HARVARD UNIVERSITY

FAS RC

FAS Research Computing
Division of Science
https://rc.fas.harvard.edu

New Users Training

Introduction to FASRC clusters

Learning objectives 1 – FASRC account

- Learn how to request an FASRC account
- Activate your new account
- How to modify your account or add groups

Learning objectives 2 – Intro to HPC

- What is high-performance computing (HPC)? How is it different from a desktop/laptop?
- Laptop vs. Cannon
- Why HPC?
- FASRC clusters
- Cluster architecture
- Job scheduler
- Choose compute resources for jobs
  - Memory, cores
  - Partitions, file systems
- Storage
- Data Management
- Cluster customs and responsibilities

Learning objectives 3 – Documentation and help

- FASRC docs
- GitHub User_codes
- Office hours
- Tickets

Request FASRC account

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

1. Request an account using Account Request Tool https://portal.rc.fas.harvard.edu/request/account/new
   - Use Harvard Key option
2. Set FASRC password https://portal.rc.fas.harvard.edu/p3/pwreset/
3. Set two-factor authentication https://docs.rc.fas.harvard.edu/kb/openauth/
4. Set FASRC VPN (needed for mounting storage, OOD, level 3 data, license server access) https://docs.rc.fas.harvard.edu/kb/vpn-setup/
5. Review intro training

How to modify your account

- Change labs: https://docs.rc.fas.harvard.edu/kb/change-lab-group/
- Add a lab:
  - Portal gives access to lab storage: https://docs.rc.fas.harvard.edu/kb/additional-groups/
  - If you work for more than 1 PI, and need access to lab slurm account (more on slurm later), send a ticket
- Never request a second account!!
- Membership in the FASRC mailing-list is required
- Account needs to be used in the last 12 months to be active
- After 12 months of inactivity
  - Account is disabled, but nothing is deleted
  - Can be reactivated with PI's/admin approval

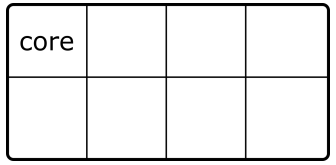
What is HPC?

- HPC: High performance computing
- HPC: biggest and fastest computing machines right now
- Supercomputers: rule of thumb - at least 100 times as powerful as a PC (personal computer)
- Jargon: other terms
  - Supercomputing
  - Cyberinfrastructure (CI)
  - Cluster computing

Laptop vs. Cannon

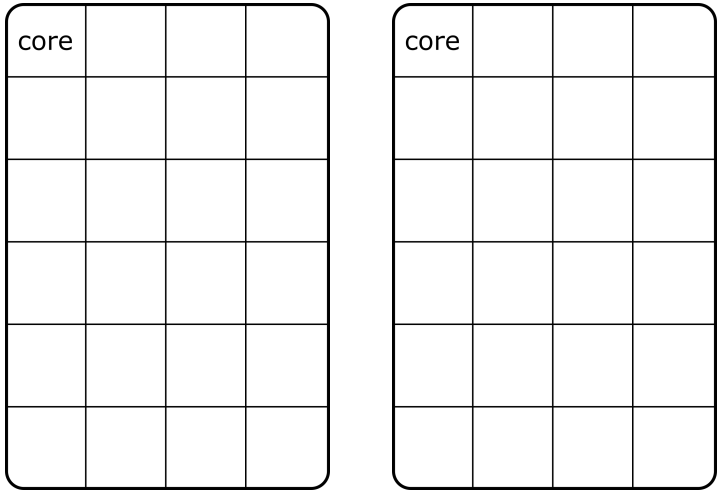
MacBook Pro

- 1 CPU (processor)
- 4-12 cores per CPU
- Memory: 16-96 GB



Cannon typical nodes

- 2 CPUs
- 24-32 cores **per CPU**
- Memory: 184-2000 GB
- **1260+ nodes!!!**



Why HPC?

- Size: problems that can't fit on a desktop/laptop, for example 500+ GB of RAM or 100s of cores
- Speed: problems that take months on a laptop may take a few hours on a supercomputer
- Amount: need 1000s of runs

45 miles/hour

600 miles/hour

What about FASRC clusters?

Massachusetts Green HPC Center (MGHPCC)

