

Alpine: New User Seminar



CURC Alpine: New User Seminar

Instructor: Trevor Hall

Website: www.rc.colorado.edu

• Helpdesk: <u>rc-help@colorado.edu</u>

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
- 5. Help!

Things to take note of:

 Confusing, ambiguous, highly nuanced concepts

 Our goal is to help you avoid common mistakes, pitfalls, and frustrations



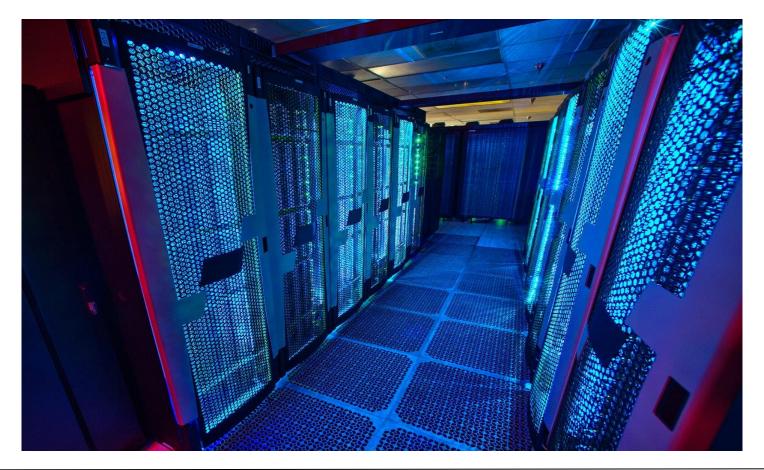
Ask Questions!

Resources Include:

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



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)



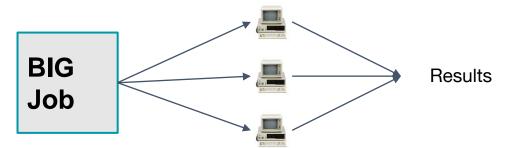
What can / use HPC for?

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

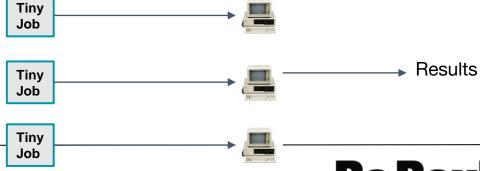


What can / use HPC for?

- 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



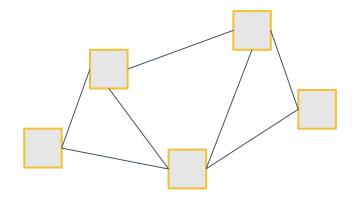


Research Computing Resources



HPC Cluster: Alpine

Alpine



- Alpine is the 3rd-generation HPC cluster at CURC, following:
 - Janus
 - RMACC Summit

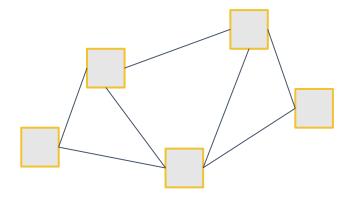
- Alpine is a heterogeneous cluster with hardware currently provided by CU Boulder, CSU, and Anschutz
- Access available to CU Boulder, CSU, AMC and RMACC users





HPC Cluster: Alpine

Alpine



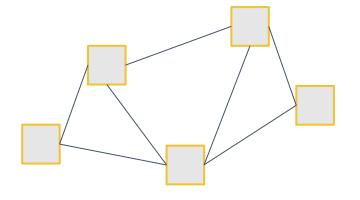
- Hardware on Alpine will continue to be purchased and released in stages:
- Alpine (stage 3):
 - 184 General CPU Nodes
 - AMD Milan, 64 Core, 3.74G RAM/Core
 - 8 NVIDIA GPU Nodes
 - 3x NVIDIA A100 (atop General CPU node)
 - 8 AMD GPU Nodes
 - 3x AMD MI100 (atop General CPU node)
 - 12 AMD High-Memory 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





