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

Slides available at
github.com/hmsrc/user-training
TroubleshootingO2Jobs.pdf

Troubleshooting O2 Jobs

kathleen_chappell@hms.harvard.edu

Some slides are courtesy of
william_rodriguez@hms.harvard.edu

HMS Research Computing:
rchelp@hms.harvard.edu

HARVARD
MEDICAL SCHOOL | Information Technology 2

Class Logistics

- Please make sure your Zoom name reflects your name in the Training Portal

- Put questions in chat, or unmute and ask

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

  ◦ TroubleshootingO2Jobs.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

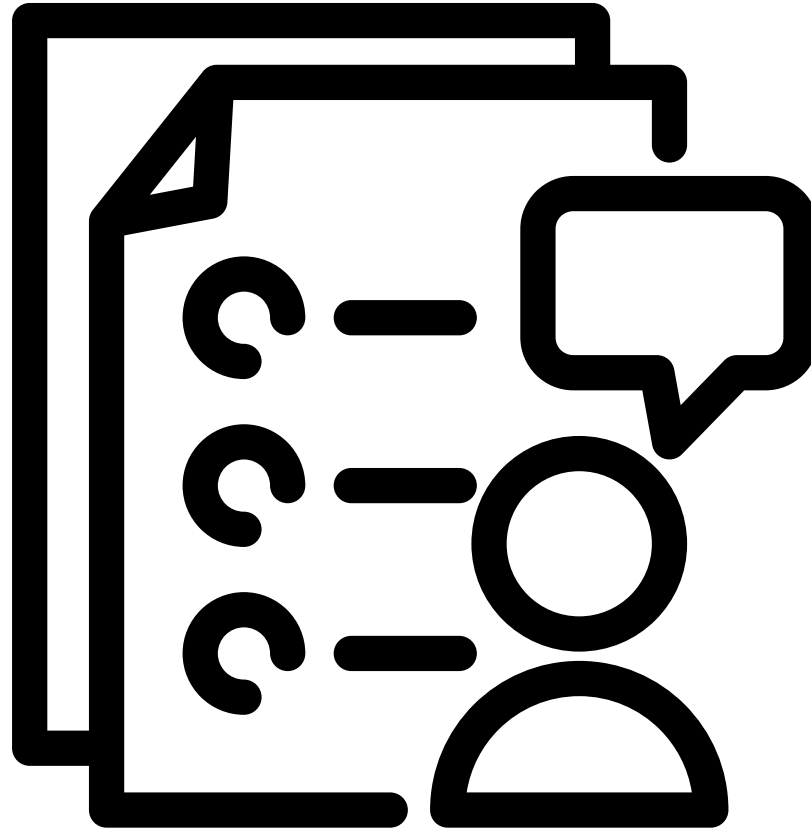- Resource for after the class: Troubleshooting Jobs wiki page

HARVARD
MEDICAL SCHOOL

Who is this class for?

- Folks who have taken "Intro to O2" or have already submitted jobs on the O2 cluster

  ◦ and who want to ***become more independent in debugging their work***.

- We assume a baseline amount of knowledge about how the cluster works, but we will have a quick review.

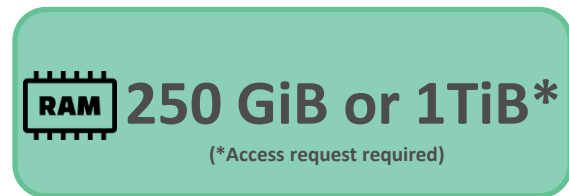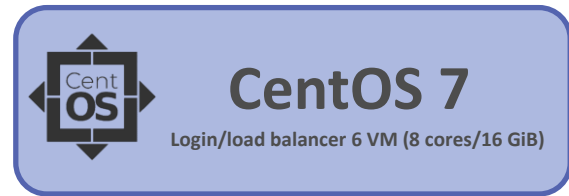- We will focus on troubleshooting jobs on the command line.