Cannon cluster

From https://www.servethehome.com/the-harvard-cannon-powered-by-lenovo-neptune/

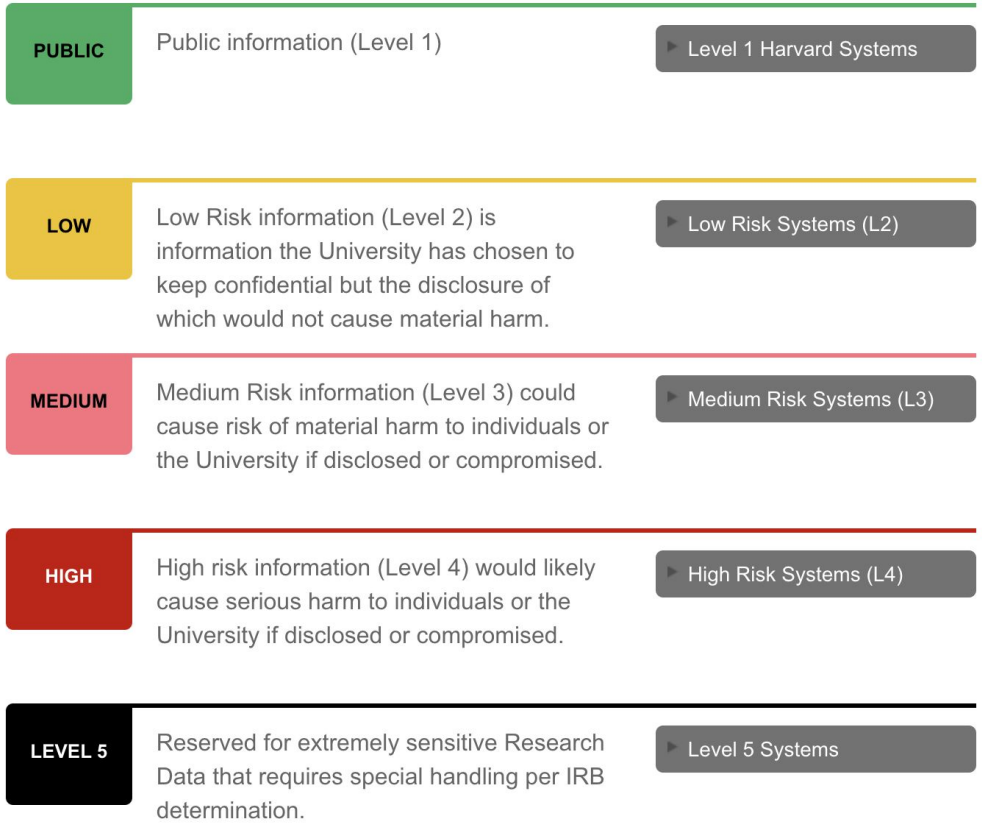
FASRC clusters: Cannon and FASSE

Cannon

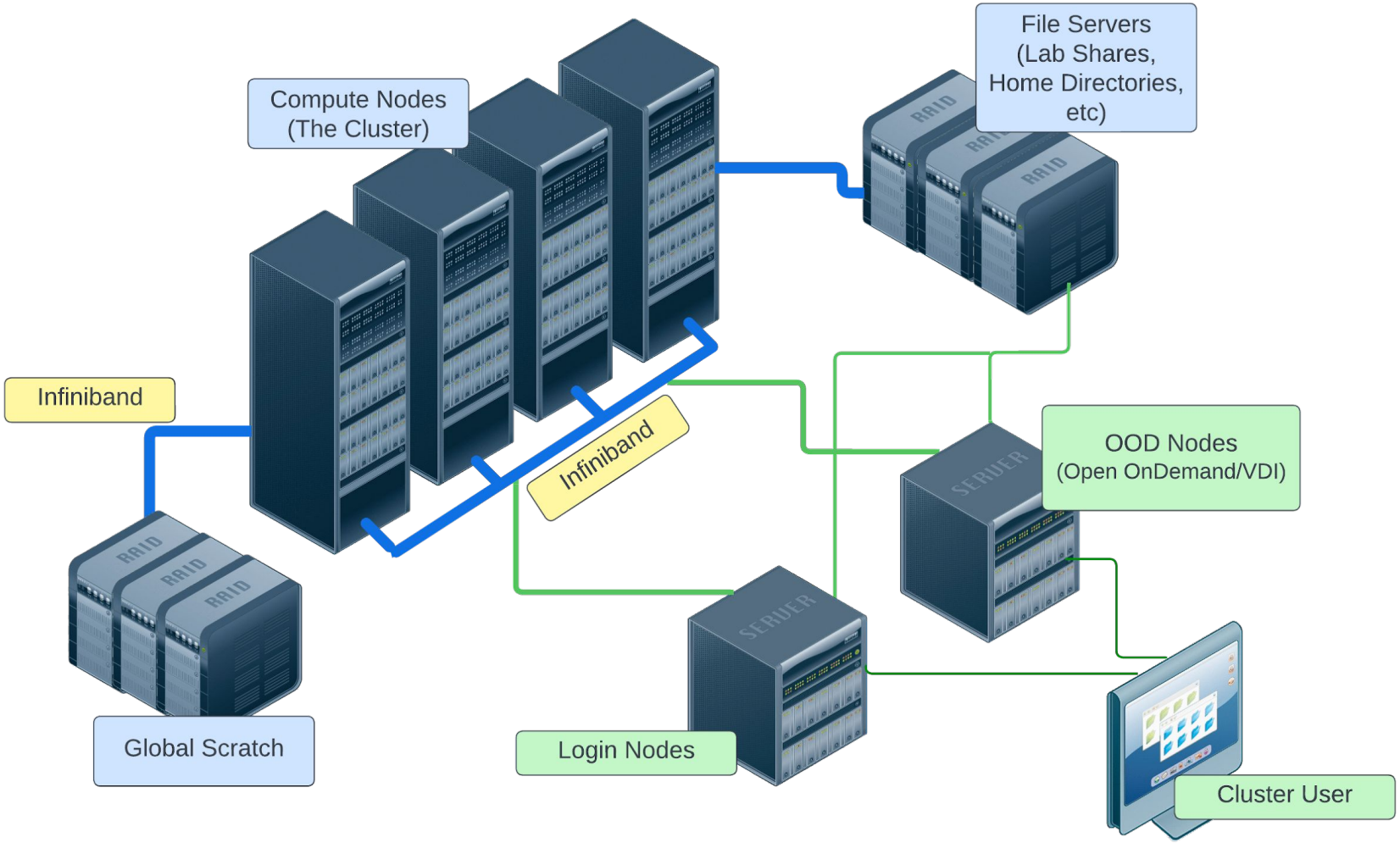
- General purpose
- Only level 1 and 2 data

