Getting Started on the FASRC clusters with Command Line Interface

Learning objectives

- Log in via `ssh` to Cannon and FASSE
- How to start an interactive job with `salloc`
- How to submit a batch job with `sbatch`
- Check job status
- Cluster software modules

Login to Cannon and FASSE – `ssh`

Documentation: https://docs.rc.fas.harvard.edu/kb/terminal-access/

- Mac: Terminal, iTerm2
- Linux: Xterm or Terminal
- Windows
  - SSH client: Putty
  - Bash emulator: Git bash

Cannon

```
$ ssh jharvard@login.rc.fas.harvard.edu
Password:
Verification code:
```

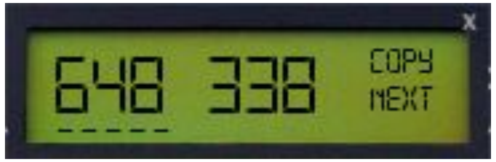
FASSE

```
$ ssh jharvard@fasselogin.rc.fas.harvard.edu
Password:
Verification code:
```

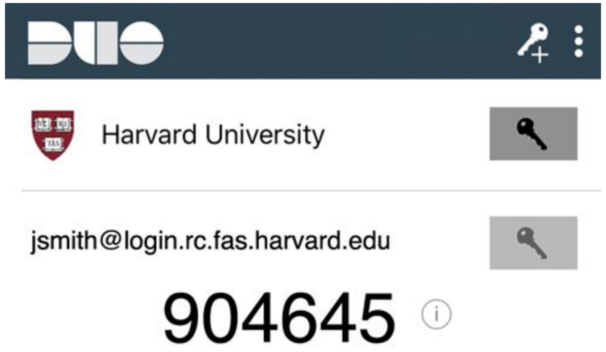
Login to Cannon and FASSE – 2 factor authentication

- Execute the ssh command, then:
  - Type your password (*cursor won't move!*), press enter
  - Type the 6-digit verification code (2-Factor Authentication)
    - Separate from HarvardKey
    - Updates token every 30 seconds
    - You can only use a token once