Poll

HARVARD
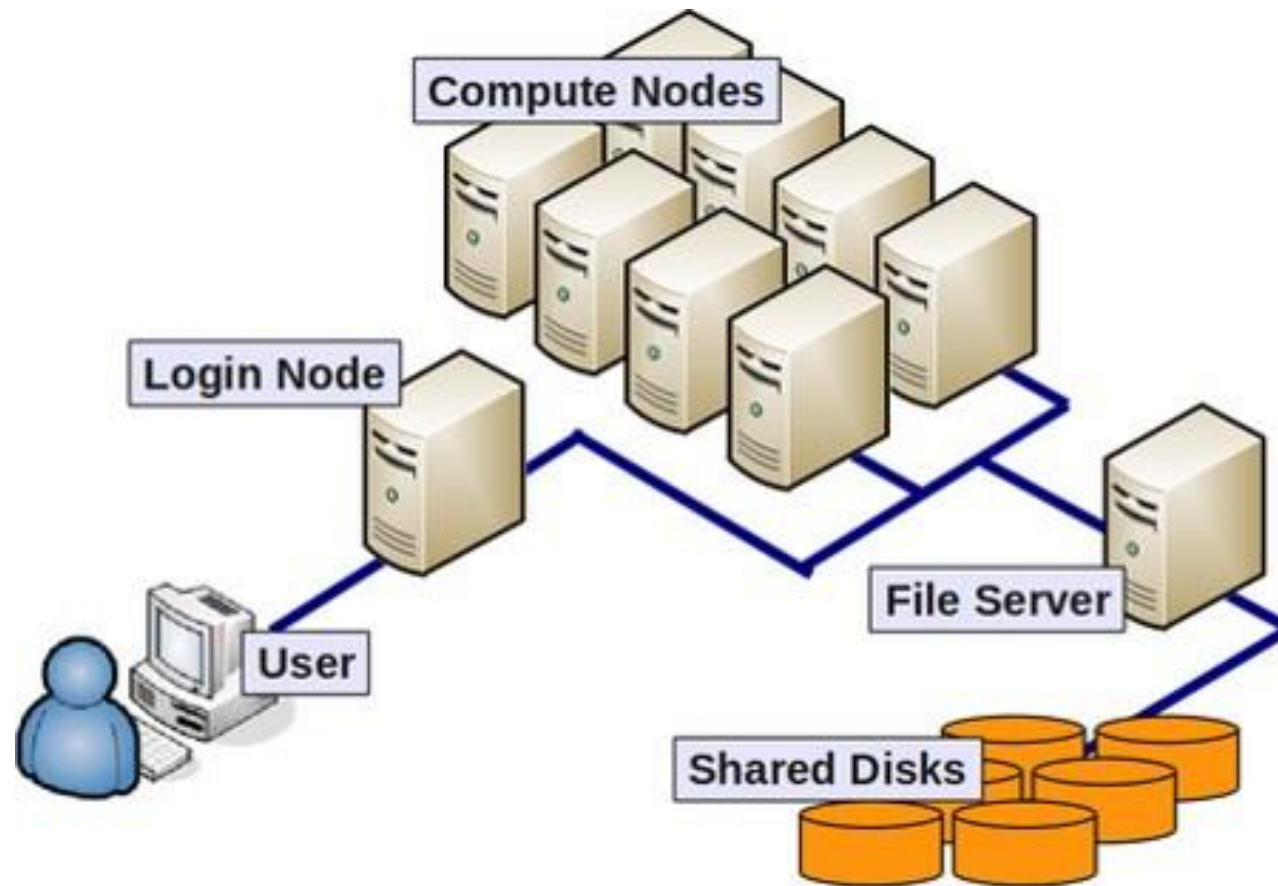MEDICAL SCHOOL

Information Technology 5

What is O2?