FASSE

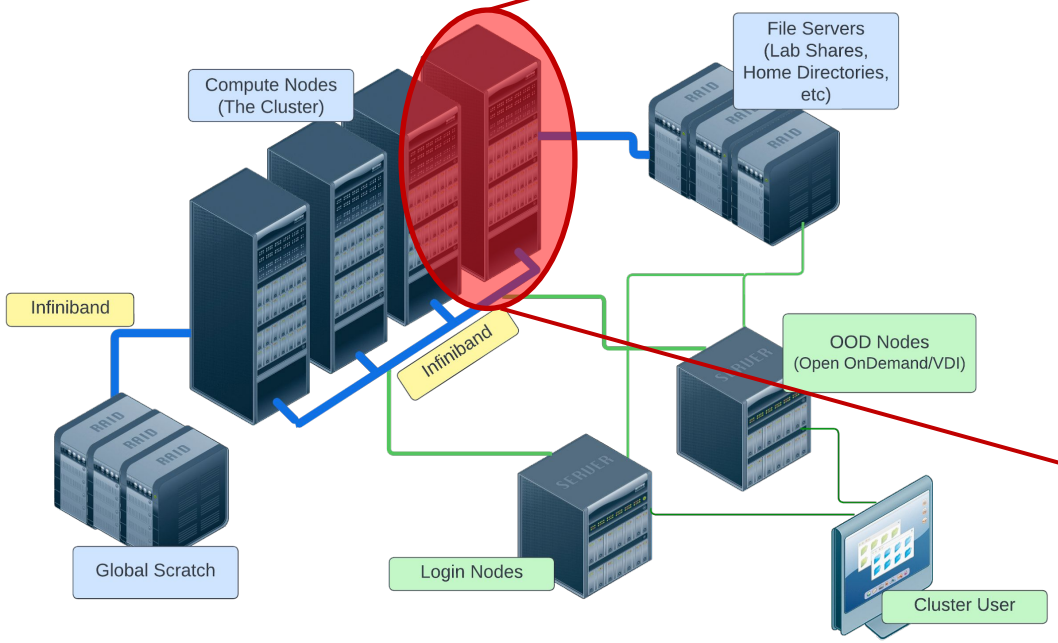
- FAS Secure Environment
- Secure multi-tenant environment
- Analysis of sensitive datasets with DUAs and IRBs
- Level 3 data, no level 4 data
- PI/lab responsibility to know their data
- https://policy.security.harvard.edu/
- https://docs.rc.fas.harvard.edu/kb/data-use-agreements/
- https://security.harvard.edu/
- https://docs.rc.fas.harvard.edu/kb/fasse/

