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

Information Technology - Research Computing
Harvard Medical School
4/09/2025

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

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

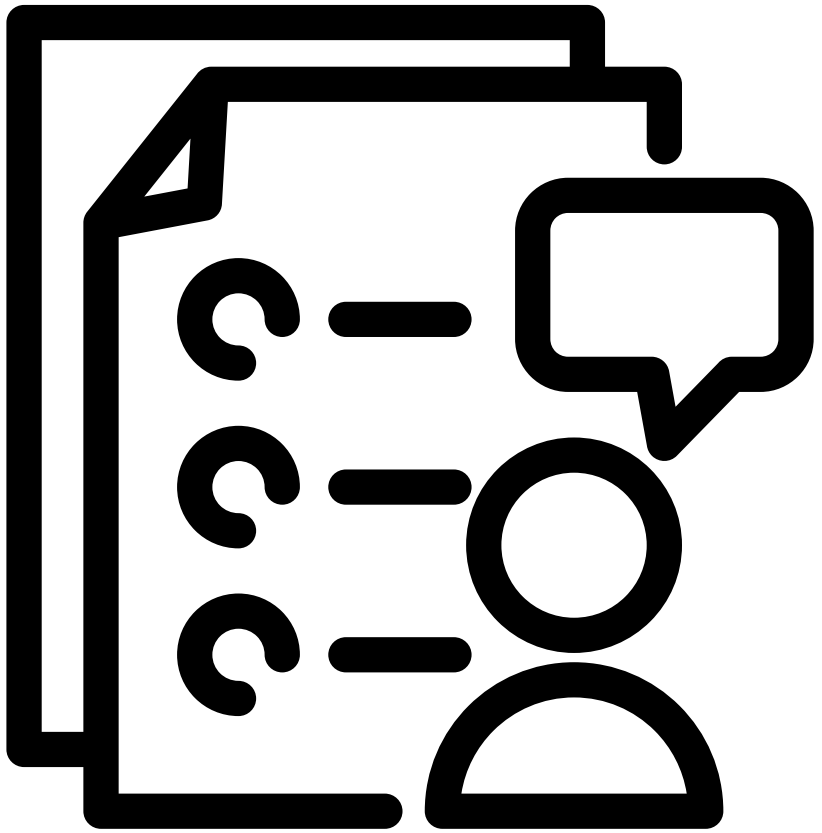
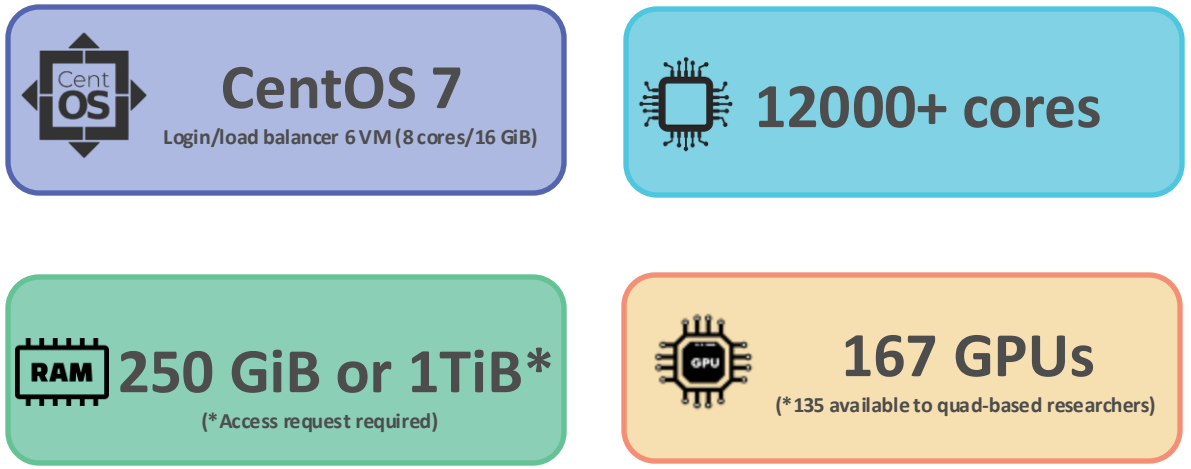