Java desktop app



648 338



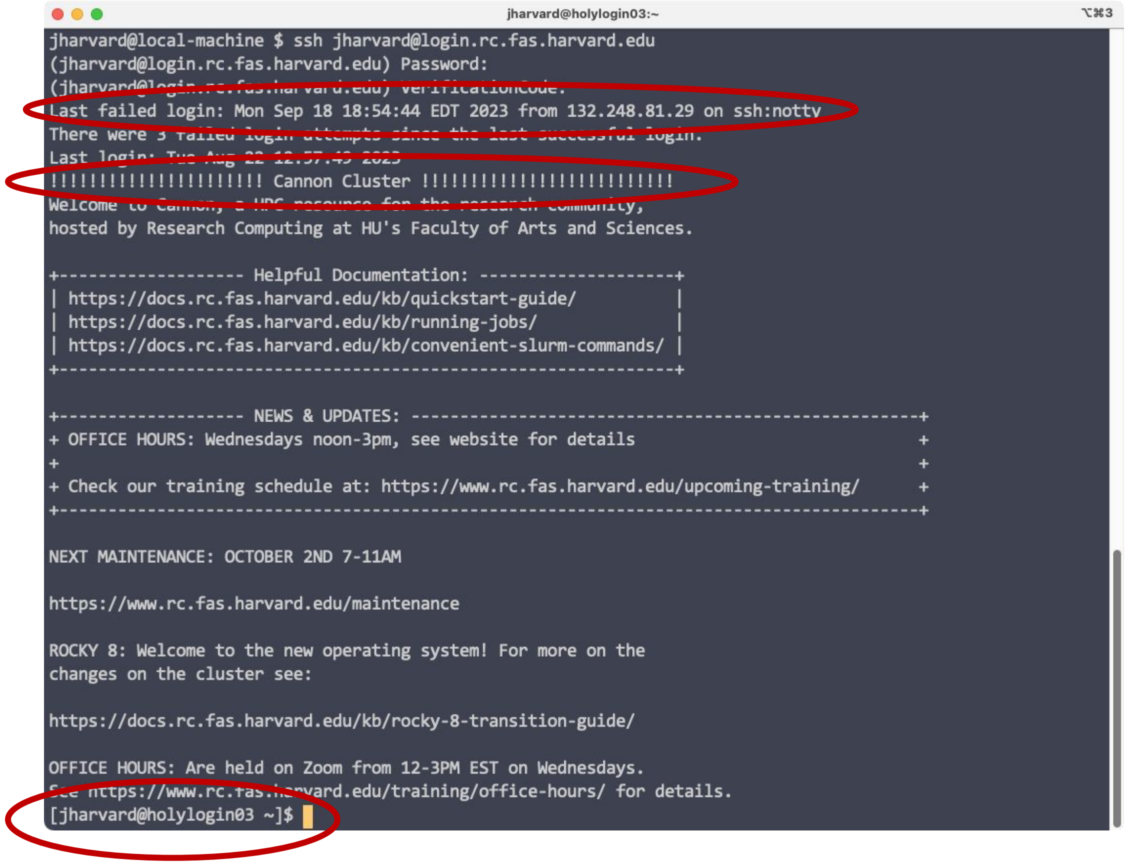
Harvard University

jsmith@login.rc.fas.harvard.edu

904645

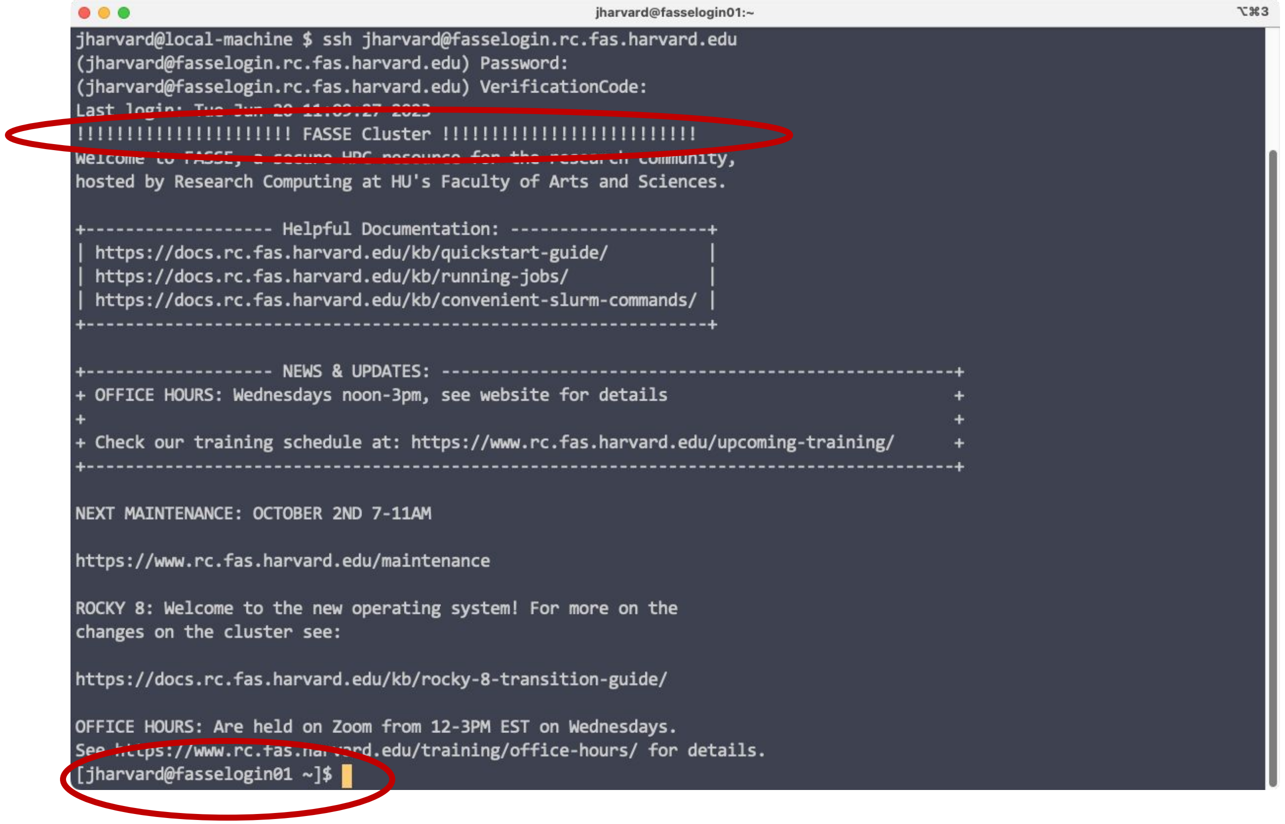
Login to Cannon and FASSE – at login node (1)