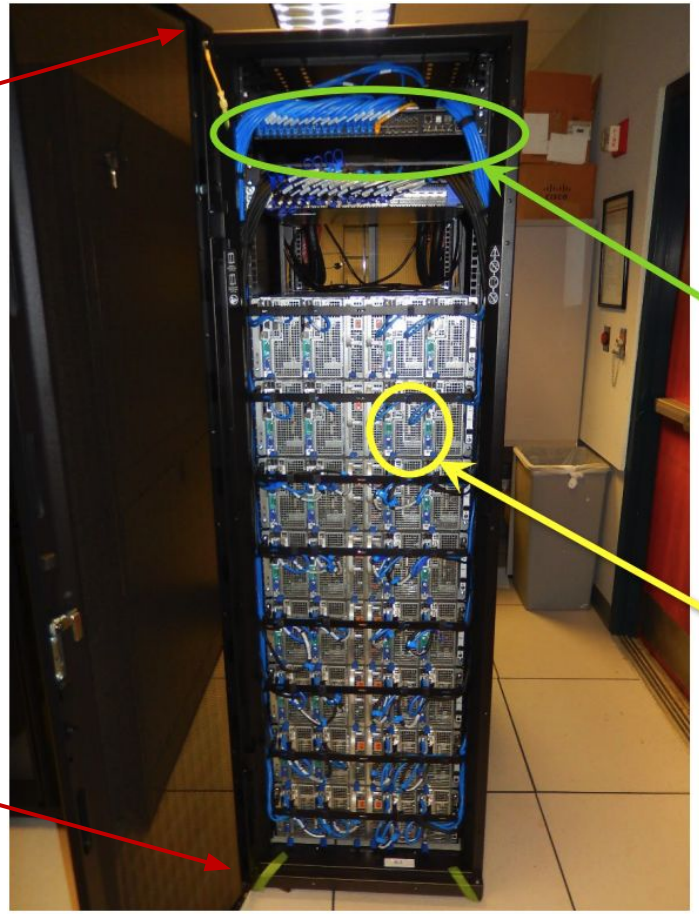


Cluster architecture



Rack



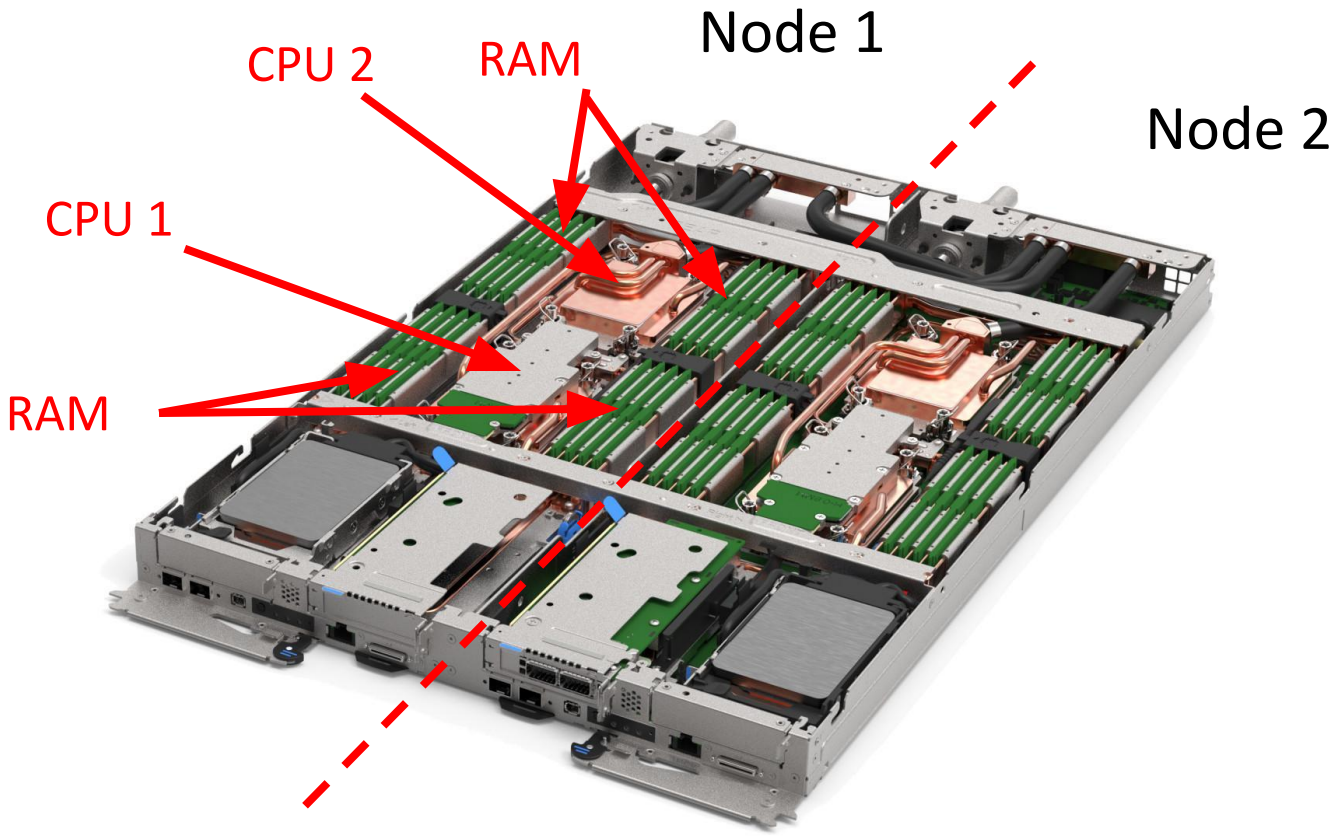


Interconnect:
Infiniband
Switch

Compute
Node

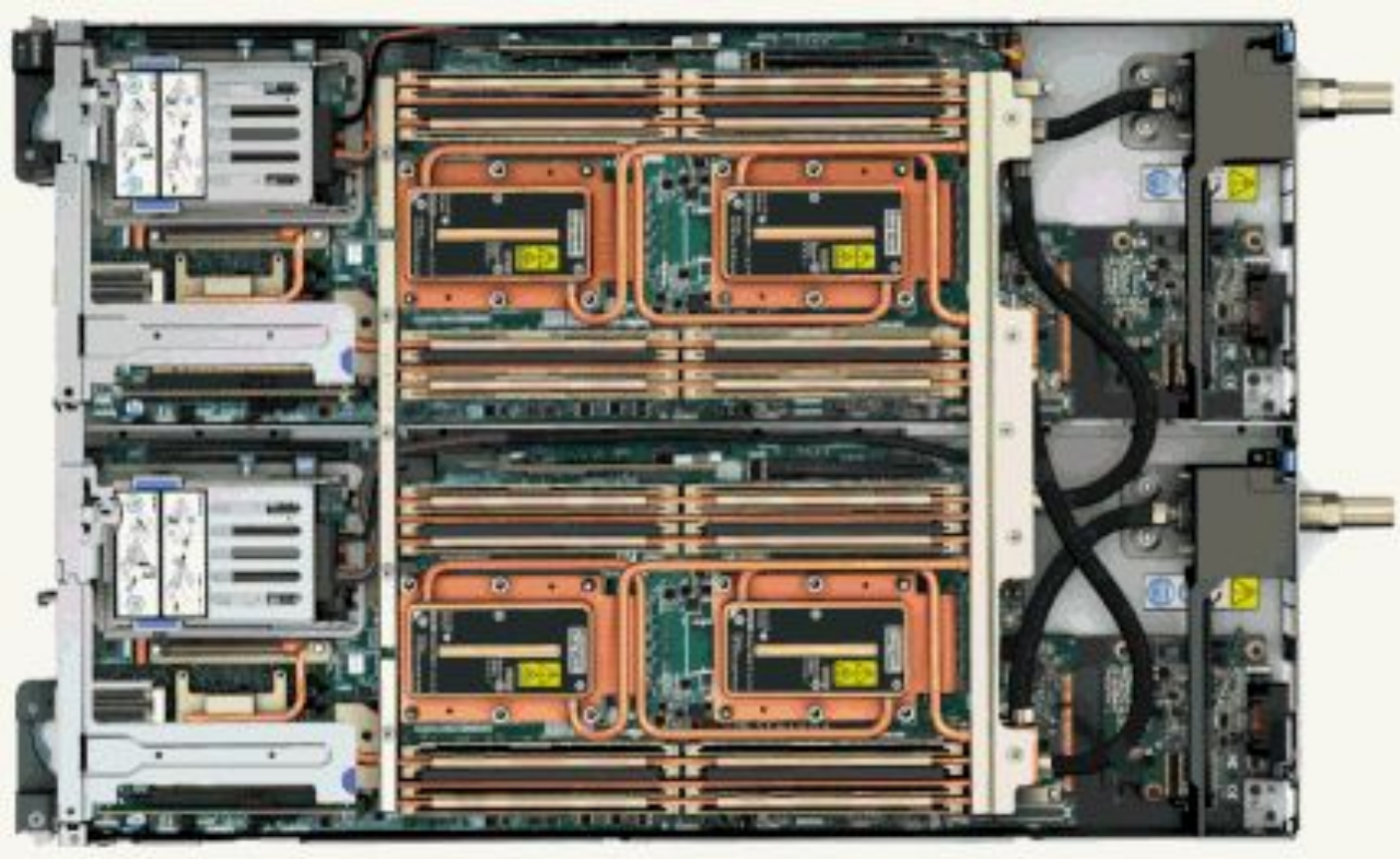
From HPC@LSU training
(http://www.hpc.lsu.edu/training/weekly-materials/2022-Fall/HPC_UserEnv1_Fall2022.pdf)