Image credit: Survey by Symbolic from Noun Project (CC BY 3.0)

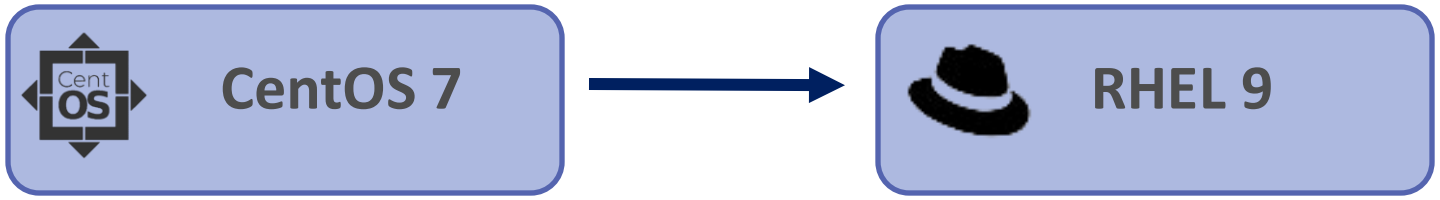
What is O2?

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

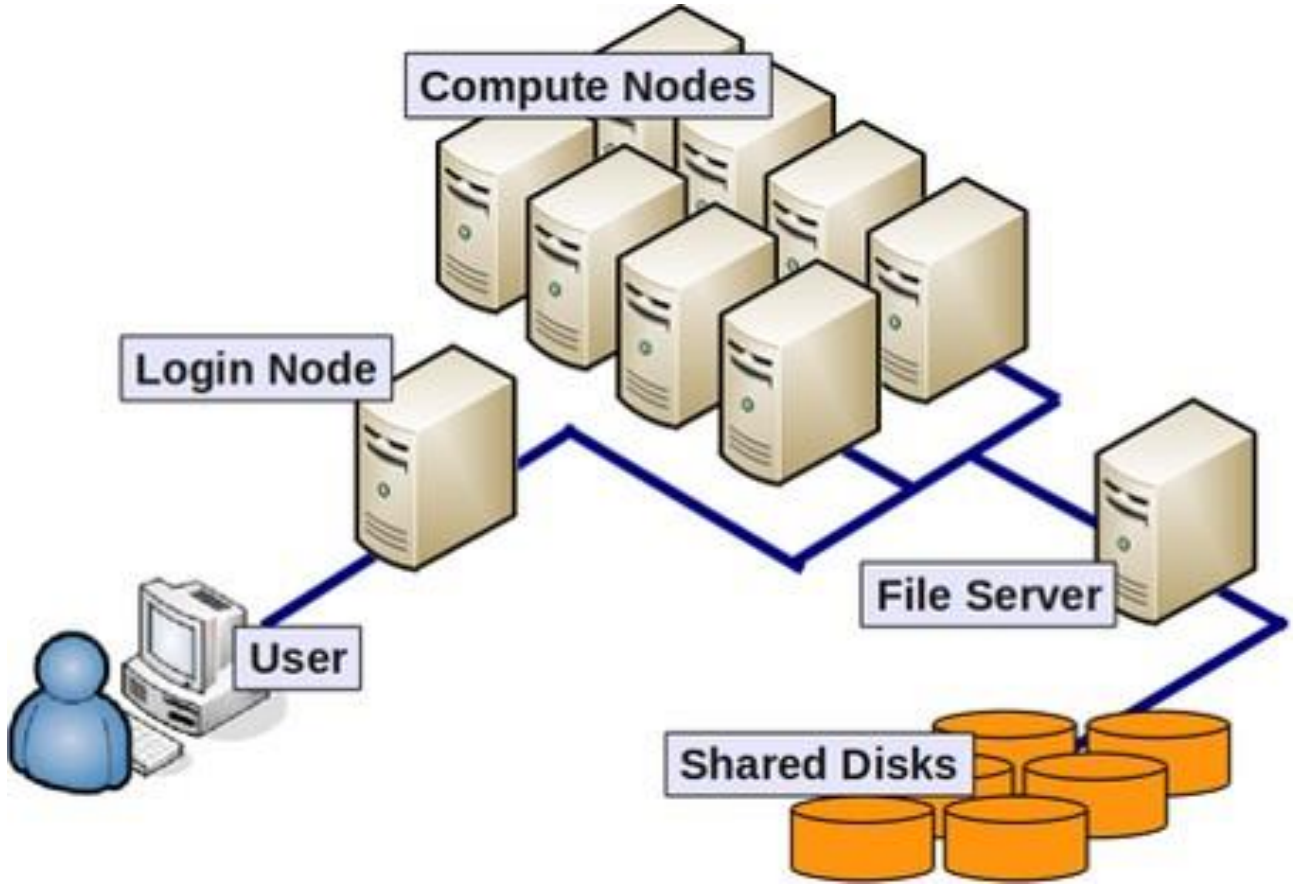


Upcoming Operating System Update

- Migrating O2 from CentOS 7 to Red Hat Enterprise Linux (RHEL) v9
  - Any software installed on CentOS 7 (including R, Python conda packages) will need to be reinstalled under RHEL
- Software freeze on CentOS 7 as of beginning of April
- Initial testing begins April 10
- If interested in testing, please contact rchelp@hms.harvard.edu
- More details are forthcoming.