Cannon



```
jharvard@local-machine $ ssh jharvard@login.rc.fas.harvard.edu
(jharvard@login.rc.fas.harvard.edu) Password:
(jharvard@login.rc.fas.harvard.edu) VerificationCode:
Last failed login: Mon Sep 18 18:54:44 EDT 2023 from 132.248.81.29 on ssh:notty
There were 3 failed login attempts since the last successful login.
Last login: Tue Aug 22 12:57:49 2023
!!!!!!!!!!!!!!!!!!!!!! Cannon Cluster !!!!!!!!!!!!!!!!!!!!!!!!!
Welcome to Cannon, a HPC resource for the research community,
hosted by Research Computing at HU's Faculty of Arts and Sciences.

+------------------- Helpful Documentation: --------------------+
| https://docs.rc.fas.harvard.edu/kb/quickstart-guide/          |
| https://docs.rc.fas.harvard.edu/kb/running-jobs/              |
| https://docs.rc.fas.harvard.edu/kb/convenient-slurm-commands/ |
+---------------------------------------------------------------+

+------------------- NEWS & UPDATES: --------------------------------------------------+
+ OFFICE HOURS: Wednesdays noon-3pm, see website for details                         +
+                                                                                    +
+ Check our training schedule at: https://www.rc.fas.harvard.edu/upcoming-training/  +
+------------------------------------------------------------------------------------+

NEXT MAINTENANCE: OCTOBER 2ND 7-11AM

https://www.rc.fas.harvard.edu/maintenance

ROCKY 8: Welcome to the new operating system! For more on the
changes on the cluster see:

https://docs.rc.fas.harvard.edu/kb/rocky-8-transition-guide/

OFFICE HOURS: Are held on Zoom from 12-3PM EST on Wednesdays.
See https://www.rc.fas.harvard.edu/training/office-hours/ for details.
[jharvard@holylogin03 ~]$ 
```

FASSE



```
jharvard@local-machine $ ssh jharvard@fasselogin.rc.fas.harvard.edu
(jharvard@fasselogin.rc.fas.harvard.edu) Password:
(jharvard@fasselogin.rc.fas.harvard.edu) VerificationCode:
Last login: Tue Jun 20 11:09:27 2023
!!!!!!!!!!!!!!!!!!!!!! FASSE Cluster !!!!!!!!!!!!!!!!!!!!!!!!!
Welcome to FASSE, a secure HPC resource for the research community,
hosted by Research Computing at HU's Faculty of Arts and Sciences.

+------------------- Helpful Documentation: --------------------+
| https://docs.rc.fas.harvard.edu/kb/quickstart-guide/          |
| https://docs.rc.fas.harvard.edu/kb/running-jobs/              |
| https://docs.rc.fas.harvard.edu/kb/convenient-slurm-commands/ |
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OFFICE HOURS: Are held on Zoom from 12-3PM EST on Wednesdays.
See https://www.rc.fas.harvard.edu/training/office-hours/ for details.
[jharvard@fasselogin01 ~]$ 
```

Login to Cannon and FASSE – at login node (2)