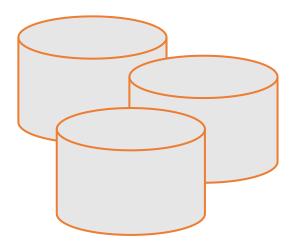
Storage at CURC

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

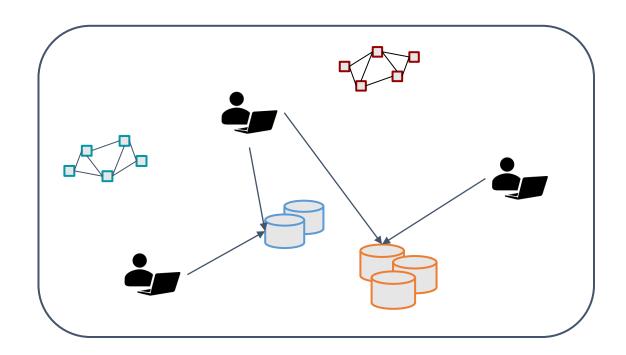




Data Sharing: Within RC

- Sharing workspaces

 - Project spaceScratch Space
 - PetaLibrary Space*



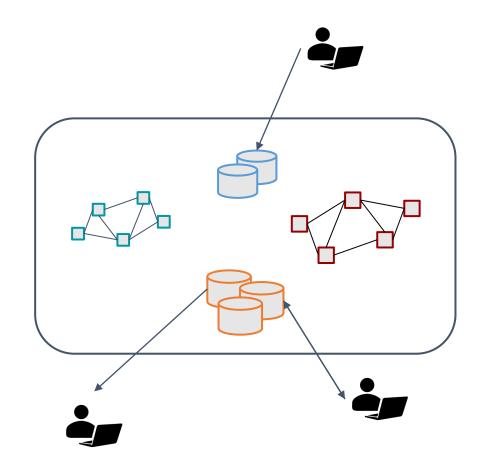
*If you have purchased PetaLibrary space



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 onpremise 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 <u>rc-help@colorado.edu</u>

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 elD 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 <u>rc-help@colorado.edu</u> 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/)



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

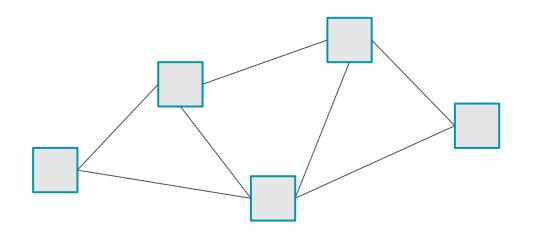


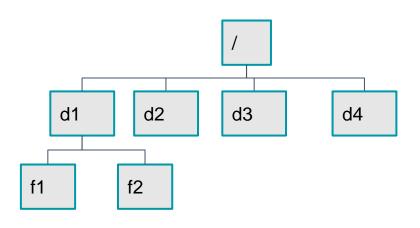
Node

File System

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

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





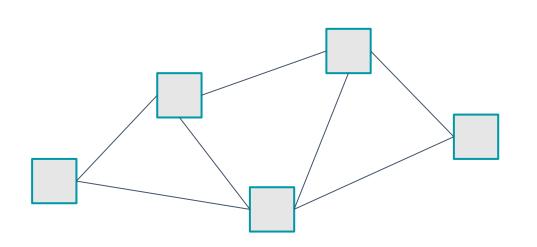


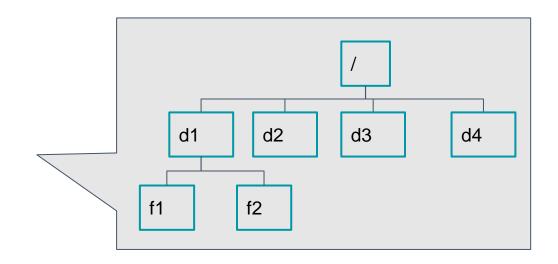
Node

File System

- One computing server
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Node Types