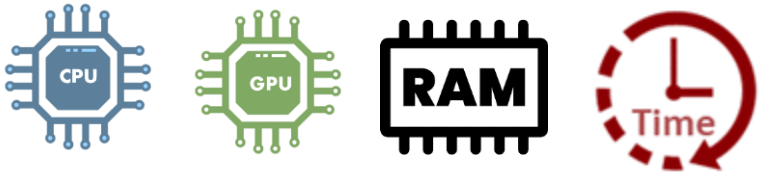
Generic Cluster Architecture



Job submissions

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

Resources

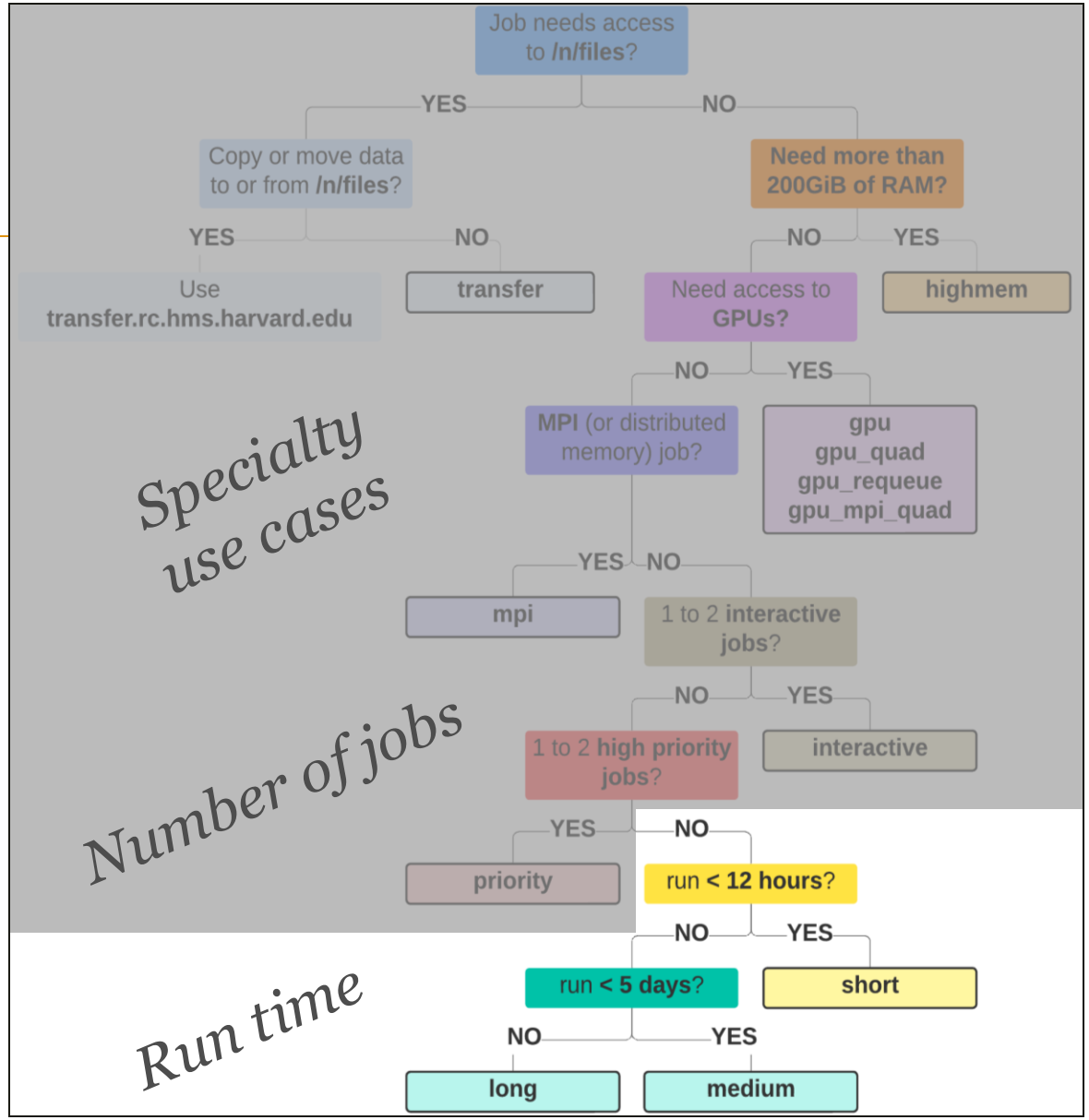


	srun interactive	**sbatch** batch
Requires a script?	No	Yes
Run analyses in real-time on the compute node(s)?	Yes	No