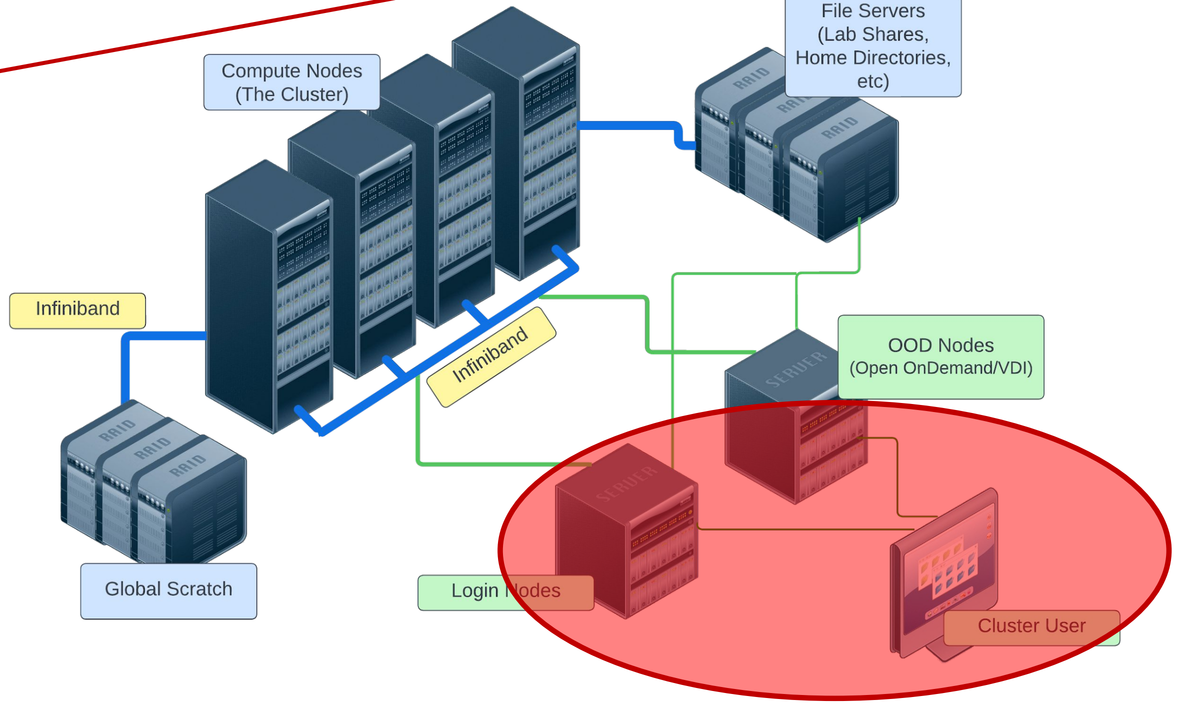
Cannon

```
[jharvard@boslogin01 ~]$
```

FASSE

```
[jharvard@fasselogin01 ~]$
```

Name of the login node assigned to you



Login vs. compute nodes

- Login nodes
  - limited to 1 core and 4G of memory
  - not designed for analysis
  - not anything compute- or memory-intensive
  - best practice is to request a compute node as soon as you login
- Compute node via interactive job
  - work a compute node interactively – testing, debugging, installing software
  - request resources from slurm using `salloc` command
  - session will only last as long as the network connection is active
  - cannot be idle for more than 1h, session will freeze

Interactive job on Cannon (1)

Requesting an interactive job

```
[jharvard@boslogin01 ~]$ salloc --partition test --mem-per-cpu 1G --time 01:00:00
salloc: Pending job allocation 2741096
salloc: job 2741096 queued and waiting for resources
salloc: job 2741096 has been allocated resources
salloc: Granted job allocation 2741096
salloc: Nodes holy7c02410 are ready for job
[jharvard@holy7c02410 ~]$
```

Name of the compute node assigned to you

`salloc` – slurm command to request interactive job

`--partition test` – requesting a compute node in a specific partition

`--mem-per-cpu 1G` – memory requested in GB (if no unit is specified, the default is MB)

