



Getting Familiar with Research Computing

CURC Alpine: New User Seminar

Instructor: Trevor Hall

- Website: www.rc.colorado.edu
- Helpdesk: rc-help@colorado.edu
- Slides: https://github.com/ResearchComputing/New_User_Seminar
- Survey: <http://tinyurl.com/curc-survey18>

RMACC Cyber Infrastructure Portal



- <https://ask.cyberinfrastructure.org/c/rmacc/65>
- This forum provides opportunity for RMACC members to converse amongst themselves and with the larger, global research computing community.
- The “go to” general Q&A platform for the global research computing community - researchers, facilitators, research software engineers, CI engineers, sys admins and others.

Learning Goals

1. Understand Basic CURC Resources & the Alpine cluster
2. Getting an account & logging in
3. Navigate the RC system
4. Running a job

Things to take note of:

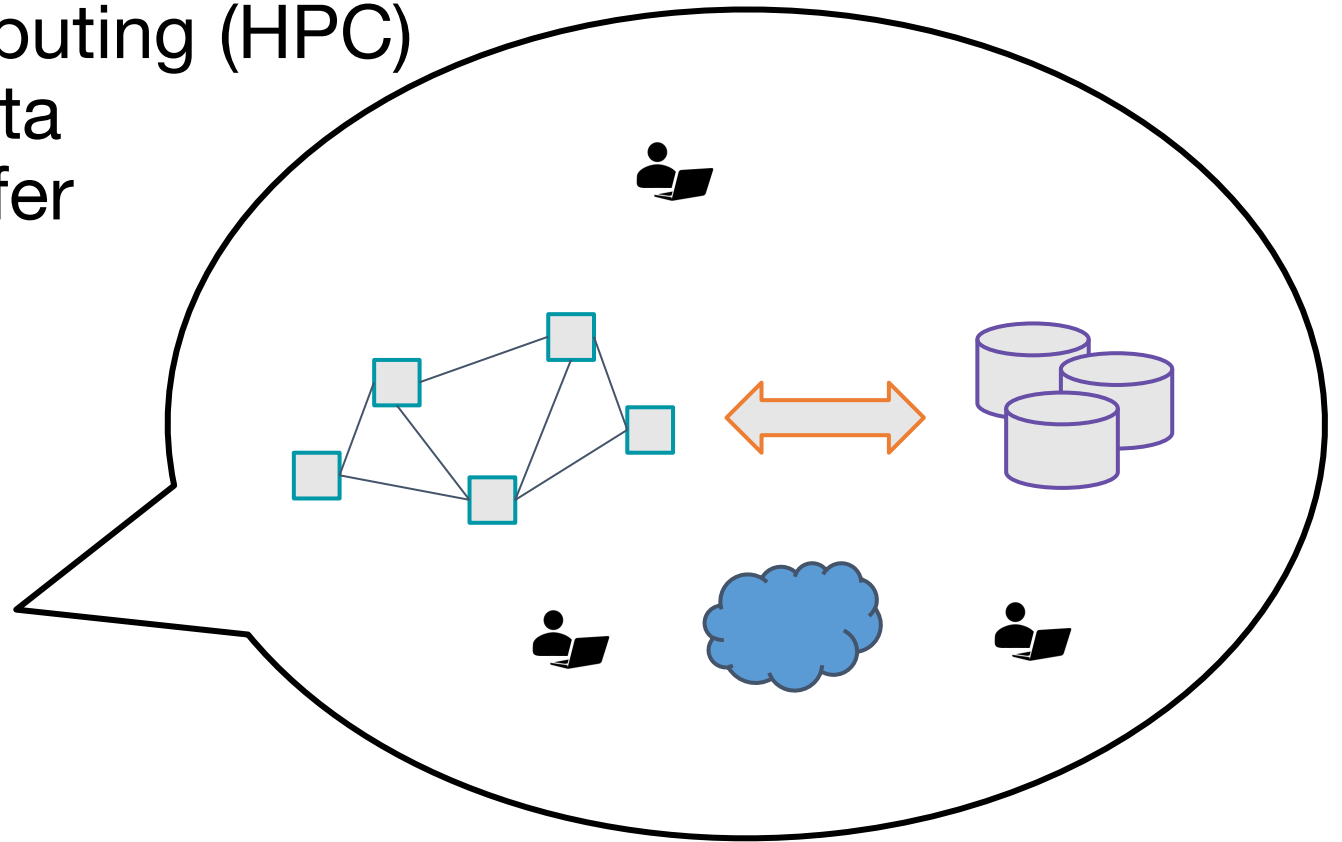
- Confusing, ambiguous, highly nuanced concepts
- Our goal is to help you avoid common mistakes, pitfalls, and frustrations