Job ends if you disconnect?	Yes	No

[Job definition from SLURM documentation]

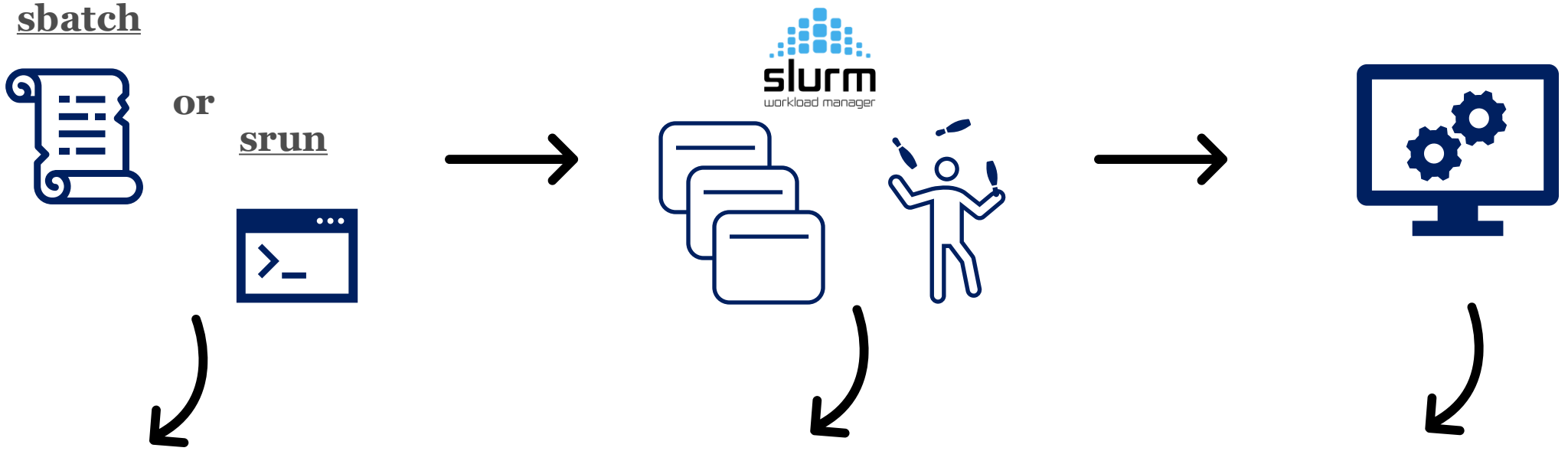
Choosing a Partition

- 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



How to Choose a Partition wiki page

Three main types of problems with jobs:



1. Job won't submit
2. Job submitted but stays pending
3. Job runs but does not complete successfully

How to debug: (1) *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 -t 0-2 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: (2) *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: (3) *Jobs that run but fail*

- Check O2_jobs_report (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
```

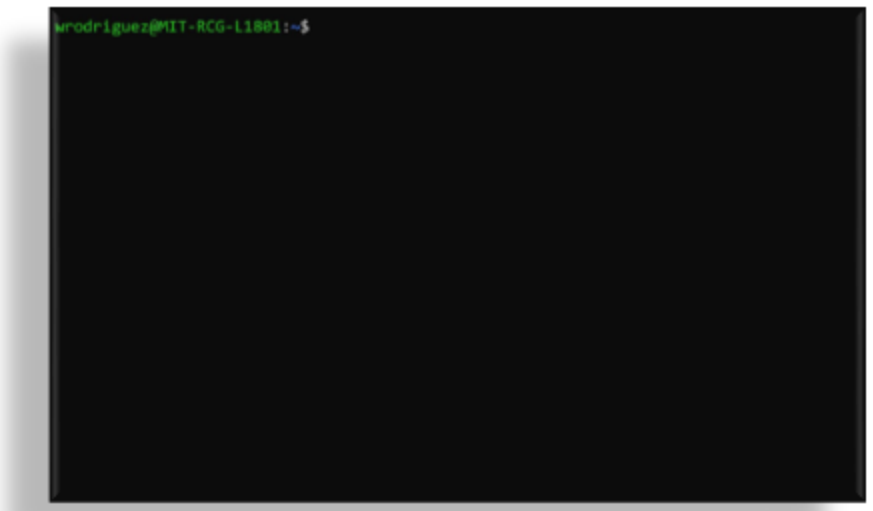
JOBID	USER	ACCOUNT	PARTITION	STATE	STARTTIME	WALLTIME(hr)	RUNTIME(hr)	nCPU,RAM(GB),nGPU	PENDINGTIME(hr)	CPU_EFF(%)	RAM_EFF(%)	WALLTIME_EFF(%)