- One of HMS Research Computing's High-Performance Compute clusters

- SLURM scheduler

CentOS 7
Login/load balancer 6 VM (8 cores/16 GiB)

12000+ cores

250 GiB or 1TiB*
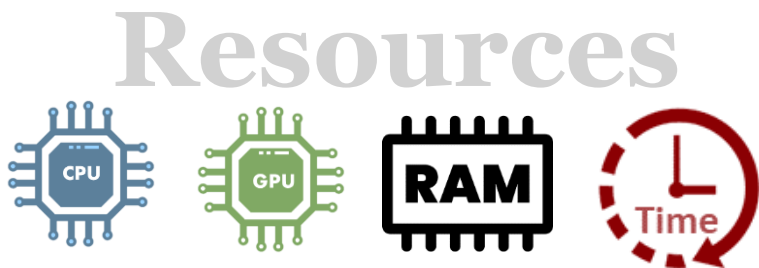(*Access request required)

167 GPUs
(*135 available to quad-based researchers)

Generic Cluster Architecture

Job submissions

A job is a **resource allocation for a user for a set amount of time**.

Resources

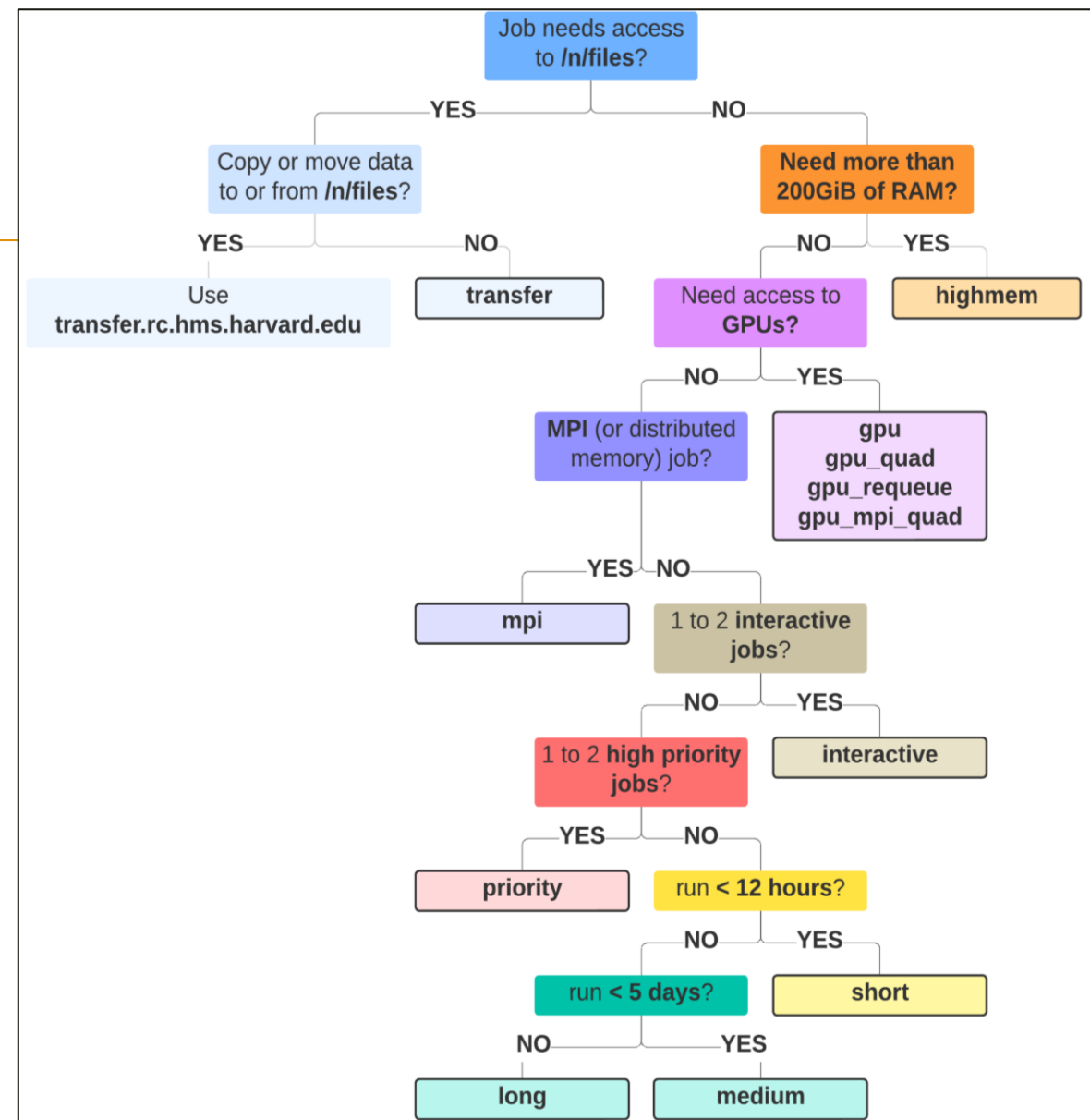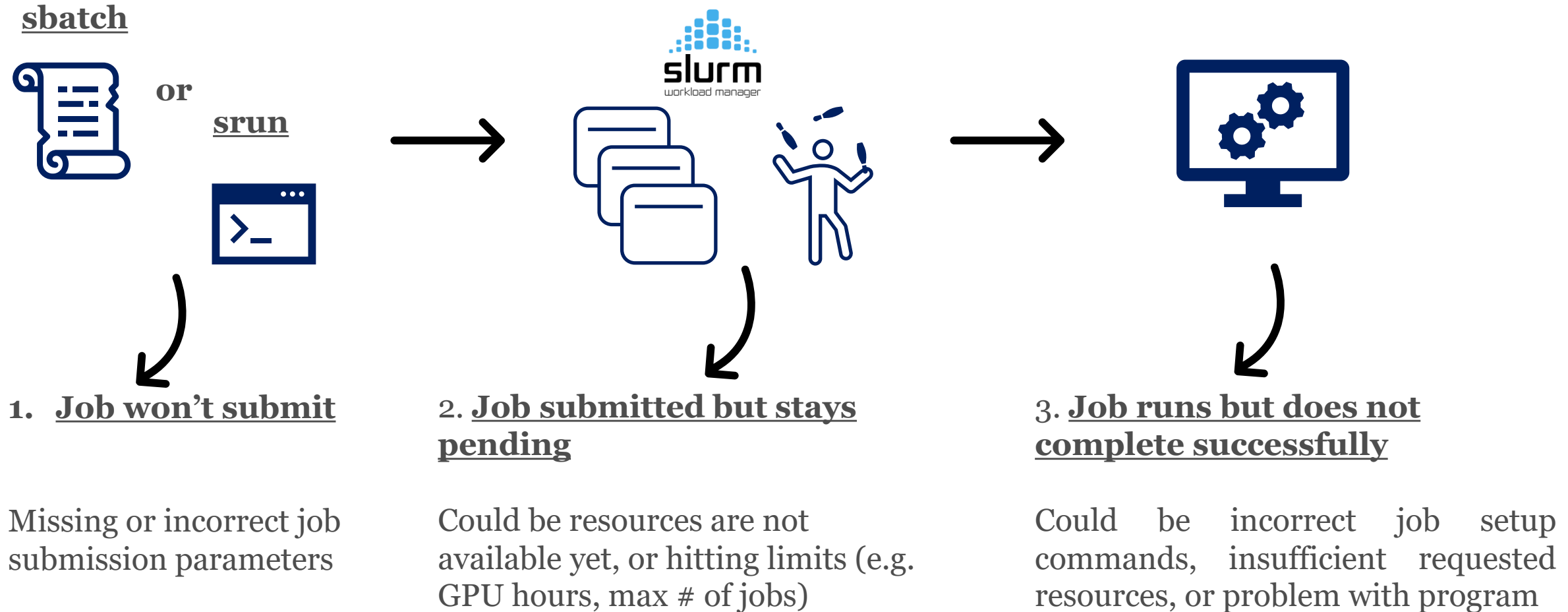|	**srun** interactive	**sbatch** batch
Requires a script?	No	Yes
Run analyses in real-time on the compute node(s)?	Yes	No
Job ends if you disconnect?	Yes	No

HARVARD
MEDICAL SCHOOL

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

Three main types of problems with jobs:

sbatch

or

srun

1. Job won't submit

Missing or incorrect job submission parameters

2. Job submitted but stays pending

Could be resources are not available yet, or hitting limits (e.g. GPU hours, max # of jobs)

3. Job runs but does not complete successfully

Could be incorrect job setup commands, insufficient requested resources, or problem with program

How to debug: *Jobs that won't submit*

- Read error messages!