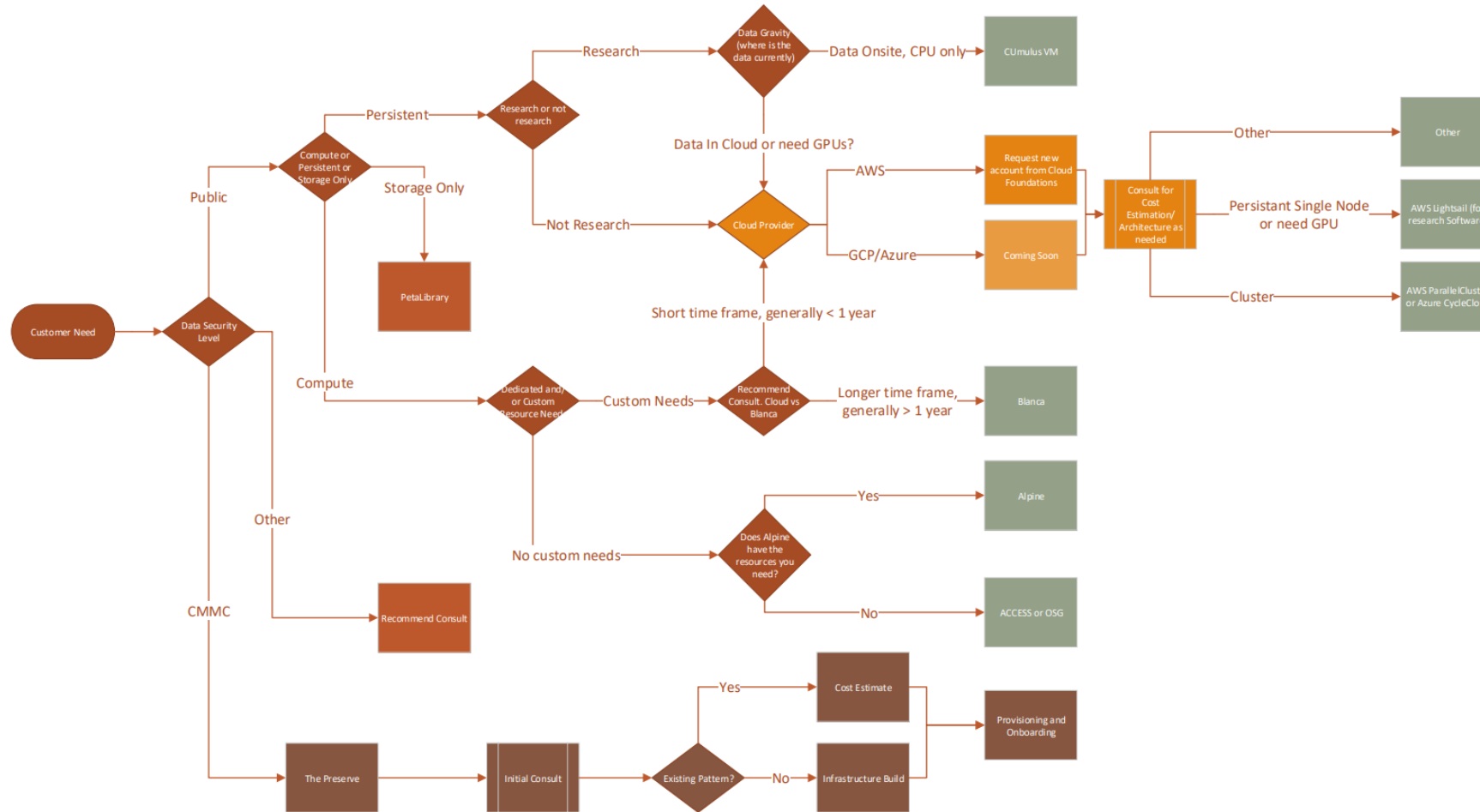
Ask Questions!

Resources Include:

- High Performance Computing (HPC)
- Storage of Research Data
- High-Speed Data Transfer
- Data Sharing
- Cloud Computing
- Training and Education
- Secure Research



How do I choose the resource for me?



Primarily known for: High Performance Computing (HPC)



High Performance Computing (HPC) vs. Traditional Computing

- Traditional computing *generally* has access to a single processor (perhaps multiple cores)

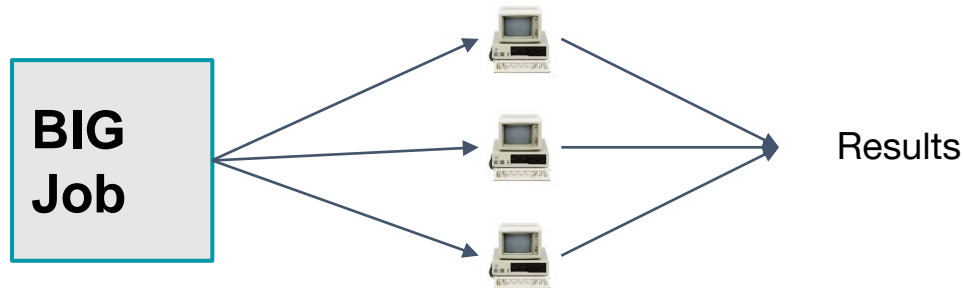


What can / use HPC for?

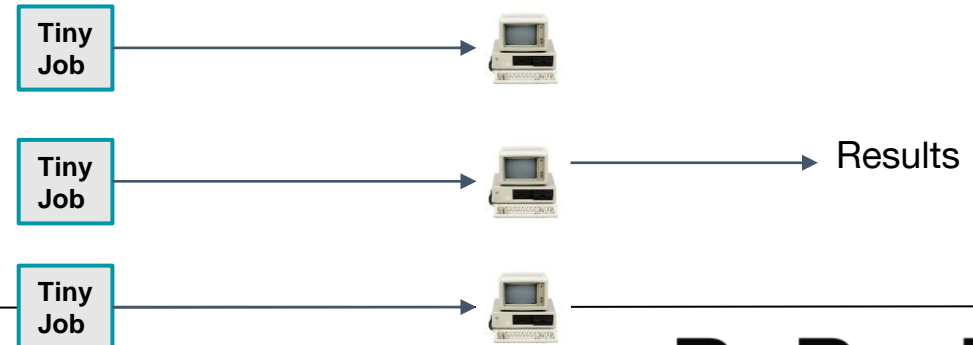
- Solving large problems that require more:
 - Memory than you have on your PC
 - cores/nodes/power than you have on your PC
- Jobs that require hardware you may not have:
 - High Performance GPU computing
 - Specific Operating System
- Visualization rendering

What can / use HPC for?

