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

Slides available at github.com/hmsrc/user-training IntroToO2.pdf

Intro to 02

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Information Technology Research Computing Harvard Medical School 2/20/2024



Class Logistics

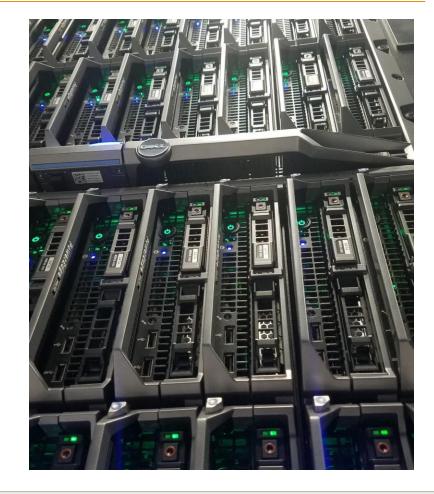
- Please make sure to sign in on the sign in sheet
- Feel free to ask questions or raise your hand if you need help
- Slides available at github.com/hmsrc/user-training
 - IntroToO2.pdf
- We will have hands-on exercises. If you do not have an O2 account, we will have training accounts (that only work for the class duration) available
- Comments/feedback welcome at course survey
- After the class:
 - Contact us at <u>rchelp@hms.harvard.edu</u>
 - Documentation available at the O2 Wiki





Welcome to O2!

- 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





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 <u>RC Core in the PPMS system</u> 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 <u>the Research Computing Core website</u>.
- Reach out to <u>rccore@hms.harvard.edu</u> with any questions.



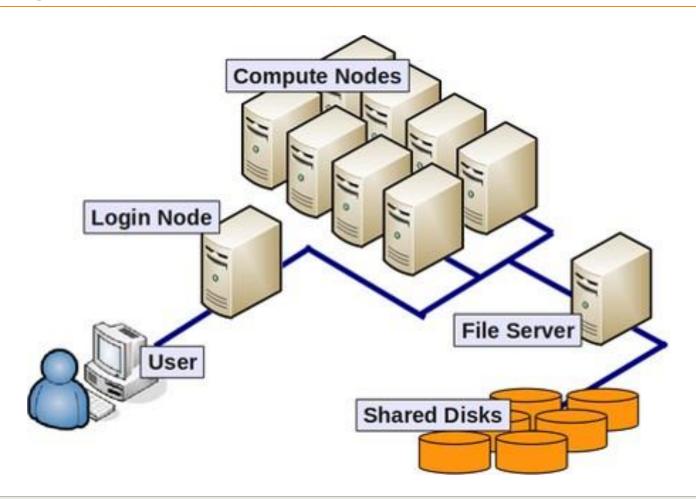


O2 Tech Specs

- 11000+ cores
- 32 cores per node
- 256 GiB RAM per node
- 8x756 GiB highmem nodes
- 200+ GPUs
 - Most GPUs available to Quad-based researchers only
- CentOS 7 Linux
 - OS will be updated later this year. Details TBA!
- Slurm job scheduler



Generic Cluster Architecture



Storage on O2

Important Note about O2 Storage

• O2 can only be used to store data of <u>Harvard Security Level 3</u> and below.

• None of the standard filesystems are automatically encrypted and cannot be used for HIPAA-protected or other secure data (above Harvard data security level 3) unless those data have been deidentified.

HMS Storage Offerings

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

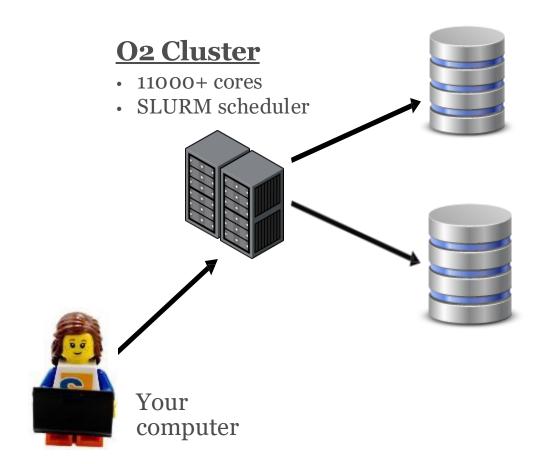
- Infrequently accessed data, that is directly available for reference, retrieval, or analysis.
- Accessible as /n/standby/institution/dept/lab on transfer cluster