Login	Compile	Compute
Where you log in to	Where you compile code, install packages	Where scheduled jobs run
 For editing code, job submission No heavy computation 	 Explore the Alpine software environment Edit code, submit jobs No heavy computation 	Intended for heavy computation
Ex. edit job script	Ex. Install python libs	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
--×11
graphical forwarding
```

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





enable

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)	/projects (250GB)	/scratch/alpine (10TB)
 Scripts, Code, Small, important files/directories Not for sharing files or job output 	 Code/files/libraries Software you are installing Sharing files Not for job output 	 Output from running jobs Large files/datasets Sharing files Cluster specific Not for long term storage
Ex .bashrc	Ex. Shared job scripts	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

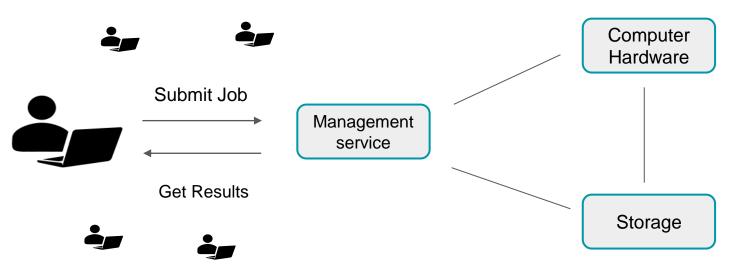
Work interactively at the command line of a compute node





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

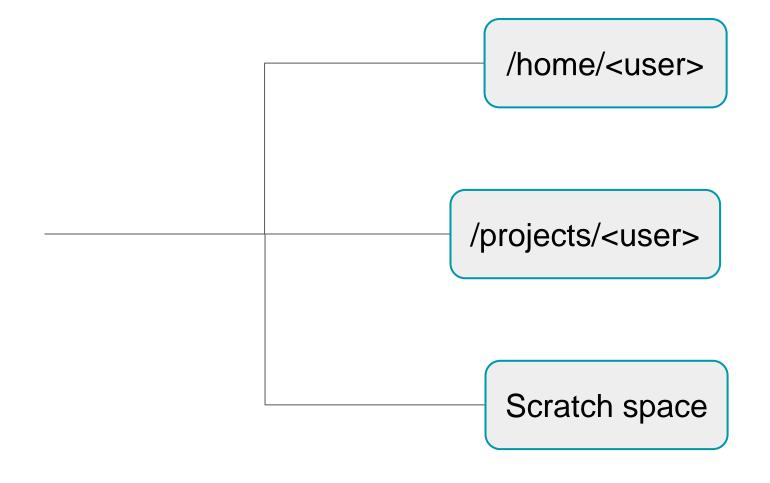
- Simple Linux Utility for Resource Management
- Through SLURM users can:
 - Schedule jobs on specific compute resources
 - Run jobs interactively or hands off
 - Query job statistics

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:

                        --aos=<aos>
 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
- 5.Help!

Help! I'm stuck, where do I go?

- Documentation: curc.readthedocs.io/
- Trainings with Center for Research Data and Digital Scholarship

(CRDDS): https://www.colorado.edu/crdds/

- Coming up:
 - Supercomputing Spin Up: Part 1 -- Working with Linux (1/25)
 - Supercomputing Spin Up: Part 2 Job Scheduling (1/31)
 - Setting up Your Research Software on Alpine (1/31)
- Helpdesk: rc-help@colorado.edu
- Consult Hours (now!)





Helpdesk Tickets

To: rc-help@colorado.edu

Dear Research Computing,

Help! My code won't run! Help!

Help please, Trevor To: rc-help@colorado.edu

Dear Research Computing,

I am running into issues running my Python script. I am using a conda environment called my_python_env with the pytorch software, and I am receiving the following error. I am not sure how to troubleshoot. My job ID is 620350. Let me know what I can try!

sbatch: error: Batch job submission failed: Invalid p artition name specified.

Thanks, Trevor





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