- Jobs that would take a long time on local machines can instead be distributed over hardware:
 - Parallelized to split up then joined (if software enabled)



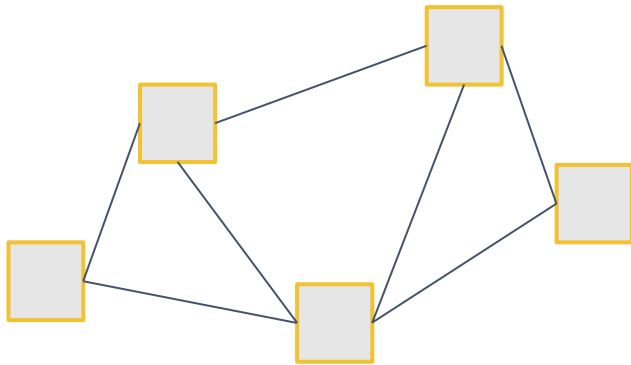
- Broken up into many serial jobs



Research Computing Resources

HPC Cluster: Alpine

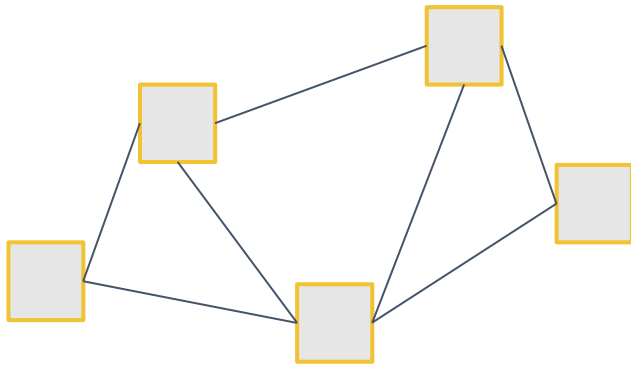
Alpine



- Alpine is the 3rd-generation HPC cluster at CURC, following:
 - Janus
 - RMACC Summit
- Alpine is a heterogeneous cluster with hardware currently provided by CU Boulder, CSU, and Anschutz
- Access available to CU Boulder, CSU, AMC and RMACC users

HPC Cluster: Alpine

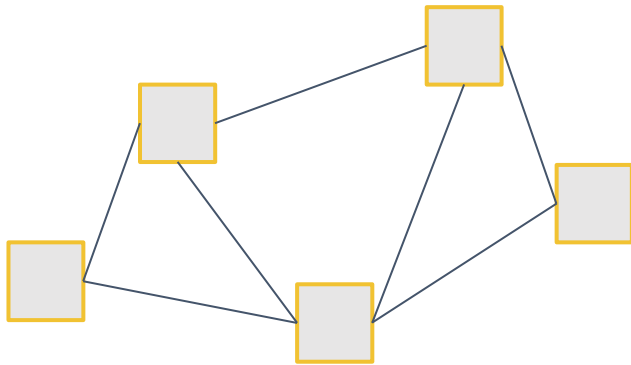
Alpine



- Hardware on Alpine will continue to be purchased and released in stages:
- Alpine (stage 3):
 - 184 General CPU Nodes
 - *AMD Milan, 64 Core, 3.74G RAM/Core*
 - 8 NVIDIA GPU Nodes
 - *3x NVIDIA A100 (atop General CPU node)*
 - 8 AMD GPU Nodes
 - *3x AMD MI100 (atop General CPU node)*
 - 12 AMD High-Memory Nodes
 - *AMD Milan, 48 Core, 21.5G RAM/Core*
 - Additional Hardware contributed by CSU, AMC
 - *Nodes which boost priority for CSU/AMC users*

HPC Cluster: Alpine

Alpine



- Interconnect

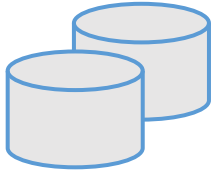
- **CPU nodes:** HDR-100 InfiniBand (200Gb inter-node fabric)
- **GPU nodes:** 2x25 Gb Ethernet +RoCE
- **Scratch Storage:** 25Gb Ethernet +RoCE

- Operating System

- RedHat Enterprise Linux version 8 operating system

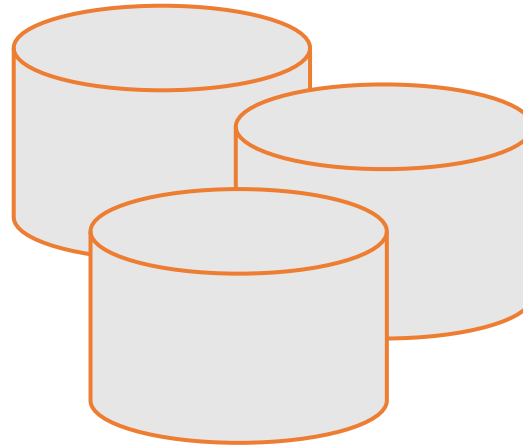
Storage at CURC

Core



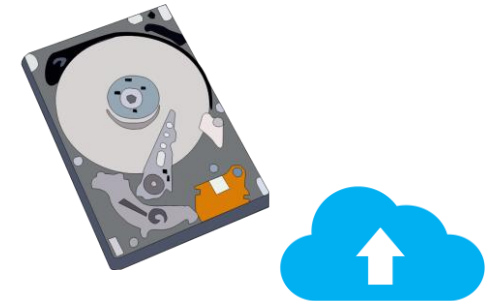
- Included with RC account
 - /home
 - /projects
 - scratch space