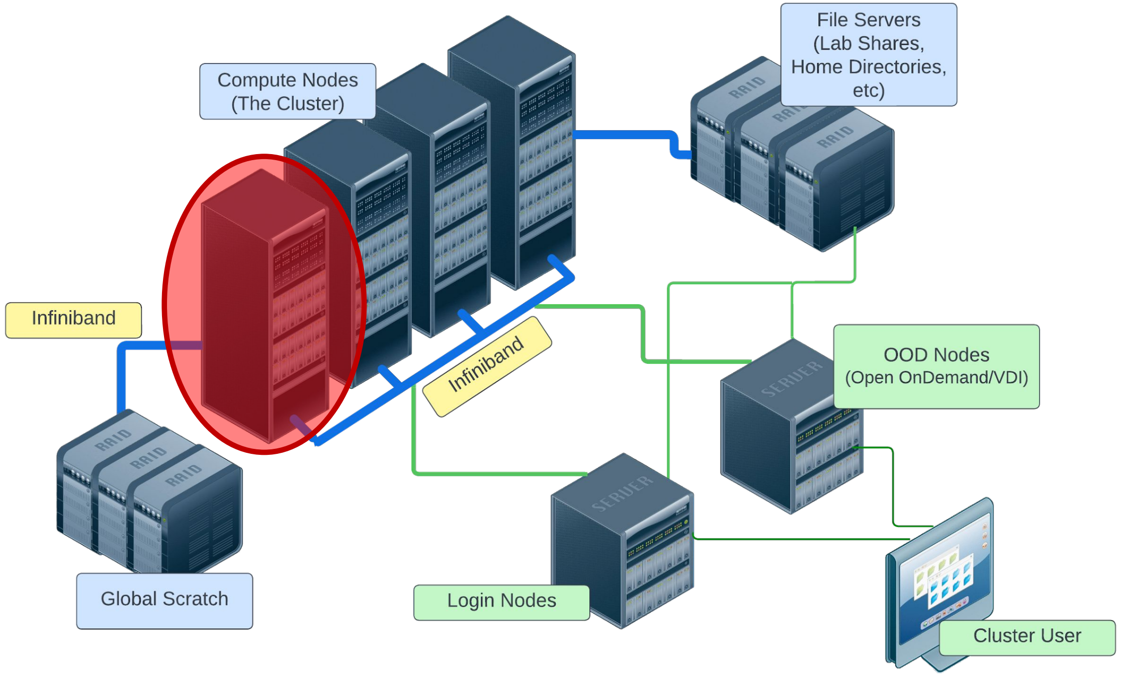
`--time 00:01:00` – time requested (1 hour, format HH:MM:SS or D-HH:MM)

Interactive job on Cannon (2)

Requesting an interactive job

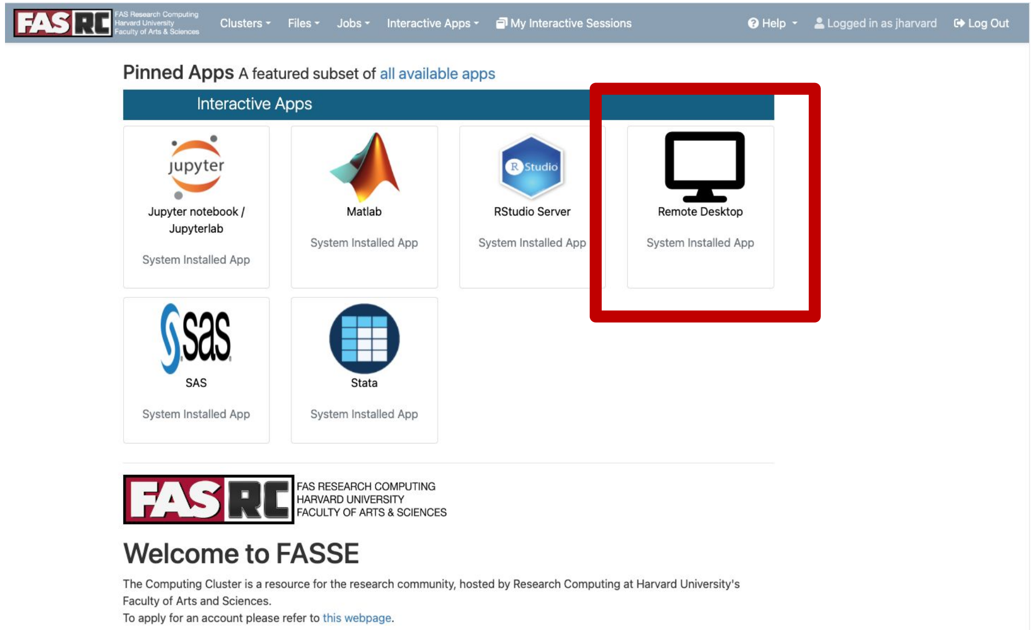
```
[jharvard@holy7c02410 ~]$
```

Name of the compute node assigned to you


File Servers (Lab Shares, Home Directories, etc)
Compute Nodes (The Cluster)
Infiniband
Infiniband
OOD Nodes (Open OnDemand/VDI)
Global Scratch
Login Nodes
Cluster User

Interactive job on FASSE

- You cannot request an interactive job on FASSE
- You must use Remote Desktop app on Open OnDemand https://fasseood.rc.fas.harvard.edu and launch terminal



Pinned Apps A featured subset of all available apps

Welcome to FASSE

The Computing Cluster is a resource for the research community, hosted by Research Computing at Harvard University's Faculty of Arts and Sciences.
To apply for an account please refer to this webpage.