Cold

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



O2 Primary Storage



/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 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!
- Location: /n/scratch/users/<first_HMS_account_char>/<HMS_account>
- Example
- mfk8@login01:~\$ cd /n/scratch/users/m/mfk8



Checking Storage Usage

To check your storage usage:

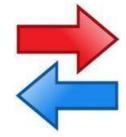
```
mfk8@login01:~$ quota-v2
```

- /home directory: each user gets 100 GiB
- /n/scratch directory: each user gets 25 TiB
- Group directories: space varies, can be increased
 - o /n/groups/lab
 - /n/data1/institution/department/lab
 - /n/data2/institution/department/lab

Snapshots

- Snapshots (frozen) are retained for up to 60 days: recover data from a hidden .snapshot directory
 - o mfk8@compute-a:~\$ cd .snapshot

 - o mfk8@compute-a:~\$ cd 02 home daily 2015-10-02-02-00
 - o mfk8@compute-a:~\$ cp MyRetreivedFile ~



Research.files O2 access

- Research.files Active filesystem is accessible on select compute nodes via the 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!

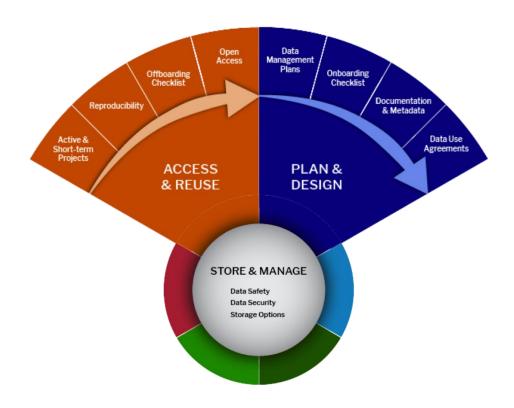


Harvard Biomedical Data Management Website: https://datamanagement.hms.harvard.edu



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

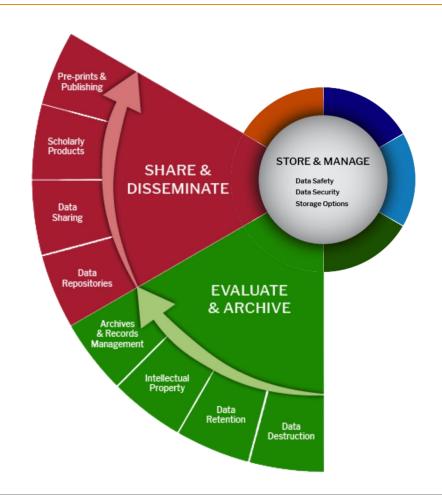
- Determine how the data will be organized including folder structure & file naming
- Consider versioning control for changes for both software and data products
- Create a README file to record the metadata that will be associated with data
- Link related code and algorithms
- Use tools & software to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

Request 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 with your HMS account password.

Get this service



2-Factor Authentication

- More secure: thing you know, and thing you have
- Easiest method: download Duo app to phone
- 2-Factor setup details here
- If you believe an email to be a phishing scheme, please forward to:
 - phishing@harvard.edu



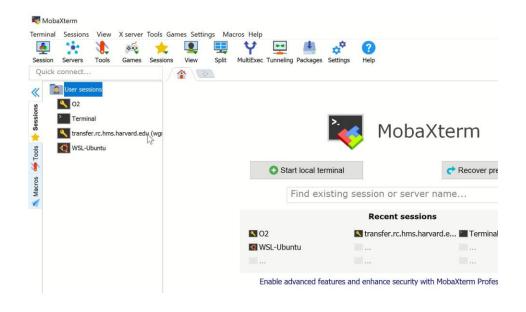
ssh hmsaccount@o2.hms.harvard.edu replace hmsaccount with your actual hmsaccount

Connecting to O2

Mac/Linux: Use Terminal



Windows: Use MobaXterm



If you do not have an O2 account, use a training account!

Please see your instructor for training account information.



Logging Into O2: X11

For most applications, using the O2 Portal is preferred to X11 forwarding.