  ◦ Missing command
  ```
  $ srun --pty -p interactive -t 0-2
  srun: fatal: No command given to execute.
  ```

  ◦ Missing partition
  ```
  $ srun --pty -t 0-2 bash
  srun: error: Job not submitted: please specify partition with -p.
  srun: error: Unable to allocate resources: Invalid partition name specified
  ```

  ◦ Missing walltime
  ```
  $ srun --pty -p interactive bash
  srun: error: Job not submitted: please specify runtime limit with -t.
  srun: error: Unable to allocate resources: Requested time limit is invalid (missing or exceeds some limit)
  ```

  ◦ Missing –account
  ```
  $ srun --pty -p interactive -t0-2 bash
  srun: error: lua: You have more than one Slurm account, must specify an account to submit
  srun: error: cli_filter plugin terminated with error
  ```

How to debug: *Jobs that won't start*

- Check O2squeue (pending/running jobs)

  ◦ For pending jobs, the "NODELIST(REASON)" will say why your job is not running

```
[kmk34@compute-a-16-160 ~ 2024-04-19 15:43:42]$ O2squeue
JOBID      PARTITION    STATE     TIME_LIMIT    TIME      NODELIST(REASON)          ELIGIBLE_TIME          START_TIME             TRES_ALLOC
36645028   interactive  PENDING   4:00:00       0:00      (Resources)               2024-04-19T15:37:09    2024-04-19T17:49:38    cpu=1,mem=250G,node=1,billing=16
36645882   interactive  PENDING   10:00         0:00      (Priority)                2024-04-19T15:43:33    N/A                    cpu=1,mem=4G,node=1,billing=1
36644759   interactive  RUNNING   2:00:00       14:06     compute-a-16-160          2024-04-19T15:28:10    2024-04-19T15:29:37    cpu=1,mem=4G,node=1,billing=1
36645850   short        PENDING   12:00:00      0:00      (None)                    2024-04-19T15:43:15    N/A                    cpu=1,mem=250G,node=1,billing=16
```

```
[kmk34@compute-a-16-160 ~ 2024-04-19 15:48:00]$ O2squeue
JOBID      PARTITION    STATE     TIME_LIMIT    TIME      NODELIST(REASON)          ELIGIBLE_TIME          START_TIME             TRES_ALLOC
36645028   interactive  PENDING   4:00:00       0:00      (QOSMaxJobsPerUserLimit)  2024-04-19T15:37:09    N/A                    cpu=1,mem=250G,node=1,billing=16
36644759   interactive  RUNNING   2:00:00       18:24     compute-a-16-160          2024-04-19T15:28:10    2024-04-19T15:29:37    cpu=1,mem=4G,node=1,billing=1
36645882   interactive  RUNNING   10:00         4:09      compute-a-16-166          2024-04-19T15:43:33    2024-04-19T15:43:52    cpu=1,mem=4G,node=1,billing=1
36646078   long         PENDING   30-00:00:00   0:00      (None)                    2024-04-19T15:47:22    N/A                    cpu=20,mem=250G,node=1,billing=35
```

  ◦ Reference here for a list of "REASONS" why a job is pending

How to debug: *Jobs that run but fail*

- Check <u>O2_jobs_report</u> (jobs that have finished running)