Batch job

Documentation: https://docs.rc.fas.harvard.edu/kb/running-jobs/

- ○ Automate job
- ○ No interaction
- ○ Can close your terminal/laptop and job will keep running

- ○ Partitions
  - Cannon: https://docs.rc.fas.harvard.edu/kb/running-jobs/
  - FASSE: https://docs.rc.fas.harvard.edu/kb/fasse/

slurm script `runscript.sh`

slurm directives

```
#!/bin/bash
#SBATCH -J py_job          # Job name
#SBATCH -p test            # Partition(s) (separate with
                           # commas if using multiple)
#SBATCH -c 1               # Number of cores
#SBATCH -t 0-00:30:00      # Time (D-HH:MM:SS)
#SBATCH --mem=500M         # Memory
#SBATCH -o py_%j.o         # Name of standard output
file
#SBATCH -e py_%j.e         # Name of standard error file

# load software environment
module load python/3.10.12-fasrc01

# print a statement
echo "This is our test slurm script"

# execute python code
python hello_world.py
```

Test first!!

ALWAYS test the job submission script first:

- To ensure the job will complete without errors
- To ensure you understand the resource needs and have requested them appropriately

Submitting a batch job

```
[jharvard@boslogin01 python]$ sbatch runscript.sh
Submitted batch job 2742999
[jharvard@boslogin01 python]$
```

Job monitoring – `sacct`

Documentation:

- `sacct`: slurm accounting database
  - every 30 sec the node collects the amount of cpu and memory usage that all of the process ID are using for a given job. After the job ends this data is sent to slurm database
- Common flags (i.e., options)
  - `-j jobid or --name=jobname`
  - `-S starttime YYYY-MM-DD and –E endtime YYYY-MM-DD`
  - `-o output_options`
  - See slurm docs for more options: https://slurm.schedmd.com/sacct.html

```
[jharvard@boslogin01 ~]$ sacct --format=JobID,Jobname,partition,state,time,start,end,elapsed,MaxRss,MaxVMSize,nnodes,ncpus,nodelist --units=G -j 2742999
JobID           JobName  Partition      State  Timelimit               Start                 End    Elapsed     MaxRSS  MaxVMSize   NNodes      NCPUS        NodeList
------------ ---------- ---------- ---------- ---------- ------------------- ------------------- ---------- ---------- ---------- -------- ---------- ---------------
2742999          py_job       test  COMPLETED   00:30:00 2023-09-21T12:03:20 2023-09-21T12:03:21   00:00:01                              1          1     holy7c02410
2742999.bat+      batch             COMPLETED            2023-09-21T12:03:20 2023-09-21T12:03:21   00:00:01      0.01G      0.21G        1          1     holy7c02410
2742999.ext+     extern             COMPLETED            2023-09-21T12:03:20 2023-09-21T12:03:21   00:00:01      0.00G      0.17G        1          1     holy7c02410
```