36454631	kmk34	rccg	interactive	TIMEOUT	2024-04-16	2.0	2.0	1,10.0,0	0.03	3.8	32.6	100.2
36511328	kmk34	rccg	short	TIMEOUT	2024-04-17	1.0	1.0	1,1.0,0	0.04	0.1	0.7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

  - Reference here for a list of “STATES” that a job could end in
- 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

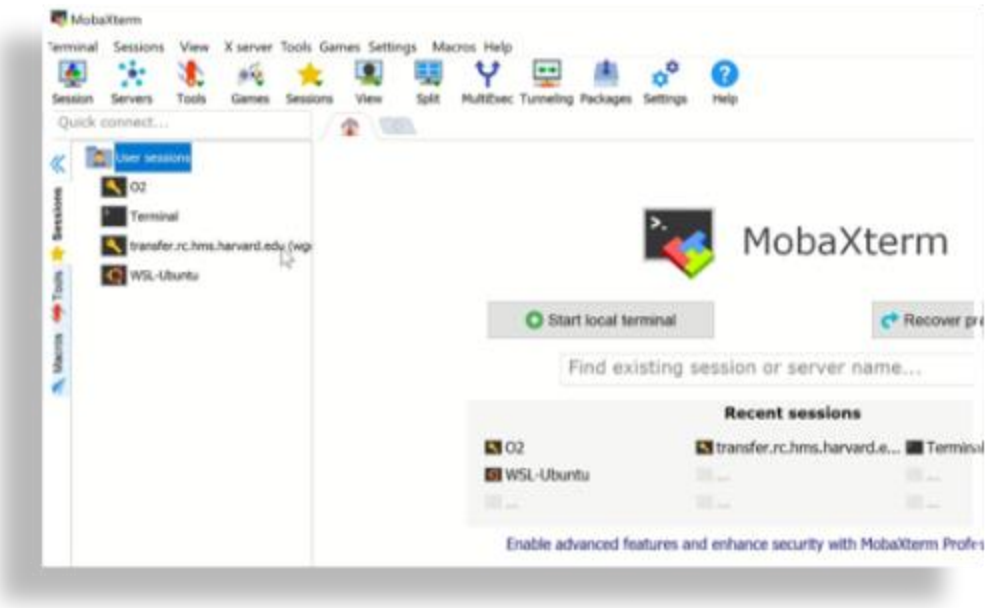
Login to the O2 cluster

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

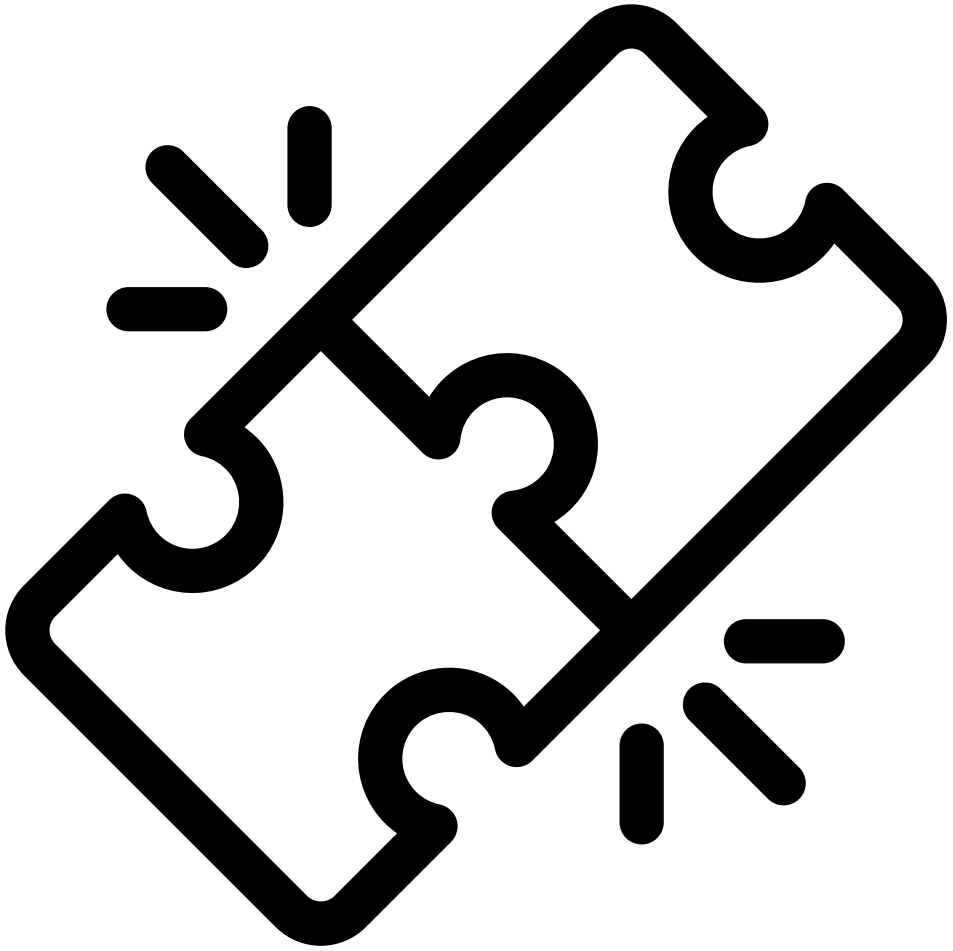


Image credit: Problem Solving by Symbolon from Noun Project (CC BY 3.0)

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)
```