PetaLibrary



- Paid Service for:
 - Storage
 - Archive
 - Sharing of research data

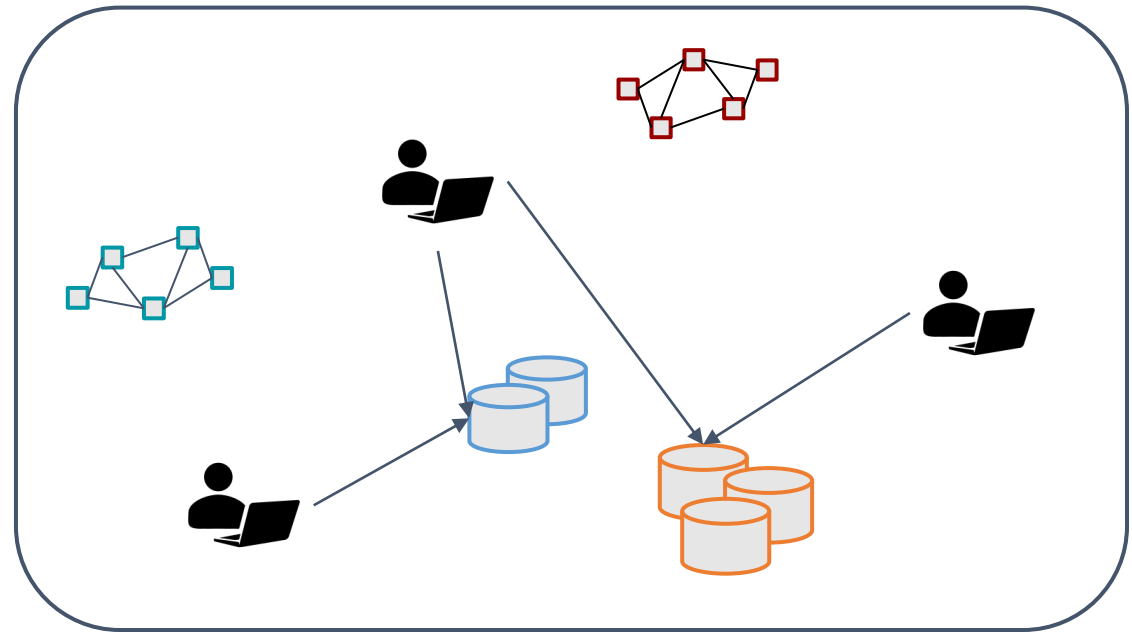
Local or Cloud



- You can download your data locally or to a variety of other cloud resources
- Cloud Foundations at Research Computing

Data Sharing: Within RC

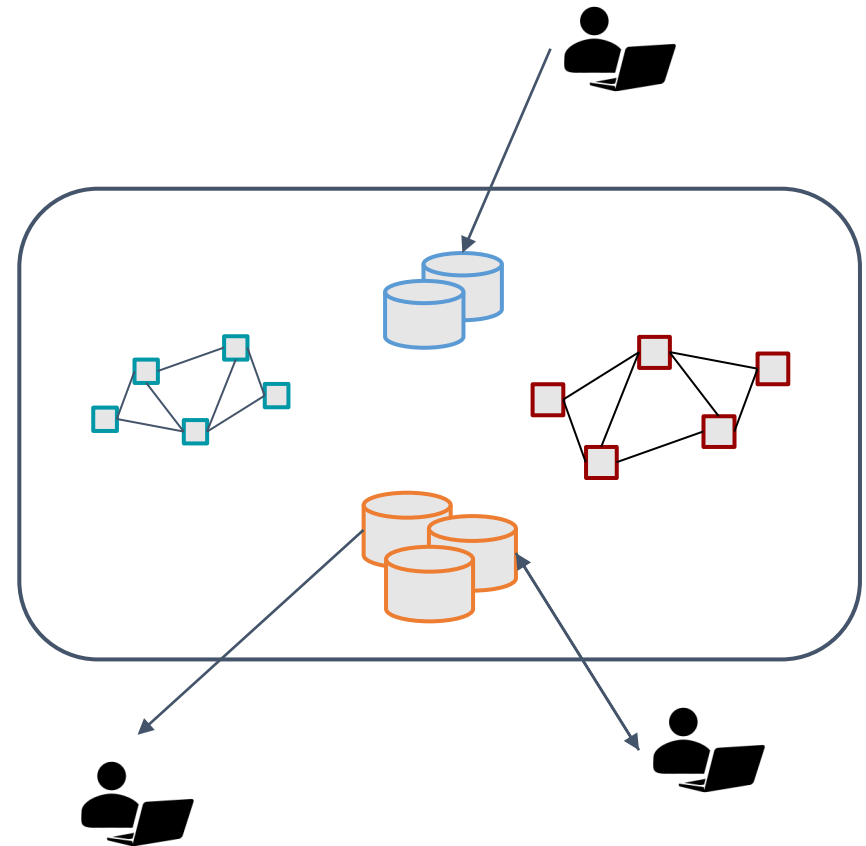
- Sharing workspaces
 - Project space
 - Scratch Space
 - PetaLibrary Space*



*If you have purchased PetaLibrary space

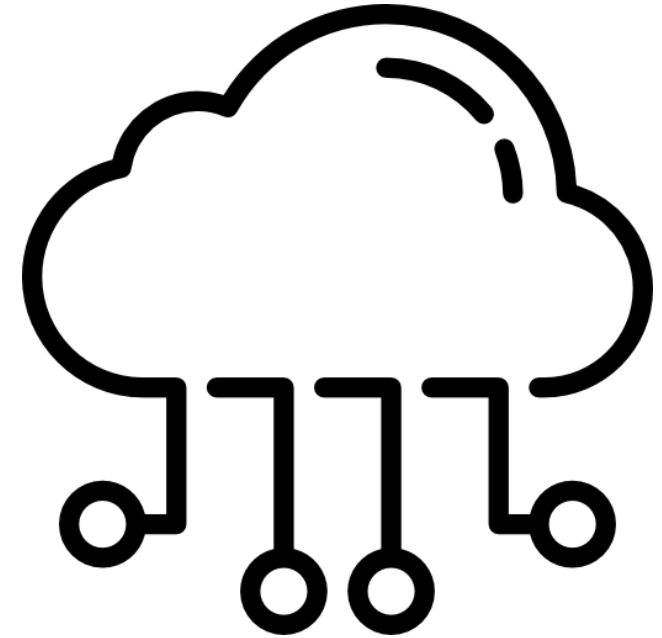
Data Sharing: Outside RC

- Globus (recommended):
 - GUI Web Application
 - Automates large transfers
 - Resumes failed transfers
 - Distributes large transfers across DTNs
 - Endpoints that can shared
- Data Transfer Nodes (DTN)
 - Internal CU network needed (VPN)
- Command line tools
 - scp, sftp, rsync, rclone



Cloud Computing

- CURC supports both AWS and on-premise cloud via CUMulus
 - For use cases not well-supported by HPC
- Can be used as an alternative to HPC
- Can be used to enhance HPC
 - Automatic job submission, high availability, etc.



