

# Alpine: New User Seminar



### CURC Alpine: New User Seminar

Instructor: Trevor Hall

Workshop Type: Primer

Website: www.rc.colorado.edu

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

Slides: <a href="https://github.com/ResearchComputing/New\_User\_Seminar">https://github.com/ResearchComputing/New\_User\_Seminar</a>

• Survey: <a href="http://tinyurl.com/curc-survey18">http://tinyurl.com/curc-survey18</a>





#### 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



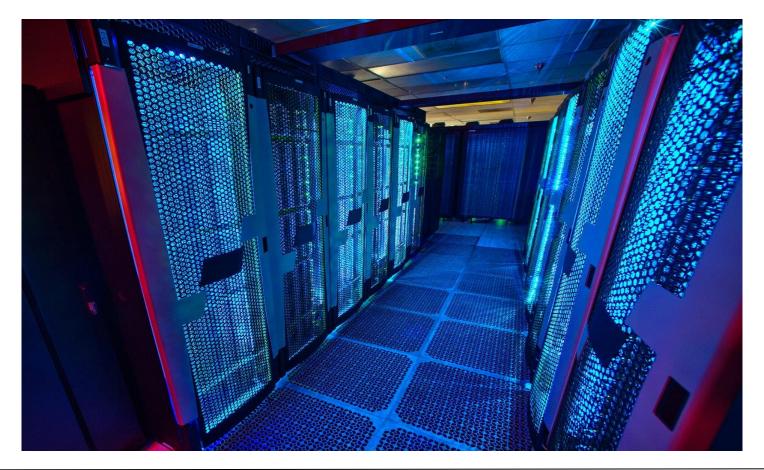
**Ask Questions!** 

#### 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)





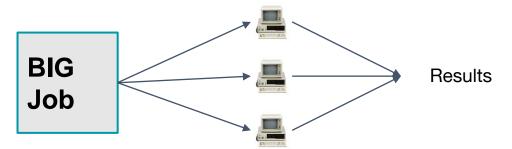
# High Performance Computing (HPC) vs. Traditional Computing

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

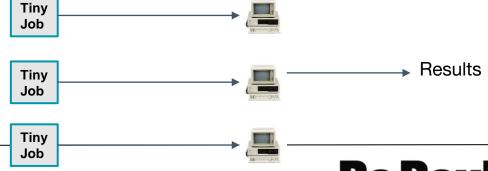


#### What can / use HPC for?

- 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





#### 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

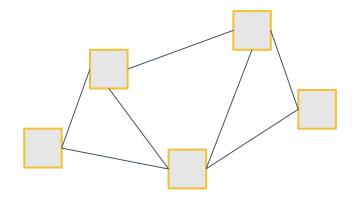


### Research Computing Resources



# HPC Cluster: Alpine

#### **Alpine**



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

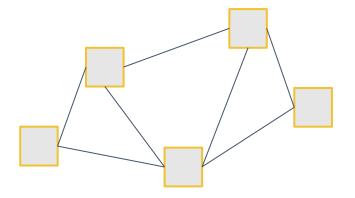
- Alpine is a heterogeneous cluster with hardware currently provided by CU Boulder, CSU, and Anschutz
- Access available to CU Boulder, CSU, AMC and RMACC users





### HPC Cluster: Alpine

#### **Alpine**



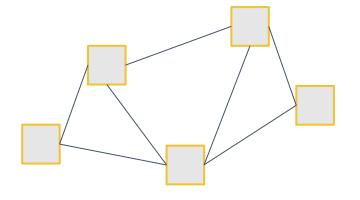
- Hardware on Alpine will continue to be purchased and released in stages:
- Alpine (stage 4):
  - 256 General CPU Nodes
    - AMD Milan, 64 Core, 3.74G RAM/Core
  - 12 NVIDIA GPU Nodes
    - 3x NVIDIA A100 (atop General CPU node)
  - 8 AMD GPU Nodes
    - 3x AMD MI100 (atop General CPU node)
  - 22 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