Node



From https://lenovopress.lenovo.com/lp1603-thinksystem-sd650-v3-server

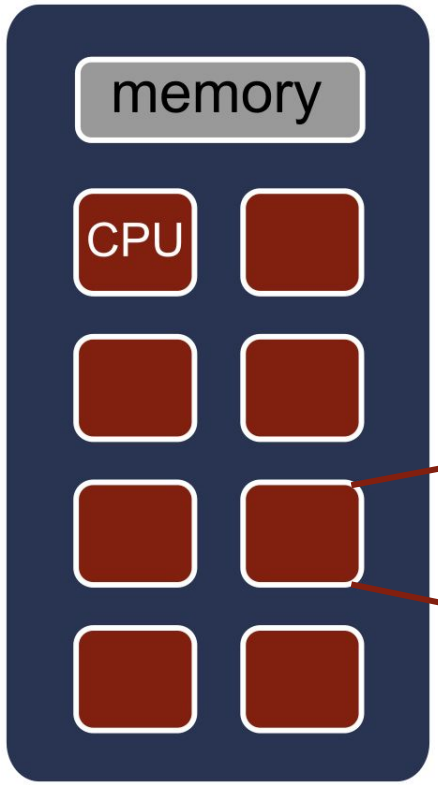
Node water cooling



From https://www.rc.fas.harvard.edu/blog/cannon-makes-top-500-list/

Node, processors, core

Node: a computer in the cluster

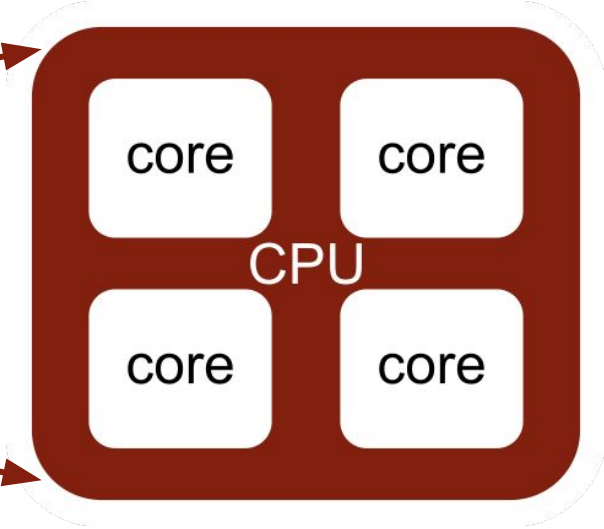


CPU

- Central processing unit, processor
- Can have many cores

Cores

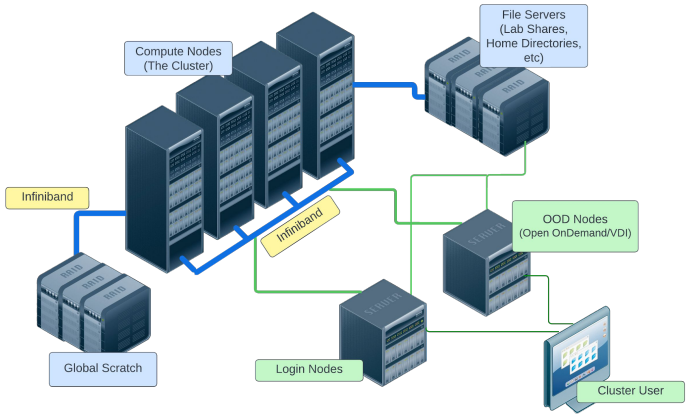
- Basic unit of compute
- Runs a single instruction of code



Nomenclature summary

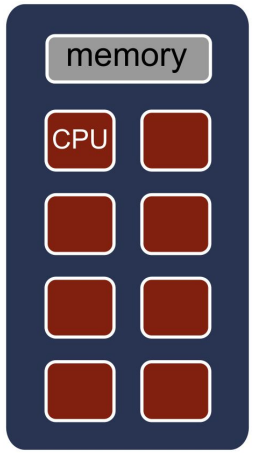
Cluster

Top level unit of a supercomputer



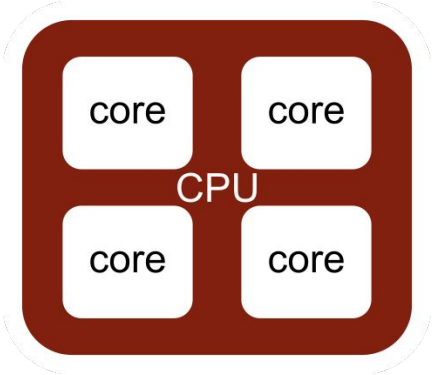
Node

One host in the cluster
(i.e., one computer)



Core

Basic unit of computer



New term: Job

A user's request to use a certain amount of resources for a specific amount of time

Glossary: https://docs.rc.fas.harvard.edu/kb/glossary/

Adapted from HPC@LSU training (http://www.hpc.lsu.edu/training/weekly-materials/2021-Summer/HPC_UserEnv_2021_Summer_session_2.pdf)

Job scheduler

- The Cluster is a multi-tenant environment, so how can everyone use it fairly?
- Job scheduler!
- Slurm: Simple Linux Utility for Resource Management
  - Manages job queue for a cluster of resources
  - Prioritizes jobs
  - Provides status of running, queue, completed and failed jobs
  - Determines the order jobs are executed
  - On which node(s) jobs are executed

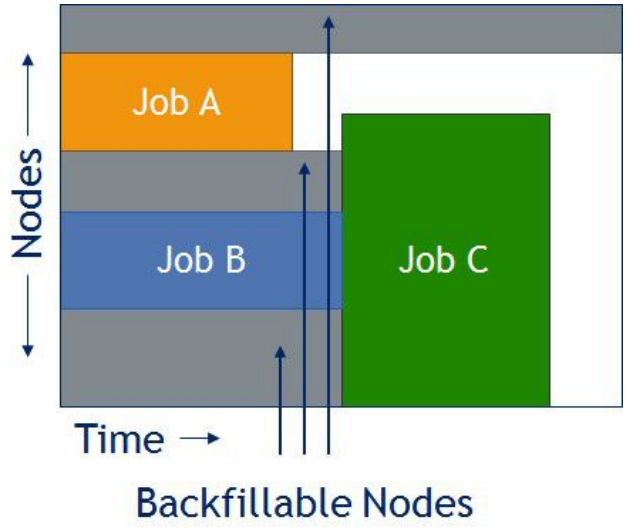
Adapted from HPC@LSU training (http://www.hpc.lsu.edu/training/weekly-materials/2021-Summer/HPC_UserEnv_2021_Summer_session_2.pdf)