Request a CUMulus application by contacting the RC helpdesk at rc-help@colorado.edu

Accessing Research Computing

How to Access RC Resources?

1. Get an RC account
2. Set up two-factor authentication with Duo
3. (Inform us of any specific needs)
4. Log in
5. Create greatness! (responsibly)

Getting an RC Account

- **University of Colorado, Boulder users and affiliates:**

- Request an account through the RC Account request portal
- <https://rcamp.rc.colorado.edu/accounts/account-request/create/organization>

- **Colorado State University users:**

- Request an CSU eID if you don't have one
- Fill out account application form
- Duo authentication
- <https://it.colostate.edu/research-computing-and-cyberinfrastructure/compute/get-started-with-alpine/>

- **RMACC Users:**

- Create an [ACCESS-CI](#) Account in the ACCESS user portal
- Email us at rc-help@colorado.edu and request an account. Please include the following information: your ACCESS username, your institutional affiliation, your role, your department, your first and last name, your preferred email address for communication

Demo: Getting an Account

- CU Boulder users and affiliates:
 - Request an account through the RC Account request portal
 - <https://rcamp.rc.colorado.edu/accounts/account-request/create/organization>

Your RC Account

Access to:

1. Alpine Cluster
2. Core Storage
3. PetaLibrary Storage*
4. Open OnDemand
5. Approximately 2,000 Service Units (SUs) per month

*If purchased

Your RC Account

How can I use more computational time?:

- Trailhead Allocation (Default)
 - ~2,000 SUs / Month
- Ascent Allocation
 - 250,000 SUs
- Peak Allocation
 - >250,000 SUs

Request an allocation at

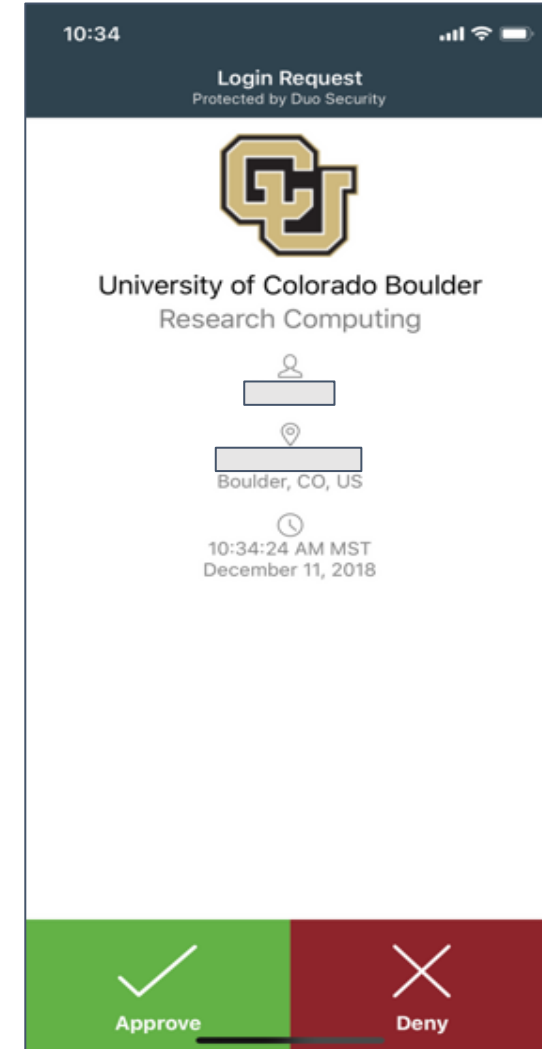
<https://curc.readthedocs.io/en/latest/clusters/alpine/allocations.html?highlight=alpine%20allocation#comparing-trailhead-auto-allocation-ascent-allocation-and-peak-allocation-tiers>

Two Factor Authentication (Duo)

- Provides an extra level of authentication
 - We are outside the firewall!
 - Valuable resources
 - Inviting, high-profile target
 - Lost time investigating/fixing
- Duo
 - You will receive a Duo invitation when your RC account is created

Duo Authentication

1. **Duo smartphone app (recommended)**
2. Phone Call/Text is an alternatives
3. Physical code generator “token” available for \$20



Linux comfort level check

- On a scale from (1-10) **how familiar/comfortable are you with Linux?**
 - The command line
 - Basic commands
 - Linux filesystem
 - Navigating the filesystem

Terminal

- Mac or Linux
 - Terminal application
- Windows
 - PuTTY
 - Powershell
- Open OnDemand (*alternative for CU affiliates*)
 - For those less familiar with Linux (ondemand.rc.colorado.edu/)

```
[user0083@tlogin1 ~]$ pwd  
/home/user0083  
[user0083@tlogin1 ~]$ █
```

Demo: Logging in via Terminal

- To login to an RC login node:

```
$ ssh <username>@login.rc.colorado.edu
```

Supply your IdentiKey password and your Duo app will alert you to confirm the login

*CU and CSU exclusive

Demo: logging in with OnDemand

CURC Open OnDemand is a browser based, integrated, single access point for all of your HPC resources at CU Research Computing.