[How to Choose a Partition wiki page]

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
```

[Using O2 GPU Resources wiki page]

Exercise 3: job runs, but fails

$ sbatch exercise3.sh

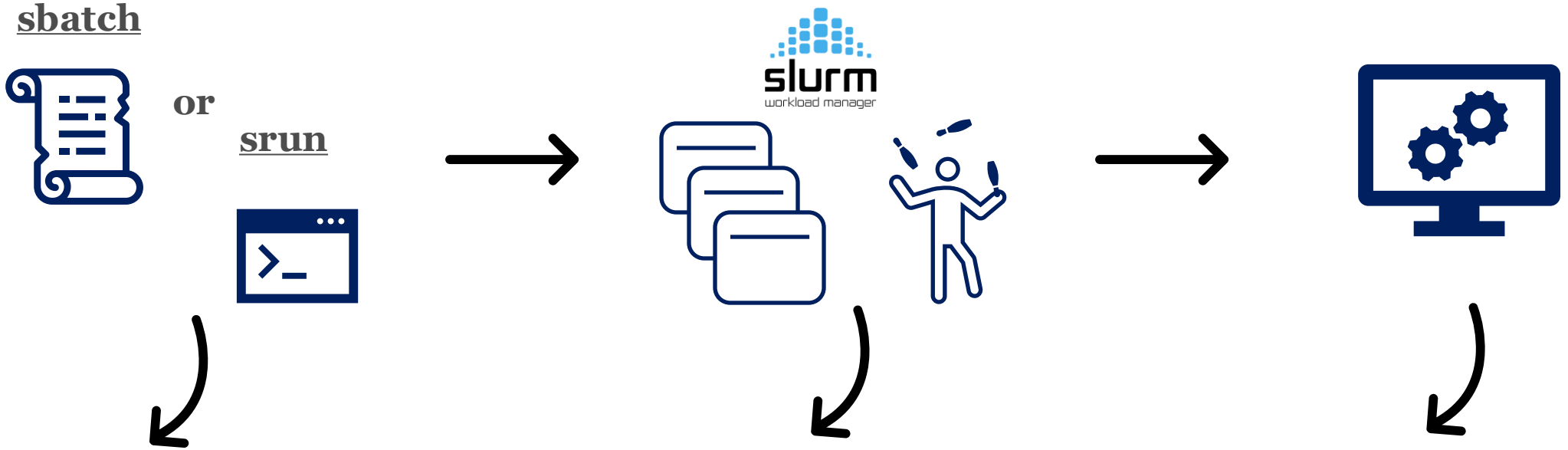
```
#!/bin/bash
#SBATCH -p short                          # Partition to submit to
#SBATCH -t 0-0:15                         # Time in days-hours:minutes format
#SBATCH -c 1                              # Number of cores requested
#SBATCH --mem=1G                          # Memory total in GB (see also --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

Revisiting a previous slide:

Three main types of problems with jobs:



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

An additional type of job problem

Check your job efficiency by

Reading weekly job usage report sent to your email!

Or use O2_jobs_report --report

4. Job runs but is inefficient

Requests more resources than are required, for example:
- Multiple cores for single threaded workflow
- 6 hours when the job finishes in 30 minutes
- 50GiB of RAM when the maximum used is 10GiB