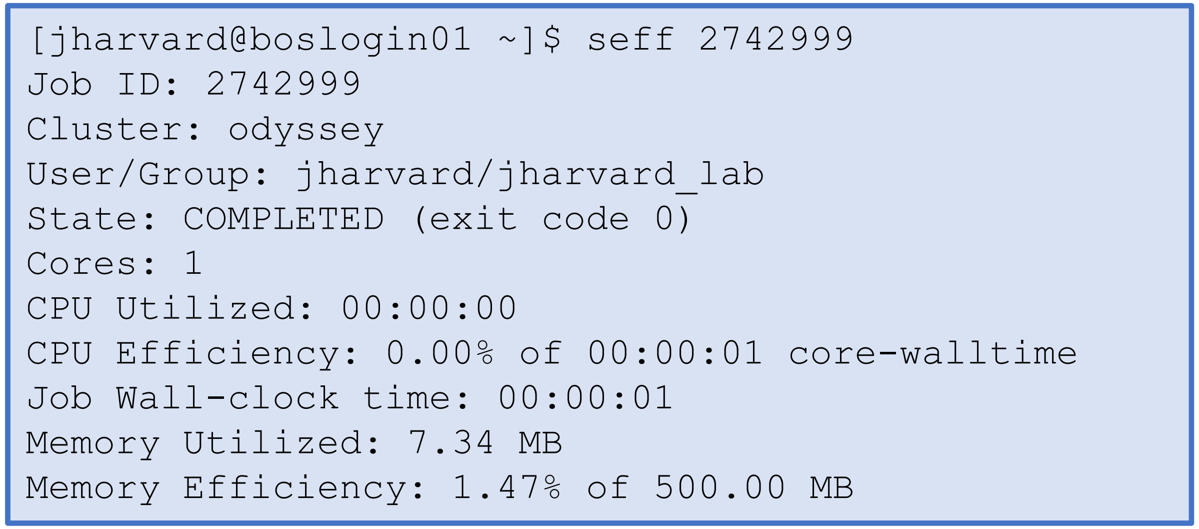
Memory usage

1. Run a test batch job
2. Check memory usage after the job has completed (with `sacct` command)

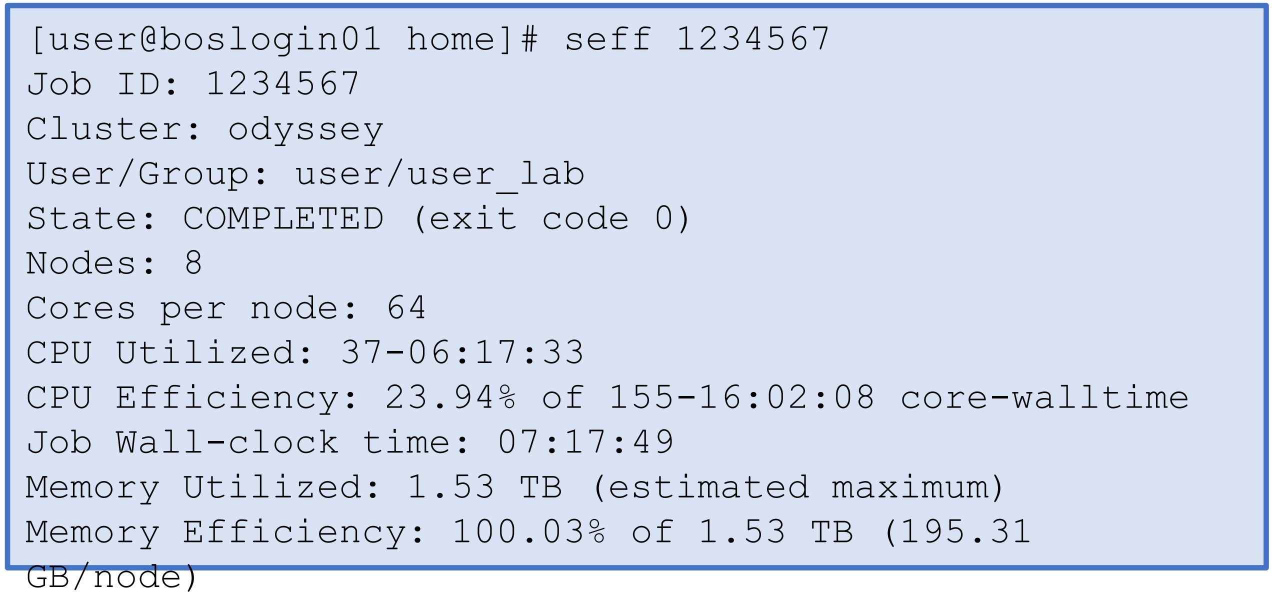
```
[jharvard@boslogin01 ~]$ sacct -j 2742999 -o ReqMem,MaxRSS
    ReqMem     MaxRSS
---------- ----------
      500M
                7512K
                4348K
[jharvard@boslogin01 ~]$ sacct -j 2742999 -o ReqMem,MaxRSS --units=G
    ReqMem     MaxRSS
---------- ----------
     0.49G
                0.01G
                0.00G
```