  ◦ Look at "STATE" column & "EFF" columns for "CPU", "RAM" and "WALLTIME"

```
[[kmk34@login02 ~ 2024-04-19 15:20:23]$ O2_jobs_report -s 2024-04-01

JOBID       USER     ACCOUNT     PARTITION      STATE      STARTTIME      WALLTIME(hr)   RUNTIME(hr)    nCPU,RAM(GB),nGPU    PENDINGTIME(hr)    CPU_EFF(%)   RAM_EFF(%)   WALLTIME_EFF(%)
---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------
36454631    kmk34    rccg        interactive    TIMEOUT    2024-04-16     2.0            2.0            1,10.0,0             0.03               3.8          32.6         100.2
36511328    kmk34    rccg        short          TIMEOUT    2024-04-17     1.0            1.0            1,1.0,0              0.04               0.1          0.7          100.2
```

  ◦ <u>Reference here for a list of "STATES" that a job could end in</u>

- Check error and output files

  ◦ Interactive jobs have messages printed to screen

  ◦ Batch jobs have error/output redirected to file(s)

    - See filenames specified in –e and –o in your job script OR will be written to slurm-jobid.out

Login to the O2 cluster

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

Mac/Linux: Terminal
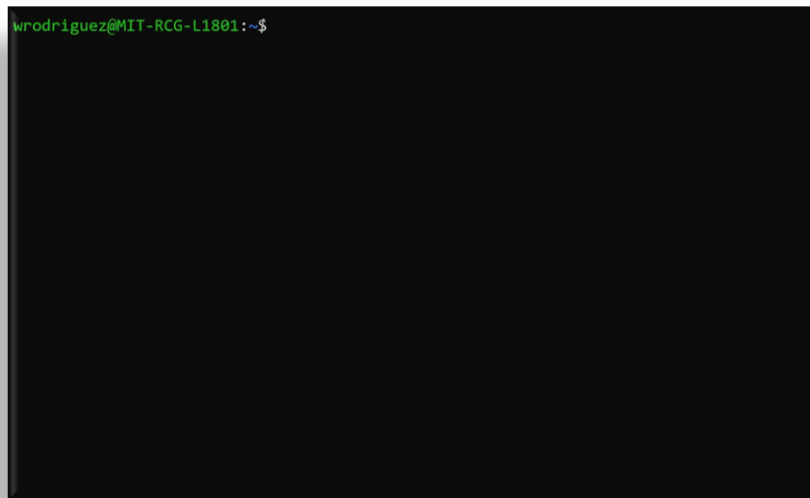
Windows: MobaXterm
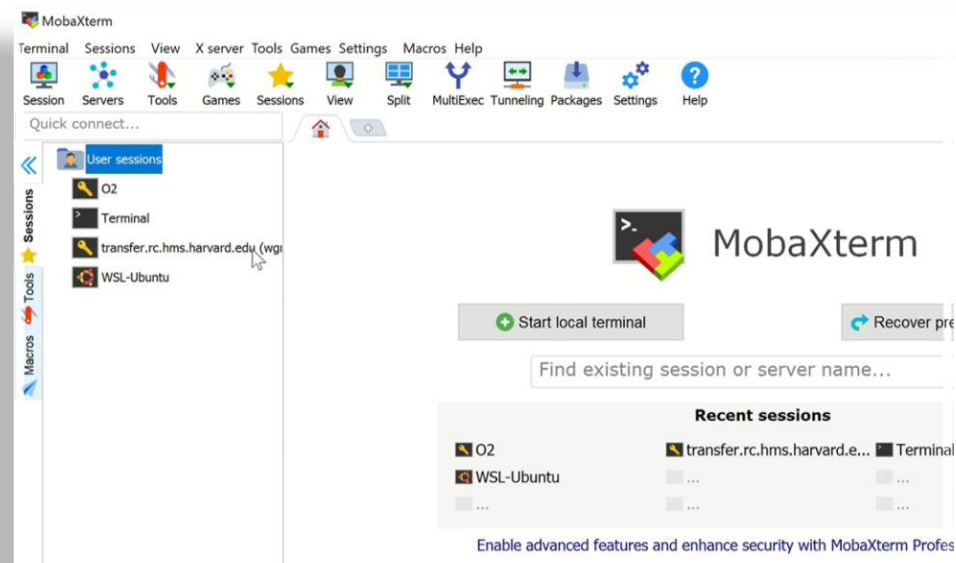
If you do not have an O2 account, use a training account!
See your instructor for training account information.