- CU Boulder: Visit <https://ondemand.rc.colorado.edu>.
- Other RMACC Institutions: Visit <https://ondemand-rmacc.rc.colorado.edu/>

Logging In

- It's important to note that you are ***NOT*** logging into any specific resource, Alpine, Blanca, etc.
- When you log in, you land on our ***login nodes***
- From ***there***, you can access our other resources:
 - Alpine
 - Blanca
 - Petalibrary

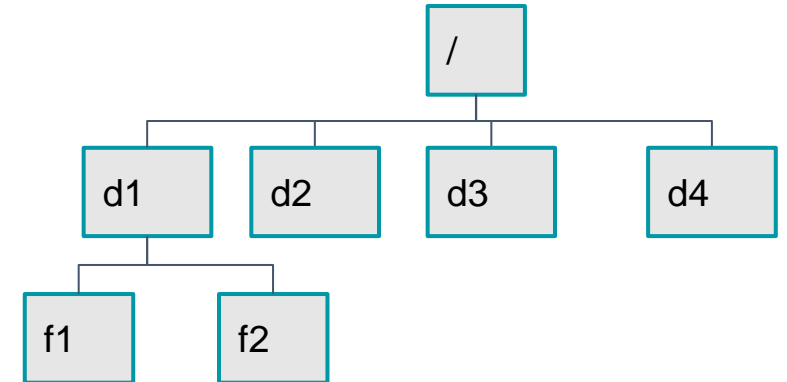
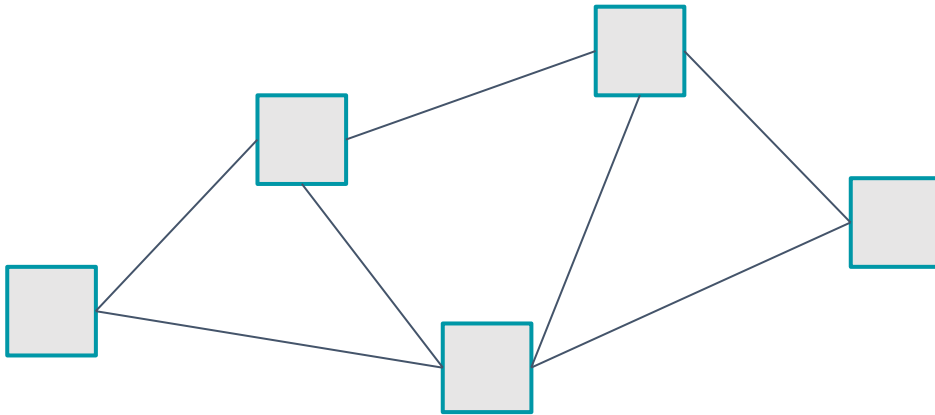
Navigating Research Computing

Node

- One computing server
- Physical hardware
- Work together in parallel

File System

- The basic tree-like layout
- From most nodes* you have access to most file systems

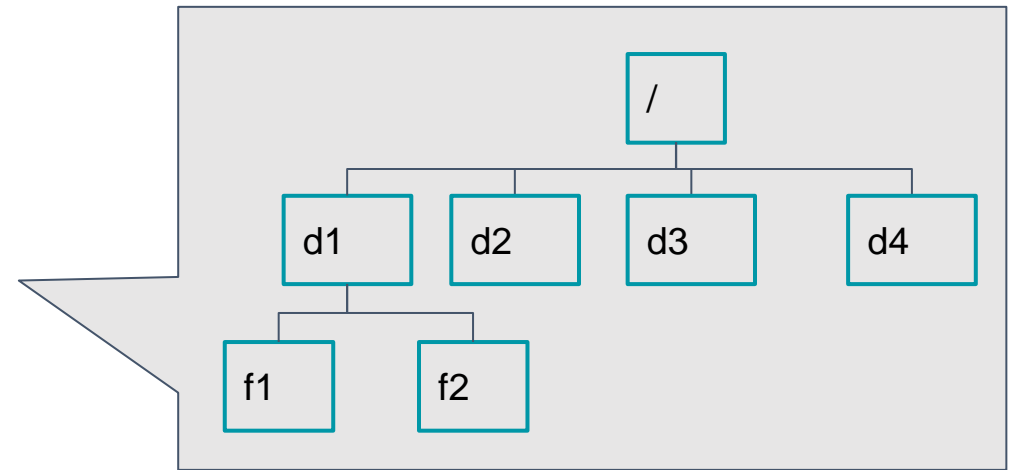
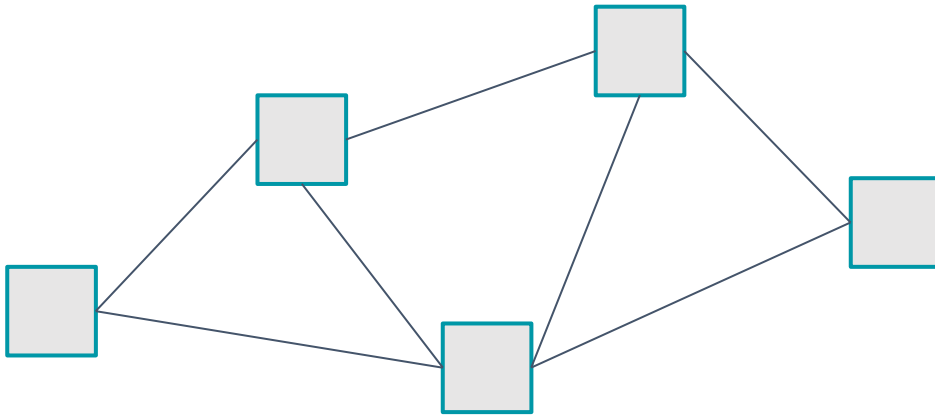