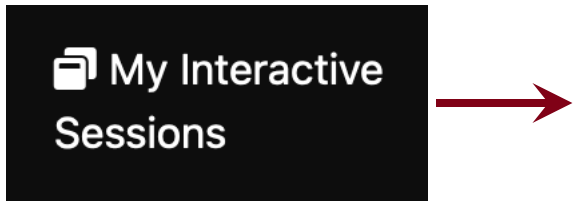
Fix by reducing job resource requests

O2 Portal: another way to access O2

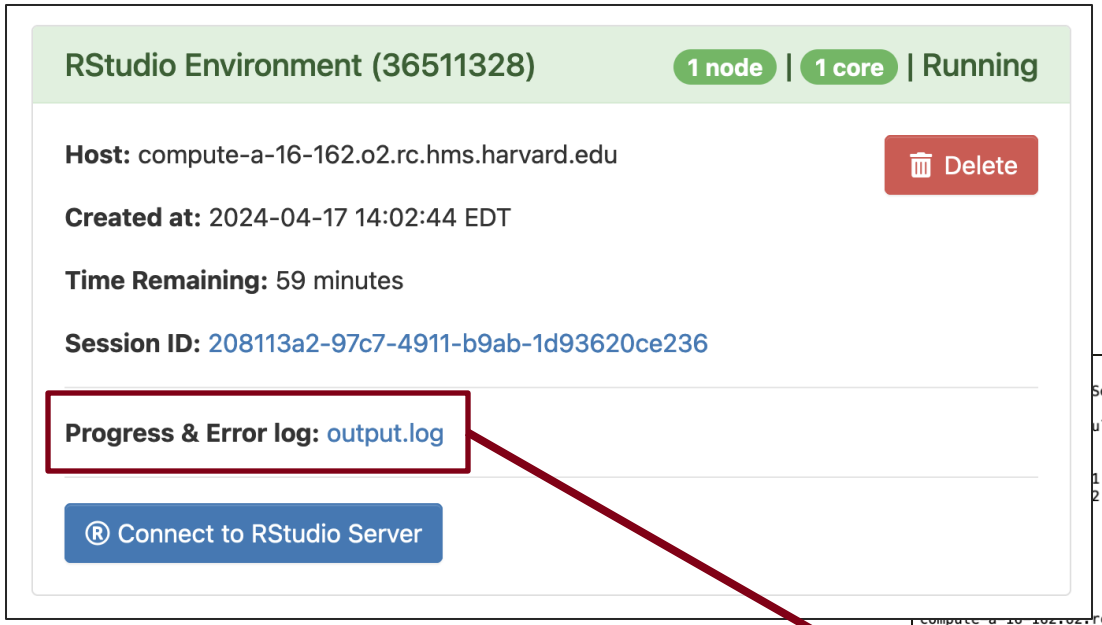
o2portal.rc.hms.harvard.edu

[O2 Portal docs](#) | [O2 Portal class slides](#)

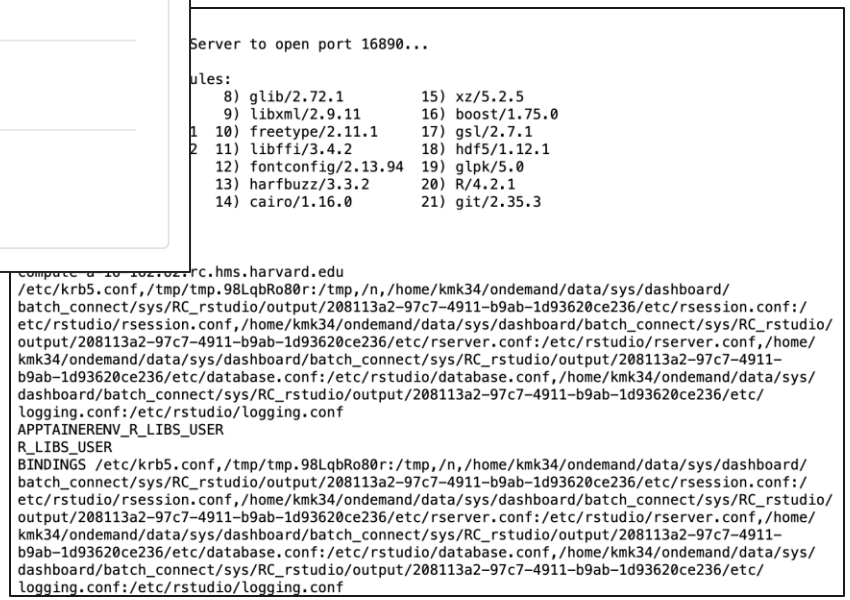
Debugging O2 Portal Jobs



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



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



Check for any error messages.

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?