



Getting started on the FASRC Cannon Cluster





Learning Objectives

- Describe the structure of a compute cluster
- Log in to Cannon
- Demonstrate how to start an interactive session and a batch job with the SLURM job scheduler
- Query job metadata
- Cluster storage
- Cluster software modules
- VDI Open OnDemand





Cluster Architecture







Cluster Terminology

- <u>Supercomputer/High Performance Computing (HPC) cluster</u>: A collection of similar computers connected by a high speed interconnect that can act in concert with each other
- <u>Node</u>: A computer in the cluster, an individual motherboard with CPU, memory, local hard drive
- <u>CPU</u>: Central Processing Unit, it can contain multiple computational cores (processors)
- <u>Core</u>: Basic unit of compute that runs a single instruction of code (a single process)
- <u>GPGPU/GPU</u>: General Purpose Graphics Processing Unit, a GPU designed for supercomputing.





https://docs.rc.fas.harvard.edu/kb/quickstart-guide/

Cluster Quick Start Guide

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This guide will provide you with the basic information needed to get up and running on the FASRC cluster for simple command line access. If you'd like more detailed information, each section has a link to fuller documentation

PREREQUISITES

1. Get a FASRC account using the account request tool.

Before you can access the cluster you need to request a Research Computing account.

See How Do I Get a Research Computing Account for instructions if you do not yet have an account.

See the account confirmation email for instructions on setting your password and getting started.





Once you have an account you can use the Terminal to connect to Cannon

- Mac: Terminal
- 🗴 Linux: Xterm or Terminal
- Windows: SSH client Putty or Bash Emulator Git Bash

\$ ssh username@login.rc.fas.harvard.edu

- ssh stands for Secure SHell
- ssh is a protocol for data transfer that is secure, i.e the data is encrypted as it travels between your computer and the cluster (remote computer)
- Commonly used commands that use the ssh protocol for data transfer are, scp and sftp





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Cannon

Login issues? See https://rc.fas.harvard.edu/resources/support/

Password: Verification code:





https://docs.rc.fas.harvard.edu/kb/quickstart-guide/

Once you have run the ssh command:

- Enter your password (*cursor won't move!*)
- Add a verification code (2-Factor Authentication)

2. Setup OpenAuth for two factor authentication



Open Auth

Once you have your new FASRC account, you will need to set up our OpenAuth tool for two-factor authentication.

See the OpenAuth Guide for instructions if you have not yet set up OpenAuth.

For troubleshooting issues you might have, please see our troubleshooting page.

OpenAuth is 2-factor authentication separate from HarvardKey and updates the token every 30 seconds





| ● ● ●rsk394 — rkhetani@holylogin03:~ — ssh rkhetani@login.rc.fas.harvard.edu — 92×40 | |
|---|------------------|
| IIIIIIIIIIIIIIIII Cannon IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII | |
| 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://rc.fas.harvard.edu/resources/quickstart-guide/ https://rc.fas.harvard.edu/running-jobs/ https://rc.fas.harvard.edu/convenient-slurm-commands/ ++ | (|
| <pre>+ NEWS & UPDATES:</pre> | + + + + |
| NEXT MAINTENANCE: NOVEMBER 4TH 7-11AM | |
| https://www.rc.fas.harvard.edu/maintenance | |
| CANNON: Cannon is live! See the Running Jobs page for information about the updated partitions. | |
| https://www.rc.fas.harvard.edu/resources/running-jobs/#Slurm_partitions | |
| For more about the new cluster see: | |
| https://www.rc.fas.harvard.edu/fasrc-cluster-refresh-2019/ | |
| GENERAL: The general partition has been decommissioned. Please use the shared partition. For high memory jobs use bigmem. | |
| WINTER MAINTENANCE DECEMBER 3RD 7AM-5PM: We are doing an all day major maintenance on December 3rd which will involve all running jobs being cancelled. More details forthcoming soon. Please plan accordingly. | |

You have logged into the login node!