Exercises

HARVARD
MEDICAL SCHOOL

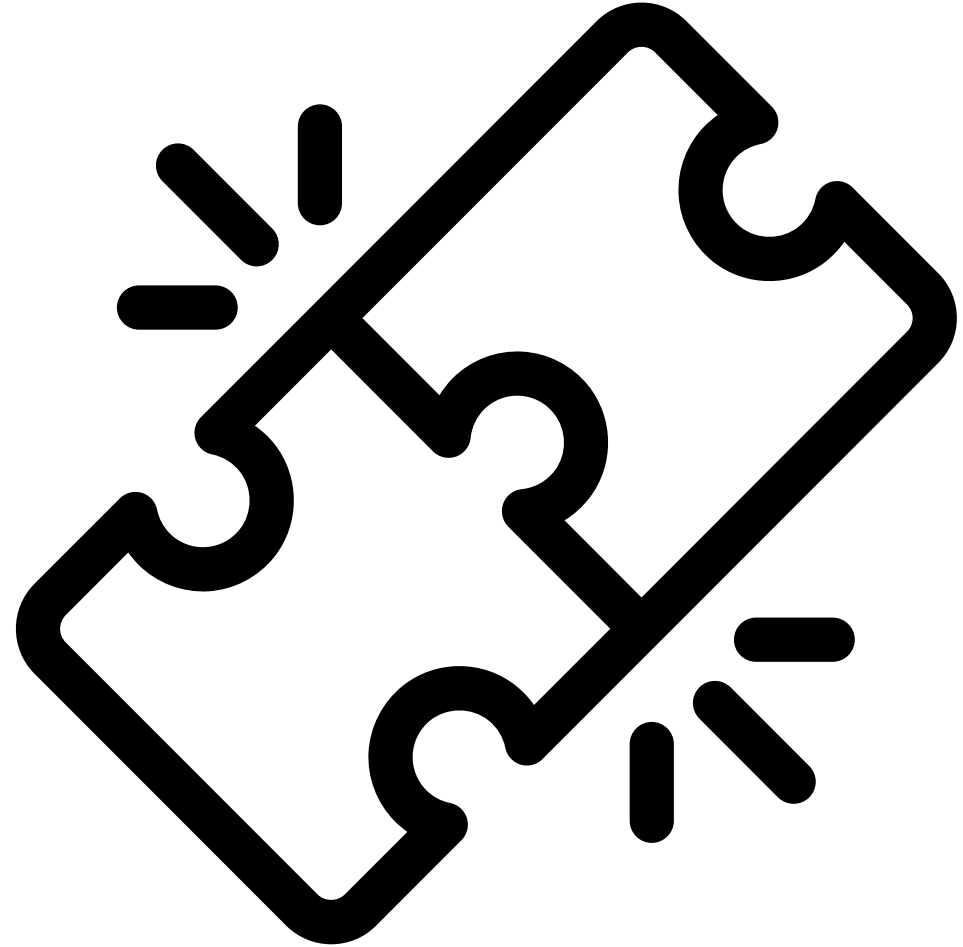Information Technology

Copy class materials

$ cp –r /n/groups/rc-training/troubleshooting_jobs/ ~

$ cd troubleshooting_jobs/

```
├── example_proteins.fasta
├── exercise1.sh
├── exercise2.sh
├── exercise3.sh
└── solutions
        ├── exercise1.sh
        ├── exercise2.sh
        └── exercise3.sh
```

The exercise scripts will fail on purpose, so we can debug them.

There are "corrected" scripts in the solutions/ subdirectory for your future reference.

Exercise 1: job won't submit!

