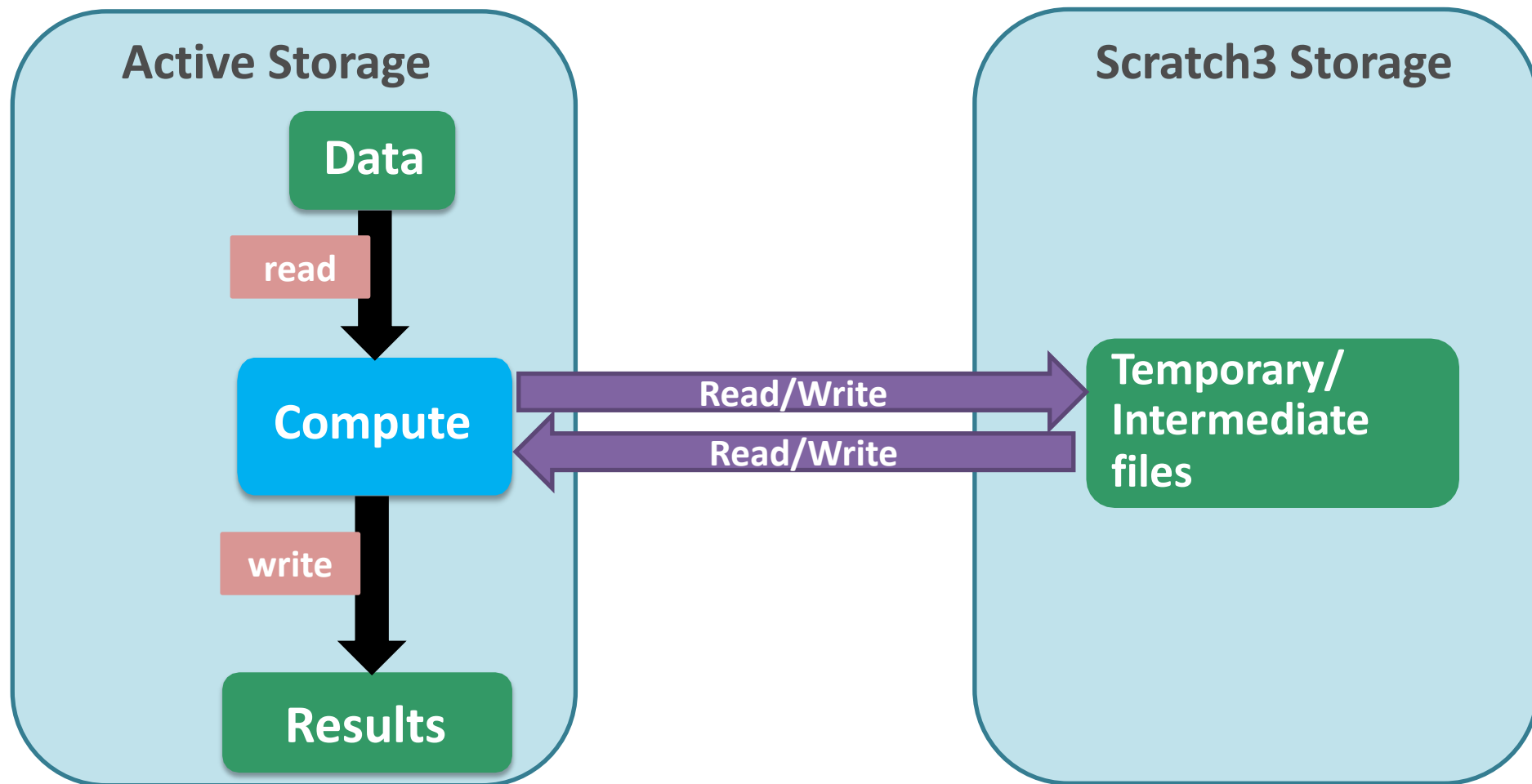
Utilizing /n/scratch3



/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

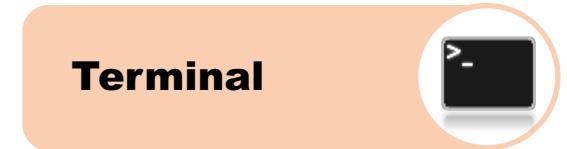
```
$ chmod u+x myfile
```
 - To take away permission from others to read/write/execute for the same file

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

O2 Portal: another way to access O2



 **Portal**

The logo consists of a red circle with a white number "2" inside, and a mouse cursor arrow pointing at the bottom right of the circle.

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

O2 Portal applications



O2 Portal documentation



O2 Portal applications

Upcoming class on O2 Portal:

September 21, 2022

[Registration details 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

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>)



Please fill out the survey

- Accessible through the Harvard Training Portal
 - <https://trainingportal.harvard.edu/>
- Click on “Me” then “Intro to O2”
- Scroll to “Evaluations” and click on the survey
- We appreciate any feedback or comments!