Node

- One computing server
- Physical hardware
- Work together in parallel

File System

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Node Types

Login

- Where you log in to
- For editing code, job submission
- No heavy computation

Ex. edit job script

Compile

- Where you compile code, install packages
- Explore the Alpine software environment
- Edit code, submit jobs
- No heavy computation

Ex. Install python libs

Compute

- Where scheduled jobs run
- Intended for heavy computation

Ex. Running Matlab

Alpine Compile Nodes

- If you have used Summit in the past, compile nodes work *slightly* differently:
 - Instead of having dedicated hardware (2 nodes) which are oversubscribed for users to `ssh` into
 - Alpine's `acompile` command starts an interactive job which users can compile in which provides the following benefits:
 - Users can request specific resources (i.e. more cores to compile with)
 - Limits dedicated hardware set aside
 - Can't accidentally run full workflows

Alpine Compile Nodes

- `$ module load slurm/alpine`
- `$ acompile`
 - starts a job with default: 1 core, 3.74GB RAM, for 60 minutes*
- `$ acompile --help`
 - `--time=<time-limit>` # set minimum runtime
 - `--ntasks=<number-of-cores>` # default 1, max 4
 - `--gpu=<nvidia|amdgpu>` # request gpu to compile with
 - `--x11` # enable
 - `graphical forwarding`

*only a single `acompile` job can be open at a time

Demo: Exploring Nodes

- Once logged in, type:

\$ acompile

To log in to an Alpine compile (or head) node.

- Once on a compile node, type:

\$ module avail

To list currently available software

Filesystem Structure

/home (2GB)

- Scripts, Code, Small, important files/directories
- Not for sharing files or job output

Ex .bashrc

/projects (250GB)

- Code/files/libraries
- Software you are installing
- Sharing files
- Not for job output

Ex. Shared job scripts

/scratch/alpine (10TB)

- Output from running jobs
- Large files/datasets
- Sharing files
- Cluster specific
- Not for long term storage

Ex. Data

Exploring the Filesystem

- Once logged in use the following commands to navigate to your different workspaces

```
$ cd /home/<user>
```

```
$ cd /projects/<user>
```

```
$ cd /scratch/alpine/<user>
```

Using RC Resources

- We have:
 - Logged in
 - Explored nodes
 - Explored filesystem
- How do we actually *use* the computing resources?

Running a Job

Jobs

What is a “**job**”?

- Work for the cluster to perform on
- Has a unique ID

1. Batch jobs

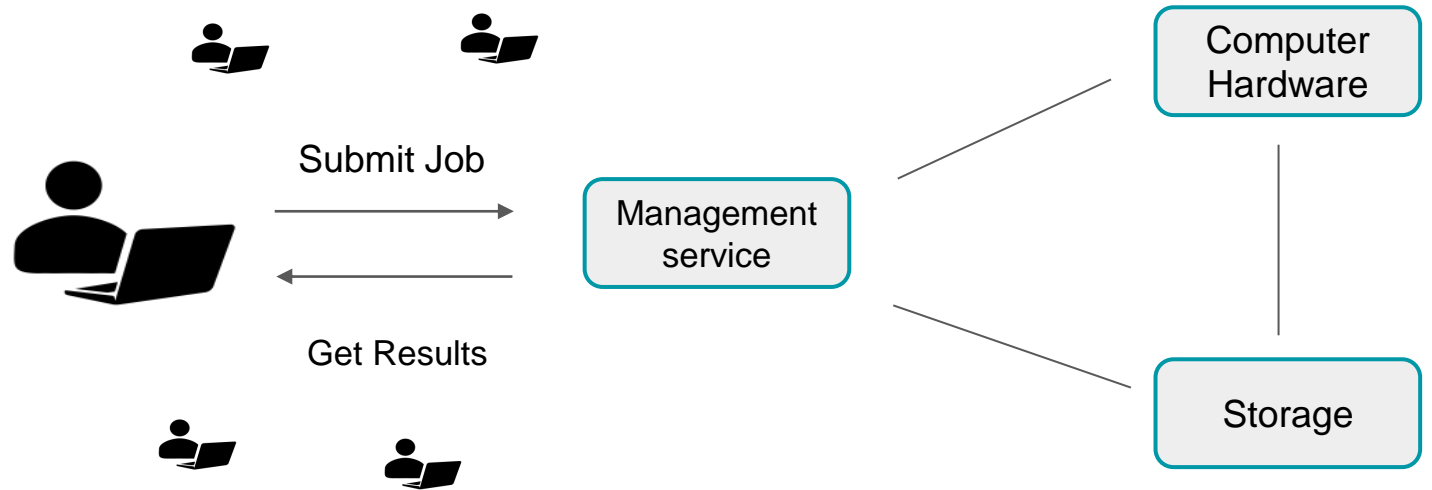
- Submit job script which will be executed when resources are available
 - Create script containing information about the job
 - Submit the job file to a queue

2. Interactive jobs

- Work interactively at the command line of a compute node

Job Scheduling

- CURC Clusters are shared resources, jobs are:
 - Submitted to a queue
 - When the required resources become available, the scheduler determines which set of nodes to use
 - Executes your job