- 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 hmsaccount@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)

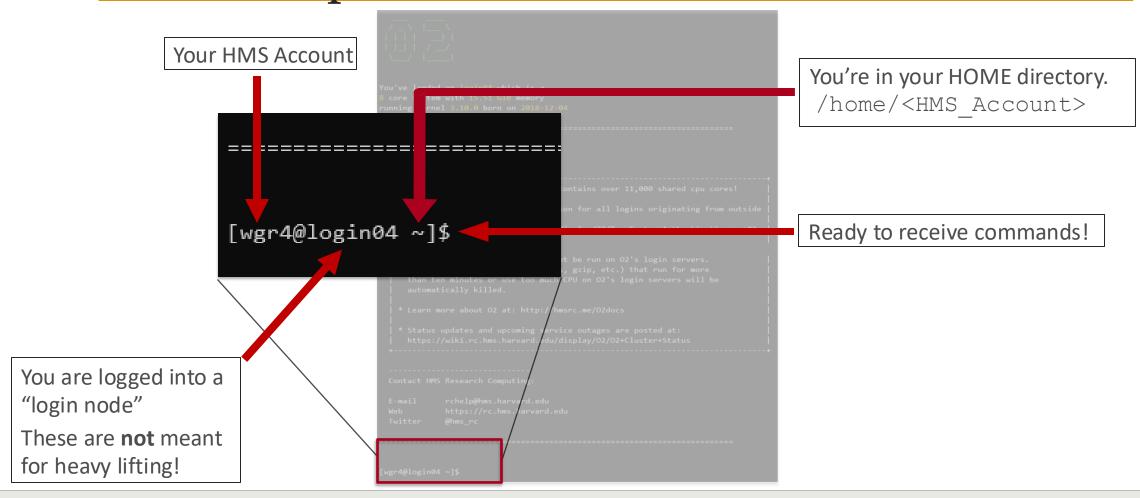


Welcome to the O2 Cluster!

```
You've landed on login@4 which is a
 core system with 15.51 GiB memory
 running kernel 3.10.0 born on 2018-12-04
    * With a recent expansion, O2 now contains over 11,000 shared cpu cores!
    * 02 requires 2-factor authentication for all logins originating from outside
    of the HMS network. Please see:
     https://wiki.rc.hms.harvard.edu/display/02/Two+Factor+Authentication+on+02
    * 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 02 at: http://hmsrc.me/02docs
   * Status updates and upcoming service outages are posted at:
    https://wiki.rc.hms.harvard.edu/display/02/02+Cluster+Status
 Contact HMS Research Computing:
 E-mail
             rchelp@hms.harvard.edu
 Web
             https://rc.hms.harvard.edu
             @hms_rc
 wgr4@login04 ~]$
```



User Prompt





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>

vord>



Port: 22

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

export DUO_PASSCODE=push/phone

Interactive Sessions

- The login nodes are not designed to handle intensive processes, and CPU usage is throttled. Start by entering your first job! This will log you into a "compute node!"
- 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:~\$



Class Practical

- Copy the class files and scripts to your /home
- 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
```

Linux Command Primer

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 "-1"

```
mfk8@compute-a:~$ ls -1
```

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

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

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 "change directory"
- 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," "vim", "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.



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 \$PATHnvariable, 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 on O2
$ module load software/version  #load software
$ module unload software/version #unload
$ module purge  #dump all modules
$ module help <software>  #displays help and setup 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 on public databases on O2, 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:~$ tar -zxvf mysoftware.tar.gz
mfk8@compute-a:~$ ls mysoftware/bin
```

Do not run the above commands. This is a demonstration of the general steps you would need to run.

Programming Languages

Python: load module (3.6.0, 3.7.4, 3.8.12, 3.9.14, 3.10.11, conda3, miniconda3)



- 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, 4.3.3, 4.4.0)
 - Setup personal R library
- <u>Perl</u>: load module (5.24.0, 5.30.0)
 - Setup local::lib (cpan/cpanm) in .bashrc
- MATLAB: load module (2022a, 2022b, 2023a, 2024a)
 - 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 a login node (and/or compute nodes), a program is submitted to O2 via an sbatch job

```
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@logino1:~\$ sbatch completeSlurmJob.run