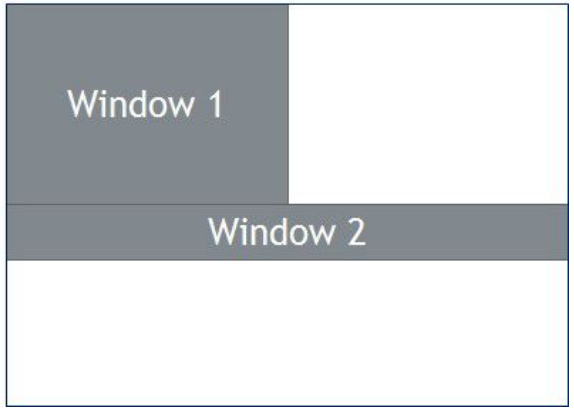
Job management philosophy

- Prioritize workload
- Backfill idle node to maximize cluster use

Job Priority

- **Not** first come, first served
- Job with higher priority scheduled ahead of jobs with lower priority
- Priority depends on
  - Fairshare
  - Amount of time pending
  - Group priority

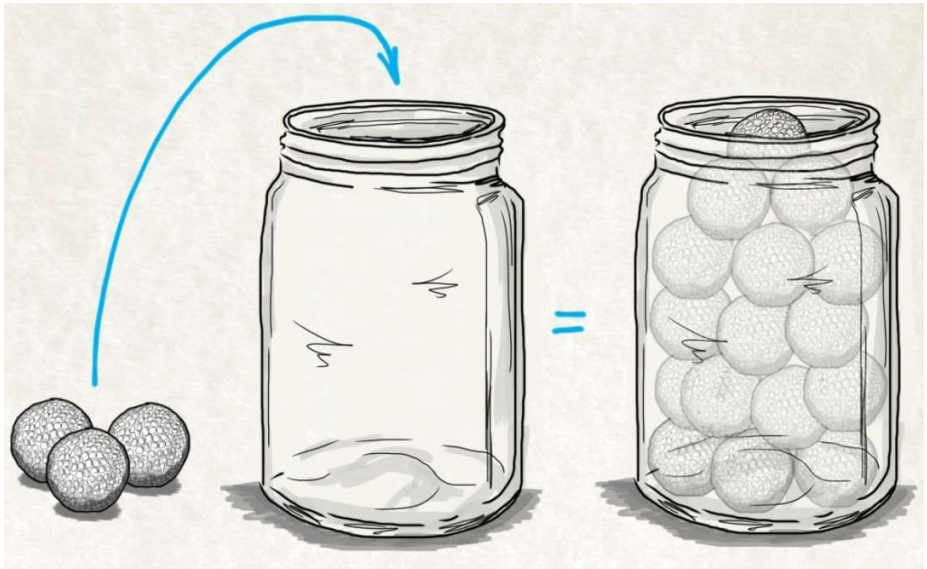




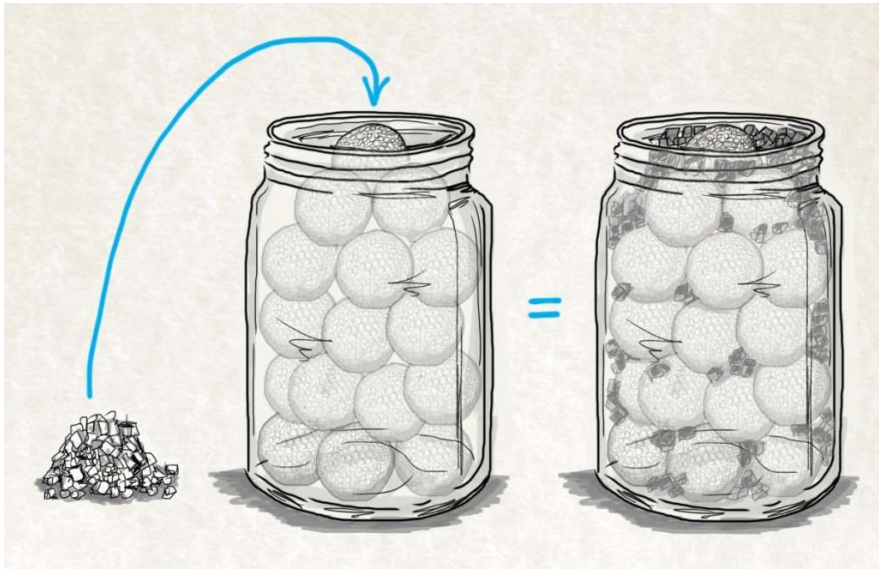
Adapted from HPC@LSU training (http://www.hpc.lsu.edu/training/weekly-materials/2021-Summer/HPC_UserEnv_2021_Summer_session_2.pdf)

How to maximize cluster usage?

1. Fill in high-priority jobs



2. Backfill with low-priority jobs



Adapted from HPC@LSU training (http://www.hpc.lsu.edu/training/weekly-materials/2021-Summer/HPC_UserEnv_2021_Summer_session_2.pdf)

Choosing computational resources

- How do we choose memory, cores, partitions, and file systems?
- First time ever running on a cluster?
  - Run a test case choosing similar resources as the machine you are currently using
  - Check how efficient your job was and adjust it accordingly
- Increasing a job/analysis/simulation?
  - Run for a small test case
  - Increase size by 1.5, 2.0, 2.5x and check how job scaled
  - Then you can have a rough estimation of how much a first trial production job of ~10x would require

Cannon partitions

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

Partitions	shared	gpu	test	gpu_test	serial_requeue	gpu_requeue	bigmem	ultramem	intermediate	bigmem_intermediate	unrestricted	**pi_lab**
Time Limit	3 days	3 days	12 h	12 h	3 days	3 days	3 days	3 days	3-14 days	3-14 days	no limit	**varies**
# Nodes	264	25	27	10	1264	138	30	3	12	4	8	**varies**
# Cores / Node	48	64 + 4 A100	48	32 + 4 V100	varies	varies	64	64	48	64	64	**varies**
Memory / Node (GB)	196	375	196	375	varies	varies	499	2000	184	499	256	**varies**