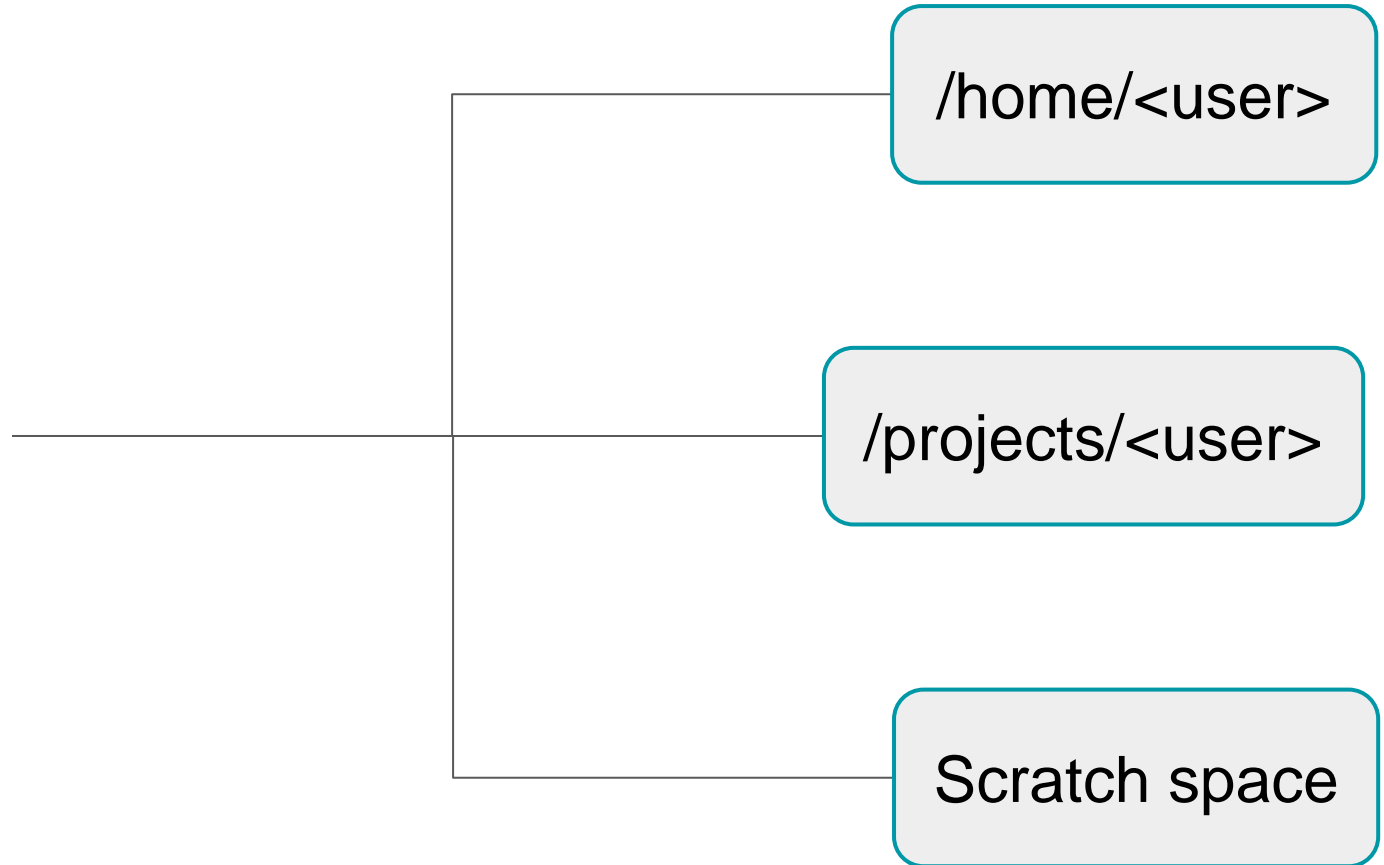


SLURM

- **S**imple **L**inux **U**tility for **R**esource **M**anagement
- Through SLURM users can:
 - Schedule jobs on specific compute resources
 - Run jobs interactively or hands off
 - Query job statistics

Your first job

- Where to write it?
- How to write it?
- How to run it?



Job Script: 3 main parts

1. Directives

- Specify resource requirements

1. Software

- Because jobs run on a different node than from where you submitted...
- ...software that is needed must be loaded via the job script

1. User scripting

- the actual user scripting that will execute when the job runs

```
#!/bin/bash

## Directives
#SBATCH --<resource>=<amount>

## Software
module purge

## User Scripting
hostname # example bash command
```


Slurm Options (directives)

`#SBATCH <options>` `sbatch <options>`

- Allocation: `--account=<account_no>`
 - Partition: `--partition=<partition_name>`
 - Sending emails: `--mail-type=<type>`
 - Output file: `--output=<file name>` (%j gives you job id)
 - Number of nodes: `--nodes=<nodes>`
 - Number of tasks: `--ntasks=<processes>`
 - Quality of service: `--qos=<qos>`
 - Reservation: `--reservation=<name>`
 - Wall time: `--time=<wall time>`
 - Job Name: `--job-name=<jobname>` ...etc...
- FYI: You do NOT actually type <> above – this designates something specific you as a user must enter about your job

Slurm Options (directives)

- There are **MANY** slurm directives, most of which are not required
 - See all options at <http://slurm.schedmd.com/sbatch.html>
- We will focus on some common options:
 - **Partition:** Nodes with the same hardware configuration
 - **Wall time:** Max time your job will run for
 - **Node count:** # of nodes requested
 - **Core count:** # of cores requested
 - **Output file:** name of output file

Alpine Partitions

Partition	Description	# of nodes	RAM/core (GB)	cores/node	GPUs/node
amilan	General Compute Node: AMD Milan	64	3.74	64	0
ami100	GPU Node: 3x AMD MI100	8	3.74	64	3
aa100	GPU Node: 3x Nvidia A100	8	3.74	64	3
amem	High-memory node	4	21.5	48	0

Review: Learning Goals

1. Understand Basic Resources (Alpine cluster)
2. Getting an account & logging in
3. Navigate the RC system
4. Running a job

Questions

CURC User Policies: <https://curc.readthedocs.io/en/latest/additional-resources/policies.html?highlight=policies#curc-user-policies>

Survey and feedback

<http://tinyurl.com/curc-survey18>