$ sbatch exercise1.sh

```
#!/bin/bash
#SBATCH -p short                # Partition to submit to
#SBATCH -t 1-0                  # Time in days-hours format
#SBATCH -c 1                    # Number of cores requested
#SBATCH --mem=1G                # Memory total in GB (see also --mem-per-cpu)
#SBATCH -o hostname.%j.out      # Standard out goes to this file
#SBATCH -e hostname.%j.err      # Standard err goes to this file

hostname
```

- Read the error message when submitting the job.

```
[kmk34@login06 troubleshooting_jobs 2024-04-23 13:49:22]$ sbatch exercise1.sh
sbatch: error: Batch job submission failed: Requested time limit is invalid (missing or exceeds some limit)
```

HARVARD
MEDICAL SCHOOL

Exercise 2: job won't dispatch

$ sbatch exercise2.sh

```
#!/bin/bash
#SBATCH -p gpu                     # Partition to submit to
#SBATCH -t 0-0:05                  # Time in days-hours:minutes format
#SBATCH -c 1                       # Number of cores requested
#SBATCH --mem=1G                   # Memory total in GB (see also --mem-per-cpu)
#SBATCH -o gpu_job.%j.out          # Standard out/err goes to this file

nvidia-smi
```

- Check O2squeue for the REASON why the job won't dispatch

```
[kmk34@login06 troubleshooting_jobs 2024-04-22 17:06:49]$ O2squeue
JOBID       PARTITION    STATE      TIME_LIMIT    TIME    NODELIST(REASON)    ELIGIBLE_TIME        START_TIME    TRES_ALLOC
36777815    gpu          PENDING    5:00          0:00    (QOSMinGRES)        2024-04-22T17:02:34  N/A           cpu=1,mem=1G,node=1,billing=1
```

Exercise 3: job runs, but fails

$ sbatch exercise3.sh

```
#!/bin/bash
#SBATCH -p short                          # Partition to submit to
#SBATCH -t 0-0:15                         # Time in days-hours:minutes format
#SBATCH -c 1                              # Number of cores requested
#SBATCH --mem=1G                          # Memory total in GB (see also --mem-per-cpu)
#SBATCH -o submits_&_fails.%j.out         # Standard out/err goes to this file

colabfold_search \
--db-load-mode 2 \
--mmseqs mmseqs \
--use-env 1 \
--use-templates 0 \
--threads 4 \
/home/$USER/troubleshooting_jobs/example_proteins.fasta /n/shared_db/misc/mmseqs2/14-7e284
/home/$USER/troubleshooting_jobs/
```

- Check O2_jobs_report and out/err file

O2 Portal: another way to access O2

Transfer Files

Submit Jobs

Monitor Jobs

②Portal

Terminal

View/Edit Files
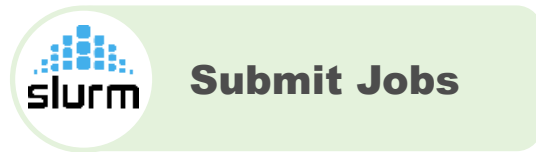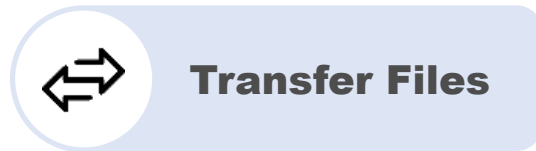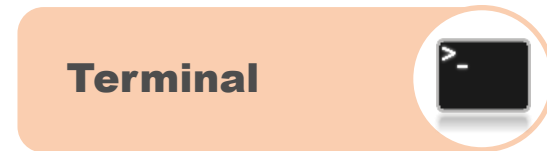
Applications

o2portal.rc.hms.harvard.edu
O2 Portal docs | O2 Portal class slides

Information Technology

Debugging O2 Portal Jobs

"My Interactive Sessions" is to the right of HMS-RC Applications in the top navigation bar

RStudio Environment (36511328)   1 node | 1 core | Running

Host: compute-a-16-162.o2.rc.hms.harvard.edu

Created at: 2024-04-17 14:02:44 EDT

Time Remaining: 59 minutes

Session ID: 208113a2-97c7-4911-b9ab-1d93620ce236

Progress & Error log: output.log

® Connect to RStudio Server

Click on the output.log link in the session card.

Check for any error messages.

HARVARD MEDICAL SCHOOL | Information Technology

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

Questions?

Information Technology