- Login node:
 - not designed for analysis
 - not anything compute- or memory-intensive
 - best practice is to request a compute node as soon as you log in
- Interactive session:
 - work on a compute node "interactively"
 - request resources from SLURM using the salloc command
 - session will only last as long as the remote connection is active

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Access to resources on a compute node

Simple Linux Utility for Resource Management - SLURM job scheduler:

- Fairly allocates access to resources to users on compute nodes
- Manages a queue of pending jobs; ensures that no single user or group monopolizes the cluster
- Ensures users do not exceed their resource requests
- Provides a framework for starting, executing, and monitoring batch jobs





Access to resources on a compute node

Requesting an interactive session:

```
[joesmith@holylogin03 ~]$ salloc -p test --mem 100 -t 0-01:00
```

salloc - is how interactive sessions are started with SLURM

-p test - requesting a compute node in a specific partition*

--mem 100 - memory requested in MB

-t 0-1:00 - time requested (1 hour)

* Partitions are groups of computers that are designated to perform specific types of computing. More on next slide







Slurm Job Script (for sbatch)



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





Test first

ALWAYS test the job submission script first:

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

Submitting a batch job:

```
[joesmith@boslogin01 ~]$ sbatch runscript.sh
Submitted batch job 20801712
[joesmith@boslogin01 ~]$
```





Partitions on Cannon

| Partitions: | shared | gpu | test | gpu_test | serial_requeue | gpu_requeue | bigmem | unrestricted | pi_lab |
|-----------------------|--------|----------------|-------|----------------|----------------|-------------|----------|--------------|--------|
| Time Limit | 7 days | 7 days | 8 hrs | 1 hrs | 7 days | 7 days | no limit | no limit | varies |
| # Nodes | 530 | 15 | 16 | 1 | 1930 | 155 | 6 | 8 | varies |
| # Cores / Node | 48 | 32 + 4 V100 | 48 | 32 + 4 V100 | varies | varies | 64 | 64 | varies |
| Memory / Node (GB) | 196 | 375 | 196 | 375 | varies | varies | 512 | 256 | varies |

Learn more about a partition:

\$ sinfo -p shared

\$ scontrol show partition shared





sacct overview

- 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 the given job. After the job ends this data is set to slurmdb.
- Common flags
 - -j *jobid* or --name=*jobname*
 - -S YYYY-MM-DD and -E YYYY-MM-DD
 - -o ouput_options

JobID, JobName, NCPUS, Nnodes, Submit, Start, End, CPUTime, TotalCPU, ReqMem, MaxRSS, MaxVMSize, State, Exit, Node





Memory Usage

Run a test batch job and check memory usage after the job has completed (with the "sacct" Slurm command)

Example:

| [joesmith@boslogin01 | ~]\$ sacct -j 3 | 3937435 - o I | ReqMem, MaxRSS |
|----------------------|-----------------|----------------------|----------------|
| ReqMem M | axRSS | | |
| 1000Mn 1000Mn 2 | 86712K | | |
| | | | |

or 286712KB = 286.712MB





seff overview

[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)





A Fairshare score

- determines what priority a user/group has to run their jobs
- is calculated for a group using various factors, including what resources/partition of the cluster groups have access.
- goes from 1 to 0 with a middle point of 0.5





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- determines what priority a user/group has to run their jobs
- is calculated for a group using various factors, including what resources/partition of the cluster groups have access.
- goes from 1 to 0 with a middle point of 0.5
 - 1.0: Unused. The account has not run any jobs recently.
 - \square 1.0 > f > 0.5: Under-utilization. The account is underutilizing their granted Share.
 - 0.5: Average utilization. The account on average is using exactly as much as their granted Share.
 - \Box 0.5 > f > 0: Over-utilization. The account has overused their granted Share.
 - 0: No share left. The account has vastly overused their granted Share.

More information: https://docs.rc.fas.harvard.edu/kb/fairshare/





A Fairshare score

- determines what priority a user/group has to run their jobs
- is calculated for a group using various factors, including what resources/partition of the cluster groups have access.
- goes from 1 to 0 with a middle point of 0.5
- dynamically updated based on usage
- ensures that no single user or group monopolizes the cluster resources





• Accounts on the cluster are assigned to a primary lab "group" based on their affiliation.