FASSE partitions

Documentation: https://docs.rc.fas.harvard.edu/kb/fasse/

Partitions	fasse	fasse_gpu	test	serial_requeue	fasse_bigmem	ultramem	remoteviz	**pi_lab**
Time Limit	7 days	7 days	12 h	7 days	7 days	7 days	7 days	**varies**
# Nodes	42	4	5	65	6	1	1	**varies**
# Cores / Node	48	32 + 4 V100	48	varies	64	64	32	**varies**
Memory / Node (GB)	184	373	5	varies	499	2000	373	**varies**

Storage

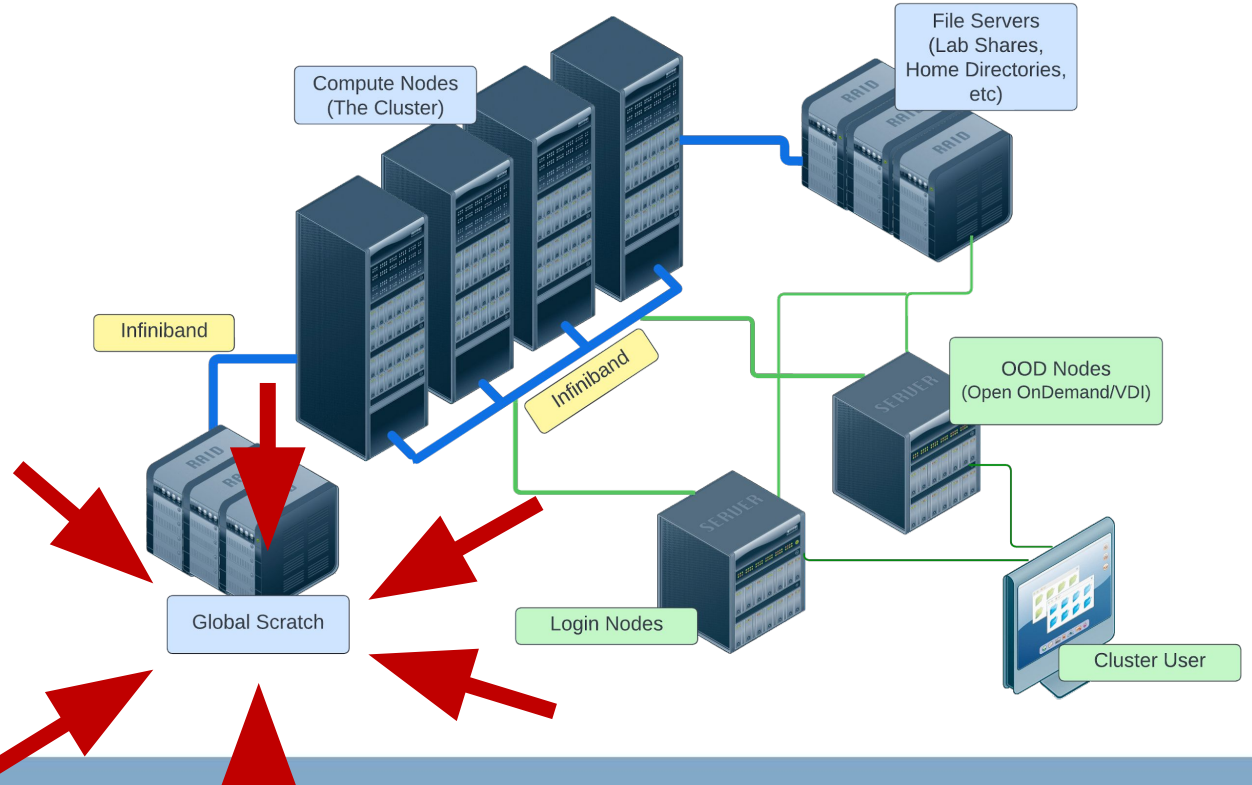
Tier storage documentation: https://www.rc.fas.harvard.edu/services/data-storage/

	Home Directories	Lab Directory (Startup)	Local Scratch	Global Scratch	Tier Storage
Mount Point	$HOME /n/home#/$USER /n/home_fasse/$USER	/n/holylabs/pi_lab	/scratch	$SCRATCH /n/holyscratch01/pi_lab	/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

Storage schematics

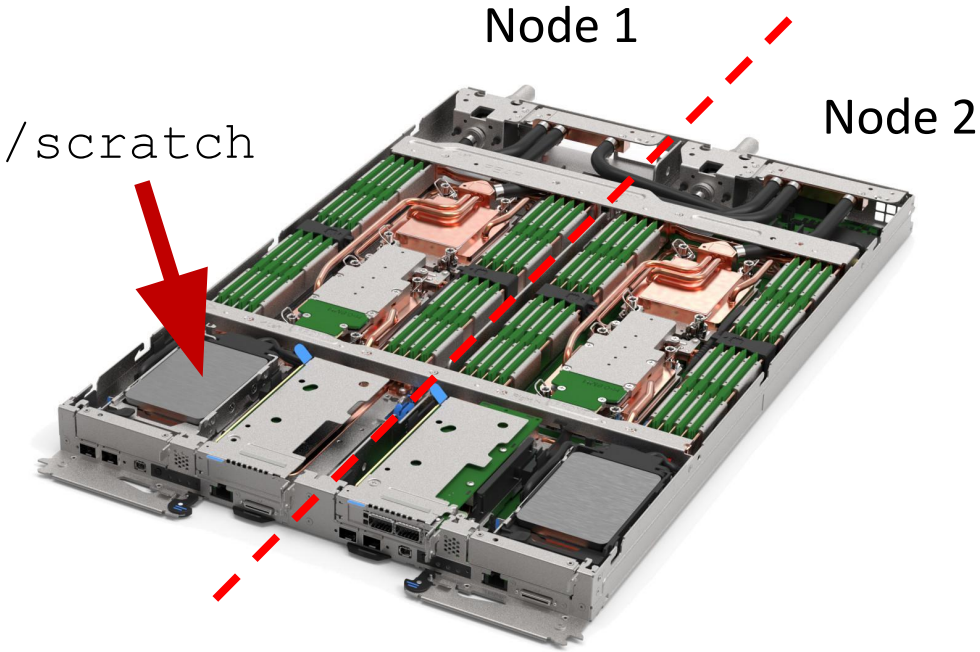
Global Scratch

- Networked scratch
- Global variable: `$SCRATCH`
- Path: `/n/holyscratch01/pi_lab`