```
Line1:#!/bin/bash
Line2:#SBATCH -p short
Line3:#SBATCH -t 0-1:00
Line4:command_here ..
```



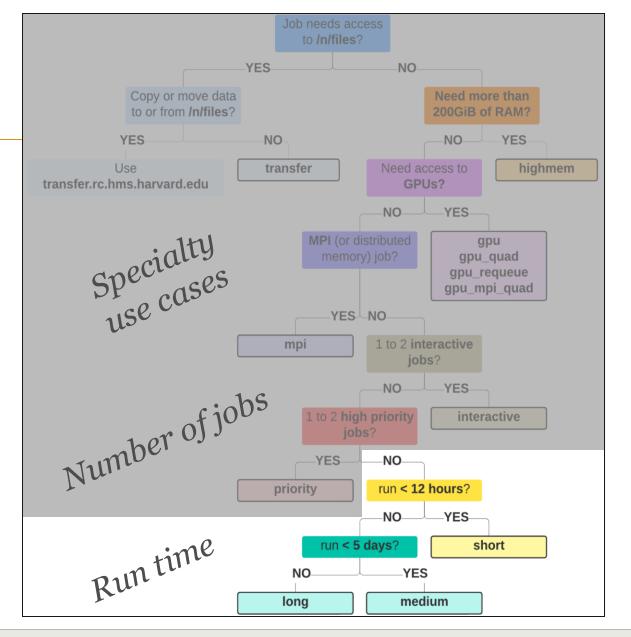
Partitions (queues): -p

Partition	Priority	Max Runtime	Max Cores	Max Memory	Limits
short	12	12 hours	20	250GiB	
medium	6	5 days	20	250GiB	
long	4	30 days	20	250GiB	
interactive	14	12 hours	20	250GiB	2 job limit, 4GiB by default
priority	14	30 days	20	250GiB	2 job limit
mpi	12	5 days	640		20 core min
highmem	16	5 days	20	990GiB	
<pre>gpu, gpu_quad, gpu_requeue</pre>	12	200 GPU hours	34 (total)	420GiB (total)	
transfer	1	5 days	4		



Choosing a Partition

- Narrow down a partition to use:
 - If you have a specialty use case (e.g. /n/files access, high memory, GPU, MPI, etc.)
 - Number of jobs to run
 - How long your job needs to run





Wall-Time: -t

- -t days-hours:minutes
- -t hours:minutes:seconds
- Need to specify how long you estimate your job will run for
- Ask for a bit more time than what you expect (e.g. 125% of expected runtime)
- 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
                      #memory per job (all cores), GiB
#SBATCH --mem=XG
#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
```



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 <u>Understanding O2 Slurm</u>
 <u>Accounts/Associations and Unix Accounts/Groups wiki page.</u>

Practical: simple sbatch script

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

```
#!/bin/bash

#SBATCH -p short  # Partition to submit to

#SBATCH -t 0-00:01  # Time in minutes

#SBATCH -c 1  # Number of cores requested

#SBATCH --mem=1G  # Memory total in GiB

#SBATCH -o hostname.%j.out  # Standard out goes to this file

#SBATCH -e hostname.%j.err  # Standard err goes to this file
hostname  # 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

For most applications, using the O2 Portal is preferred to X11 forwarding.

- To visualize or initiate plot devices, an X11 device must be active
- On Mac: install XQuartz and have it running prior to connecting to O2
- Windows: install <u>MobaXterm</u>, connect to O2 using it
- Login: ssh -XY
- To interactives, srun add: --x11
- No extra parameter required for batch jobs
- For more detail on X11 graphics forwarding, see this wiki page







Job Management

Job Monitoring: Current jobs

- \$ 02squeue
- JOBID, PARTITION, STATE, TIME_LIMIT, TIME, NODELIST(REASON), ELIGIBLE_TIME, START_TIME, TRES
- 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

- \$ 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
- O2_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>
- \$ scancel -t PENDING
- \$ scancel --name JOBNAME
- \$ scancel jobid [indices]
- \$ scontrol hold <jobid>
- \$ scontrol release <jobid>