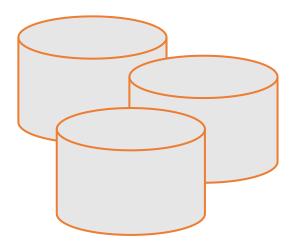
# Storage at CURC

#### 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

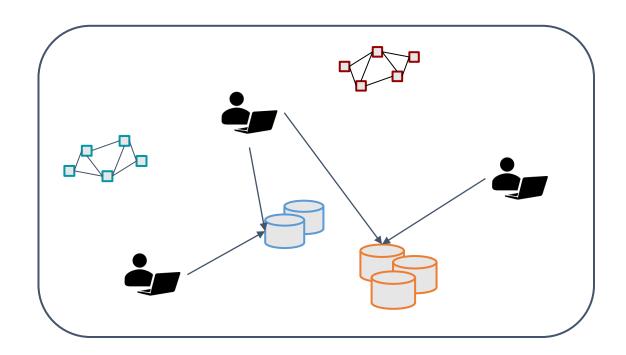




# Data Sharing: Within RC

- Sharing workspaces

  - Project spaceScratch Space
  - PetaLibrary Space\*



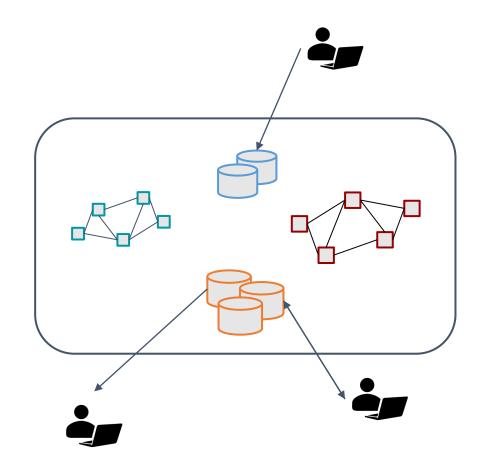
\*If you have purchased PetaLibrary space



# Data Sharing: Outside RC

- Globus (recommended):
  - GUI Web Application
  - Automates large transfersResumes 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 AWS, Azure, and GCP
  - 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 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/
- CU Anschutz Users:
  - Create an <u>ACCESS-CI</u> Account in the ACCESS user portal
  - Reach out to <a href="mailto:hpcsupport@cuanschutz.edu">hpcsupport@cuanschutz.edu</a> to receive and sign the End-User Agreement
- RMACC Users:
  - Create an <u>ACCESS-CI</u> 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, CSU users and affiliates:
  - Request an account through the RC Account request portal: <a href="https://rcamp.rc.colorado.edu/accounts/account-request/create/organization">https://rcamp.rc.colorado.edu/accounts/account-request/create/organization</a>
- AMC, RMACC users and affiliates:
  - Request an account through the ACCESS-CI User Registration Portal: <a href="https://identity.access-ci.org/new-user.html">https://identity.access-ci.org/new-user.html</a>





#### 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)

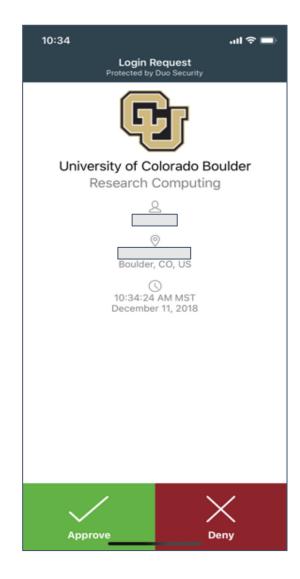
- Provides an extra level of authentication
  - We are outside the firewall!
  - Valuable resources
  - Inviting, high-profile target
  - Lost time investigating/fixing
- Duo
  - You will receive a Duo invitation when your RC account is created





#### **Duo Authentication**

- 1. Duo smartphone app (recommended)
- 2. Phone Call/Text is an alternatives







#### 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 <a href="https://ondemand.rc.colorado.edu">https://ondemand.rc.colorado.edu</a>.
- Other RMACC Institutions: Visit <a href="https://ondemand-rmacc.rc.colorado.edu/">https://ondemand-rmacc.rc.colorado.edu/</a>



# 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

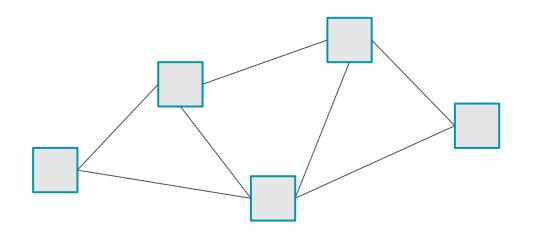


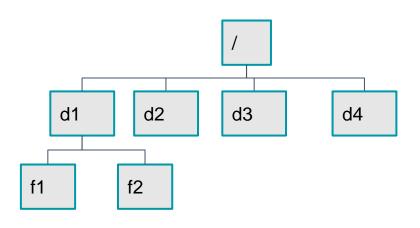
#### Node

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





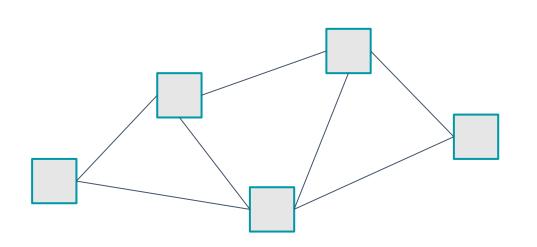


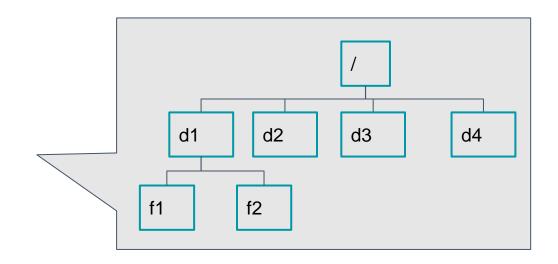
#### Node

**File System** 

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

- The basic tree-like layout
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# Node Types