[user1@holyitc01 ~]\$ groups

test_lab cluster_users





• Accounts on the cluster are assigned to a primary lab "group" based on their affiliation.

test lab cluster users

[user1@holyitc01 ~]\$ groups

sshare can be used to check the current fairshare for a whole group or a single user

```
[user1@holyitc01 ~]$ sshare --account=test lab -a
Account User RawShares NormShares RawUsage EffectvUsage FairShare
test lab
         244
                       0.001363 45566082 0.000572 0.747627
test lab user1 parent
                      0.001363 8202875 0.000572 0.747627
test lab user2 parent
                       0.001363 248820 0.000572 0.747627
test lab user3 parent
                       0.001363 163318 0.000572 0.747627
test lab user4 parent
                       0.001363 18901027 0.000572 0.747627
test lab user5 parent
                       0.001363
                                 18050039 0.000572
                                                   0.747627
```

More information: https://docs.rc.fas.harvard.edu/kb/fairshare/

| | | Storag | FASRE | | |
|------------------|---|-------------------------------------|--|---|---------------------------------|
| | Home Directories | Lab Directory (Startup) | Local Scratch | Global Scratch | Tier Storage |
| Mount Point | /n/home#/ \$USER | /n/holylabs/pi_lab | /scratch | /n/\$SCRATCH | /n/pi_lab |
| Size Limit | 100GB | 1- 4TB | 70GB/node | 2.4PB total | Based on Tier |
| Availability | All cluster nodes + Desktop/laptop | All cluster nodes | Local compute node only | All cluster nodes | All cluster nodes/ mountable |
| Retention Policy | Indefinite | Indefinite | Job duration | 90 days | Indefinite |
| Backup | Hourly snapshot + Daily Offsite | No backup | No backup | No backup | Depending on Tier |
| Performance | Moderate. Not suitable for high I/O | Moderate. Not suitable for high I/O | Suited for small file I/O intensive jobs | Appropriate for large file I/O intensive jobs | Depending on Tier |
| Cost | Free | Free max of 4TB | Free | Free | Paid |

Tier Storage: https://www.rc.fas.harvard.edu/services/data-storage/





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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)

| # recommended |
|----------------------------------|
| <pre># most recent version</pre> |
| <pre># show loaded modules</pre> |
| <pre># unload all modules</pre> |
| |

Software search capabilities similar to module-query are also available on the RC Portal: <u>https://portal.rc.fas.harvard.edu/apps/modules</u>

Module loads best placed in SLURM batch scripts:

- 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





VDI - Open OnDemand

For applications that need a GUI: <u>https://vdi.rc.fas.harvard.edu</u>

Supports:

- Remote Desktop
- Jupyter Notebooks
- Rstudio
- Matlab

Notes:

- Need to be on the RC VPN to use
- Sessions are submitted as jobs on the cluster and thus use fairshare but also can run on any partition



FASSE Cluster

determination.

The FAS Secure Environment (FASSE) is a secure multi-tenant cluster environment to provide Harvard researchers access to a secure enclave for analysis of sensitive datasets with DUA's and IRB's classified as Level 3.

RVARD

VERI

https://policy.security.harvard.edu/

https://docs.rc.fas.harvard.edu/kb/ data-use-agreements/

https://security.harvard.edu/

https://docs.rc.fas.harvard.edu/kb/f asse/

| - | | | а |
|---------|--|--------------------------|---------------------|
| PUBLIC | Public information (Level 1) | Level 1 Harvard Systems | [1 6 |
| | | | C |
| LOW | Low Risk information (Level 2) is information the University has chosen to | Low Risk Systems (L2) | E E L |
| | keep confidential but the disclosure of which would not cause material harm. | | ŀ |
| MEDIUM | Medium Risk information (Level 3) could cause risk of material harm to individuals or the University if disclosed or compromised | Medium Risk Systems (L3) | <u>(</u> II V |
| | | | Ē |
| нідн | High risk information (Level 4) would likely cause serious harm to individuals or the | ► High Risk Systems (L4) | L F |
| | University if disclosed or compromised. | | |
| LEVEL 5 | Reserved for extremely sensitive Research Data that requires special handling per IRB | ► Level 5 Systems | |





Request Help - Resources

- <u>https://docs.rc.fas.harvard.edu/kb/support/</u>
 - Documentation
 - https://docs.rc.fas.harvard.edu/
 - Portal
 - http://portal.rc.fas.harvard.edu/rcrt/submit_ticket
 - Email
 - rchelp@rc.fas.harvard.edu
 - Office Hours
 - Wednesday noon-3pm https://harvard.zoom.us/j/255102481
 - Consulting Calendar
 - https://www.rc.fas.harvard.edu/consulting-calendar/
 - Training
 - https://www.rc.fas.harvard.edu/upcoming-training/