Local Scratch

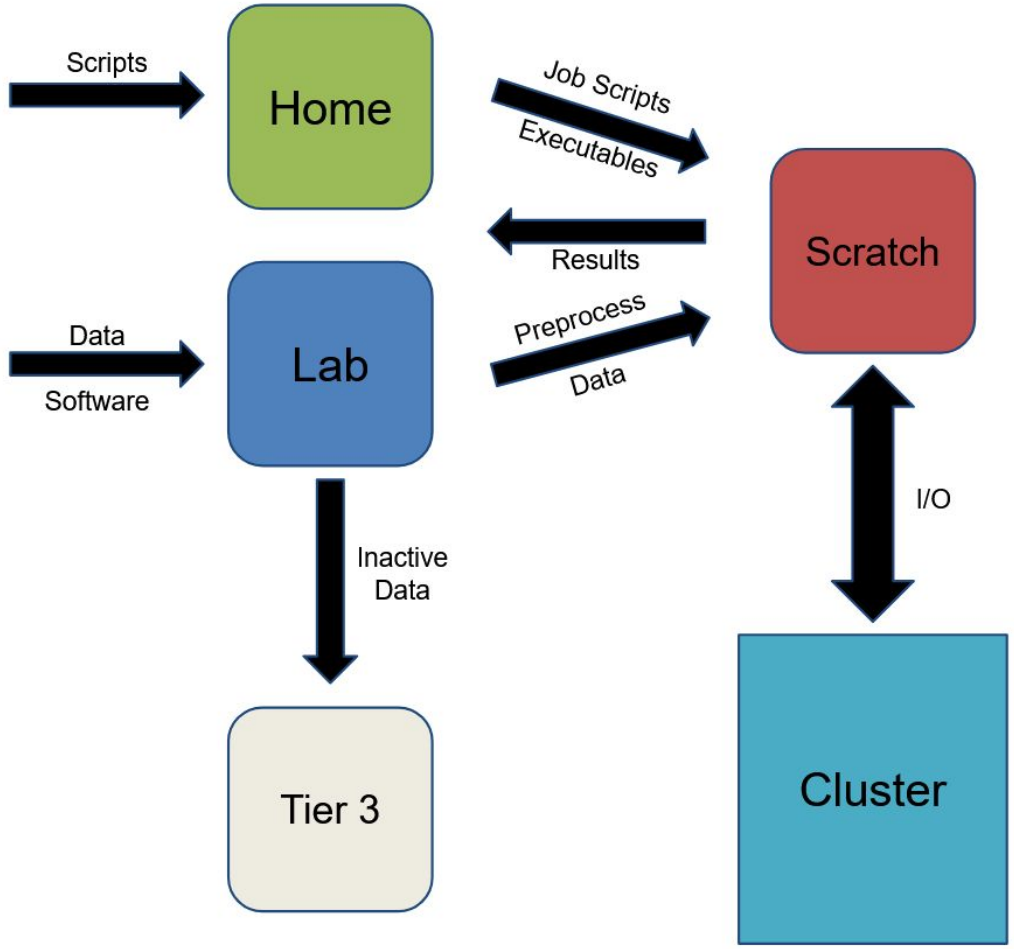
- Storage on the node
- Path: `/scratch`



From https://lenovopress.lenovo.com/lp1603-thinksystem-sd650-v3-server

Data management

- Home
  - Backed up with daily snapshots (up to 2 weeks)
  - "Valuable" and small code
- Global scratch
  - Temporary storage
  - Copy job scripts and executables for jobs
  - Input data
  - Output results
- Lab storage
  - Permanent storage
  - If you have code here and not backed up, use version control (git)!!



Cluster customs and responsibilities (1)

Documentation: https://docs.rc.fas.harvard.edu/kb/responsibilities/

- Don’t run anything on the login nodes
- Be as accurate as possible for memory requests
- Keep job counts reasonable: 10,000 job limit per user (scheduled or running)
- Request at least 10 minutes
- Don’t overwhelm scheduler: wait 0.5 to 1 sec for `sbatch` and `sacct` commands

Cluster customs and responsibilities (2)

Documentation: https://docs.rc.fas.harvard.edu/kb/responsibilities/

- Use appropriate partition
- Use `serial_requeue` and `gpu_requeue` when possible
- Heavy I/O should be done on `/scratch` and `$SCRATH`
- Keep at most 1000 files per directory (i.e., folder)
- No production work on test partitions
- Poorly behaved jobs will be terminated
- Don’t mine digital currency or misuse Harvard resources

Publications Acknowledging the FASRC Cluster

Documentation: https://docs.rc.fas.harvard.edu/kb/attribution/

- If you publish work performed on FASRC clusters, acknowledge it:

"The computations in this paper were run on the FASRC Odyssey cluster supported by the FAS Division of Science Research Computing Group at Harvard University."

FASRC documentation

- FASRC docs: https://docs.rc.fas.harvard.edu/
  - Search
- 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 trainings

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

Getting started on the FASRC clusters with Open OnDemand

- new users not familiar with command-line interface
- prefers to use a GUI
- 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

Getting started on the FASRC clusters with CLI

- Users familiar with command-line interface
- New to Cannon and FASSE, but familiar with HPC systems
- Working FASRC account with cluster access
- Content
  - Submit interactive job
  - Submit batch job
  - Monitor jobs
  - Cluster software (modules, spack)

Thank you :)

FAS Research Computing