```
#Cancels specific job
```

```
#Cancels pending jobs
```

```
#Cancels job by name
```

```
#array indices
```

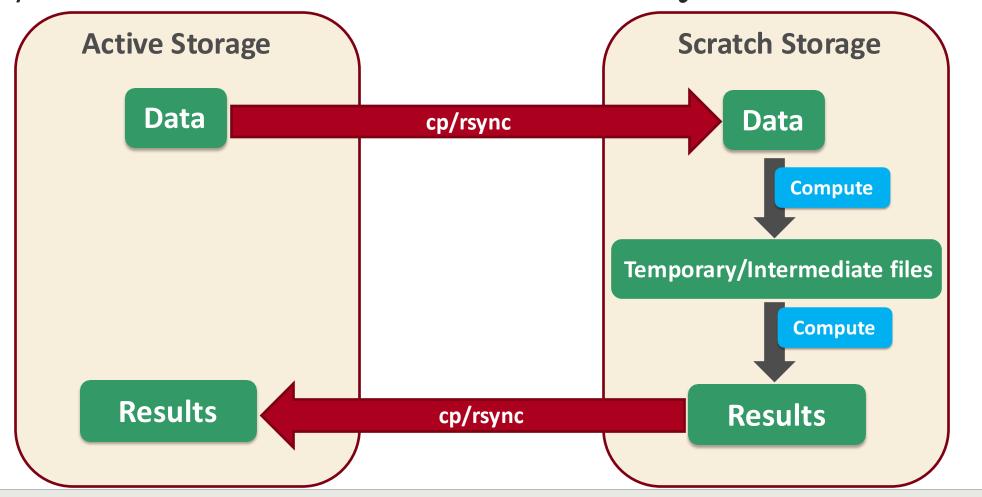
#pause pending jobs

#resume

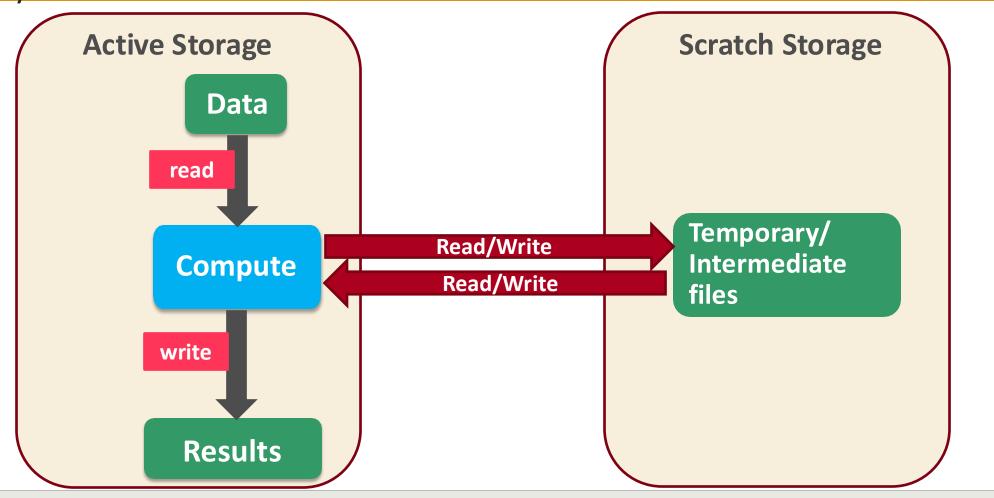


Utilizing /n/scratch

/n/scratch Workflow: Redundancy



/n/scratch Workflow: Best Practice



Utilizing /n/scratch

- 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/scratch, write final files to /n/groups (/n/data*) or /home
 - Change working directory to /n/scratch, 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/scratch, 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? user group others all (u/g/o/a)
 - What? **r**ead **w**rite execute (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



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

O2 Portal applications

Class on O2 Portal: March 6 and May 22

Slides available here











O2 Portal documentation



OMERO

- A visualization platform for the management of microscope images and metadata, available for use across the HMS research community.
- Available to HMS Quad-based faculty, staff, postdocs, and graduate students. External sponsored collaborators who are working with HMS Labs or Cores.
- An HMS ID/account is required as a prerequisite.
- 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.
- CLI environment module on O2, Java desktop client, or web interface
- Upload data from research.files, /home, /n/groups, /n/data1, /n/data2



Contact us!



Email: 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



We welcome your feedback in the survey!

https://bit.ly/hmsrc_o2 or



Questions?