Job efficiency summary – seff

1. Run a test batch job
2. Check job efficiency after the job has completed (with seff command)



```
[jharvard@boslogin01 ~]$ seff 2742999
Job ID: 2742999
Cluster: odyssey
User/Group: jharvard/jharvard_lab
State: COMPLETED (exit code 0)
Cores: 1
CPU Utilized: 00:00:00
CPU Efficiency: 0.00% of 00:00:01 core-walltime
Job Wall-clock time: 00:00:01
Memory Utilized: 7.34 MB
Memory Efficiency: 1.47% of 500.00 MB
```



```
[user@boslogin01 home]# seff 1234567
Job ID: 1234567
Cluster: odyssey
User/Group: user/user_lab
State: COMPLETED (exit code 0)
Nodes: 8
Cores per node: 64
CPU Utilized: 37-06:17:33
CPU Efficiency: 23.94% of 155-16:02:08 core-walltime
Job Wall-clock time: 07:17:49
Memory Utilized: 1.53 TB (estimated maximum)
Memory Efficiency: 100.03% of 1.53 TB (195.31
GB/node)
```

Partitions

`spart` allows you to see which partitions you have access to

Documentation: https://docs.rc.fas.harvard.edu/kb/convenient-slurm-commands/

```
[jharvard@boslogin02 ~]$ spart
Partition               State     Cores     GPUs      Average Mem/Node(GB)     Nodes     Time Limit
bigmem                  UP        448       0         2015                     4         3-00:00:00
bigmem_intermediate     UP        192       0         2015                     3
14-00:00:00
gpu                     UP        2304      144       1007                     36        3-00:00:00
gpu_requeue             UP        9184      698       772                      156       3-00:00:00
gpu_test                UP        896       112       503                      14        12:00:00
intermediate            UP        1344      0         1007                     12
14-00:00:00
remoteviz               UP        32        0         377                      1         3-00:00:00
sapphire                UP        21504     0         1007                     192       3-00:00:00
serial_requeue          UP        88300     690       438                      1457      3-00:00:00
shared                  UP        13824     0         188                      288       3-00:00:00
test                    UP        1344      0         1007                     12        12:00:00
ultramem                DRAIN     192       0         2015                     3         3-00:00:00
```

Software – LMOD module system

- Software is loaded incrementally using modules, to set up your shell environment (e.g., `PATH`, `LD_LIBRARY_PATH`, and other environment variables)
- Why add `module load` commands in a slurm batch script? (instead of `.bashrc` file)
  - Keeps your interactive working environment simple
  - Is a record of your research workflow (reproducible research!)
  - Keep `.bashrc` module loads sparse, lest you run into software and library conflicts

```
module load matlab/R2022b-fasrc01 # recommended command
module load matlab        # loads most recent version
module list            # show loaded modules
module purge              # unload all loaded modules
module spider matlab          # search for modules with matlab in the name
module display matlab/R2022b-fasrc01  # show the details of the module
```

Spack

- For software that does not have a module, you can install it with Spack: https://docs.rc.fas.harvard.edu/kb/spack/
- Install Spack in a Holyoke storage location, such as `holylabs`
    - Package installation is best done in an interactive session with 8 cores 12GB as Spack needs more resources

```
salloc --partition test --time 0-04:00 --mem 12G --cpus-per-task 8
```

Survey

Please, fill out our course survey. Your feedback is essential for us to improve our trainings!!

http://tinyurl.com/FASRCsurvey

FASRC documentation

- FASRC docs: https://docs.rc.fas.harvard.edu/
- GitHub User_codes: https://github.com/fasrc/User_Codes/
- Getting help
  - Office hours: https://www.rc.fas.harvard.edu/training/office-hours/
  - Ticket
    - Portal: http://portal.rc.fas.harvard.edu/rcrt/submit_ticket (requires login)
    - Email: rchelp@rc.fas.harvard.edu

Upcoming training sessions

Training calendar: https://www.rc.fas.harvard.edu/upcoming-training/

Getting started on the FASRC clusters with Open OnDemand

- Audience
  - New users not familiar with command-line interface
  - Wants to use a GUI
- Requirements
  - Single-node jobs
  - Working FASRC account with cluster access
- Content
  - Access Open OnDemand
  - Launch Jupyter, Rstudio Server, Remote Desktop
  - Install Rstudio Server packages
  - Install python packages for Jupyter
  - Launch software from Remote Desktop

Thank you :)

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