Login	Compile	Compute
Where you log in to	Where you compile code, install packages	Where scheduled jobs run
<ul> <li>For editing code, job submission</li> <li>No heavy computation</li> </ul>	<ul> <li>Explore the Alpine software environment</li> <li>Edit code, submit jobs</li> <li>No heavy computation</li> </ul>	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)
<ul> <li>Scripts, Code, Small, important files/directories</li> <li>Not for sharing files or job output</li> </ul>	<ul> <li>Code/files/libraries</li> <li>Software you are installing</li> <li>Sharing files</li> <li>Not for job output</li> </ul>	<ul> <li>Output from running jobs</li> <li>Large files/datasets</li> <li>Sharing files</li> <li>Cluster specific</li> <li>Not for long term storage</li> </ul>
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

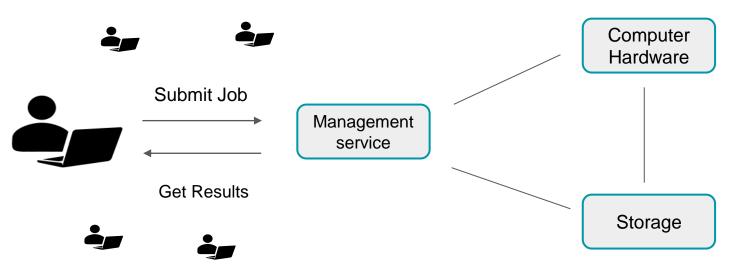
Work interactively at the command line of a compute node





## 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**

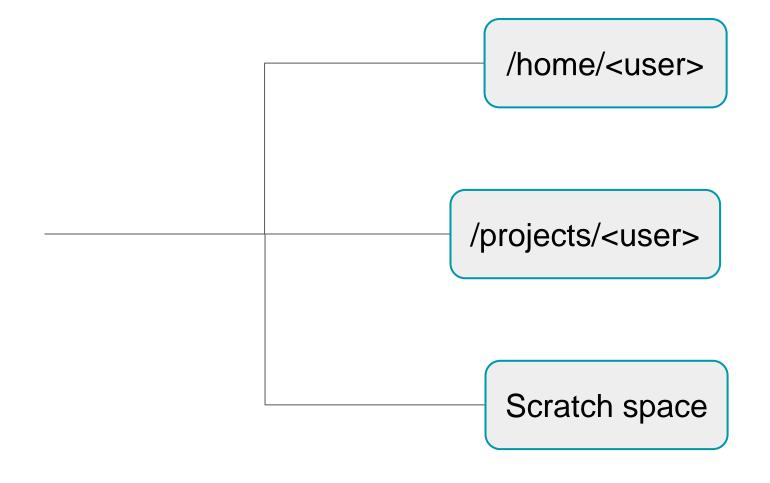
- Simple Linux Utility for Resource Management
- Through SLURM users can:
  - Schedule jobs on specific compute resources
  - Run jobs interactively or hands off
  - Query job statistics

#### 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

#### 2. Software

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

#### 3. 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 <a href="http://slurm.schedmd.com/sbatch.html">http://slurm.schedmd.com/sbatch.html</a>

- 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	256	3.74	64	0
ami100	GPU Node: 3x AMD MI100	8	3.74	64	3
aa100	GPU Node: 3x Nvidia A100	12	3.74	64	3
amem	High-memory node	22	21.5	64 (10), 48 (12)	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): <a href="https://www.colorado.edu/crdds/">https://www.colorado.edu/crdds/</a>
  - Coming up:
    - Supercomputing Spin Up: Part 1 Working with Linux (4/9)
    - Supercomputing Spin Up: Part 2 Submitting Jobs (4/11)
- Helpdesk: rc-help@colorado.edu
- Consult Hours (Tuesday 12:00-1:00 in-person, Thursday 1:00-2:00 virtually)





#### 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: <a href="https://curc.readthedocs.io/en/latest/additional-resources/policies.html?highlight=policies#curc-user-policies">https://curc.readthedocs.io/en/latest/additional-resources/policies.html?highlight=policies#curc-user-policies</a>





## Survey and feedback

http://tinyurl.com/curc-survey18

