Alpine: New User Seminar

Research Computing
UNIVERSITY OF COLORADO **BOULDER**

Be Boulder.

Alpine: New User Seminar

Instructors: Brandon Reyes, Andy Monaghan

- Website: www.rc.colorado.edu
- Documentation: https://curc.readthedocs.io
- Helpdesk: rc-help@colorado.edu

- Slides: https://github.com/ResearchComputing/rmacc_2024
  - In the directory “alpine_new_user_seminar”

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.

What is CURC?

CU Research Computing (CURC) is a group at CU Boulder that hosts a variety of resources. One of these resources is the Alpine High-Performance Computing (HPC) system. All individuals within the RMACC community can request an account with CURC, which will allow them to freely run on Alpine. Access to Alpine for the RMACC community is facilitated through Open OnDemand.

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!

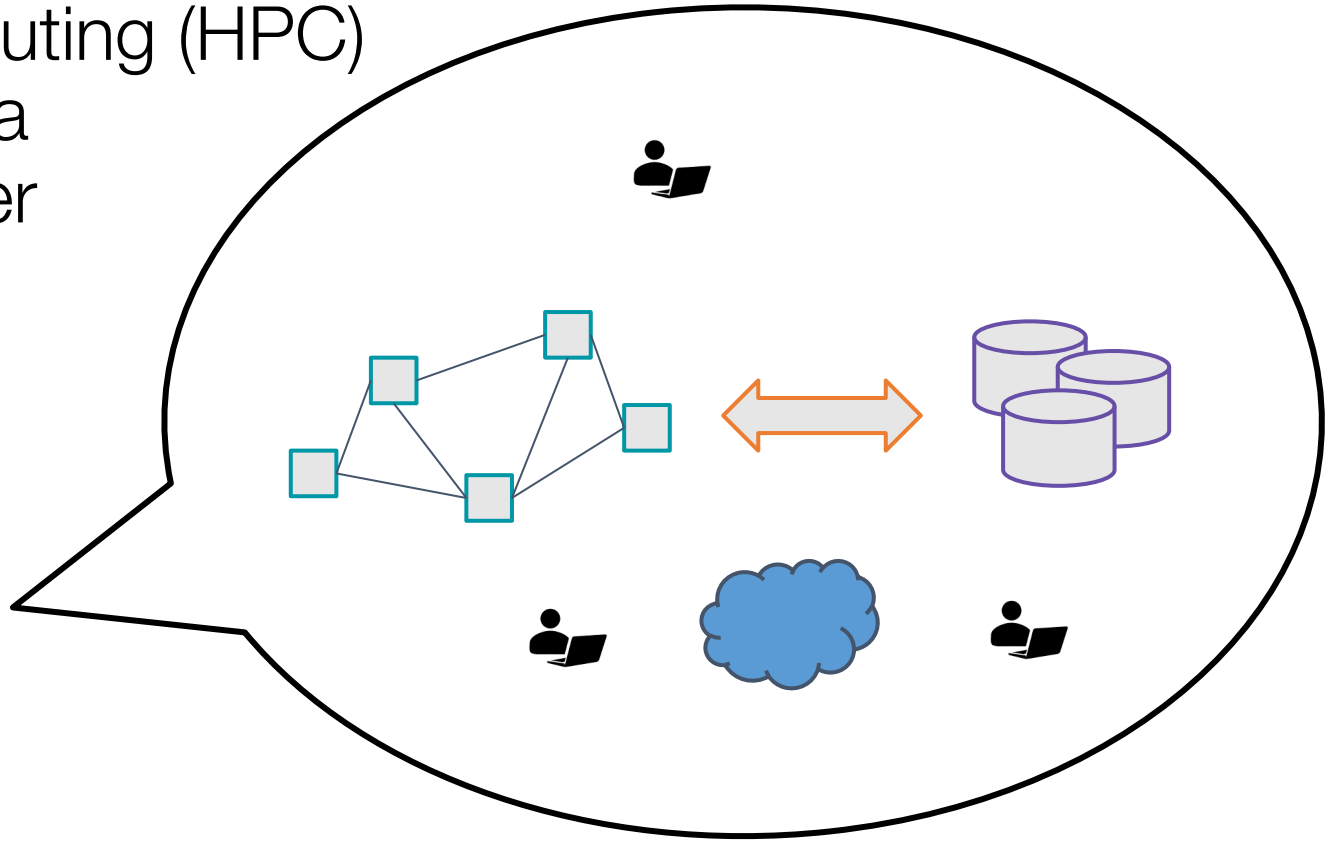
Things to take note of:

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

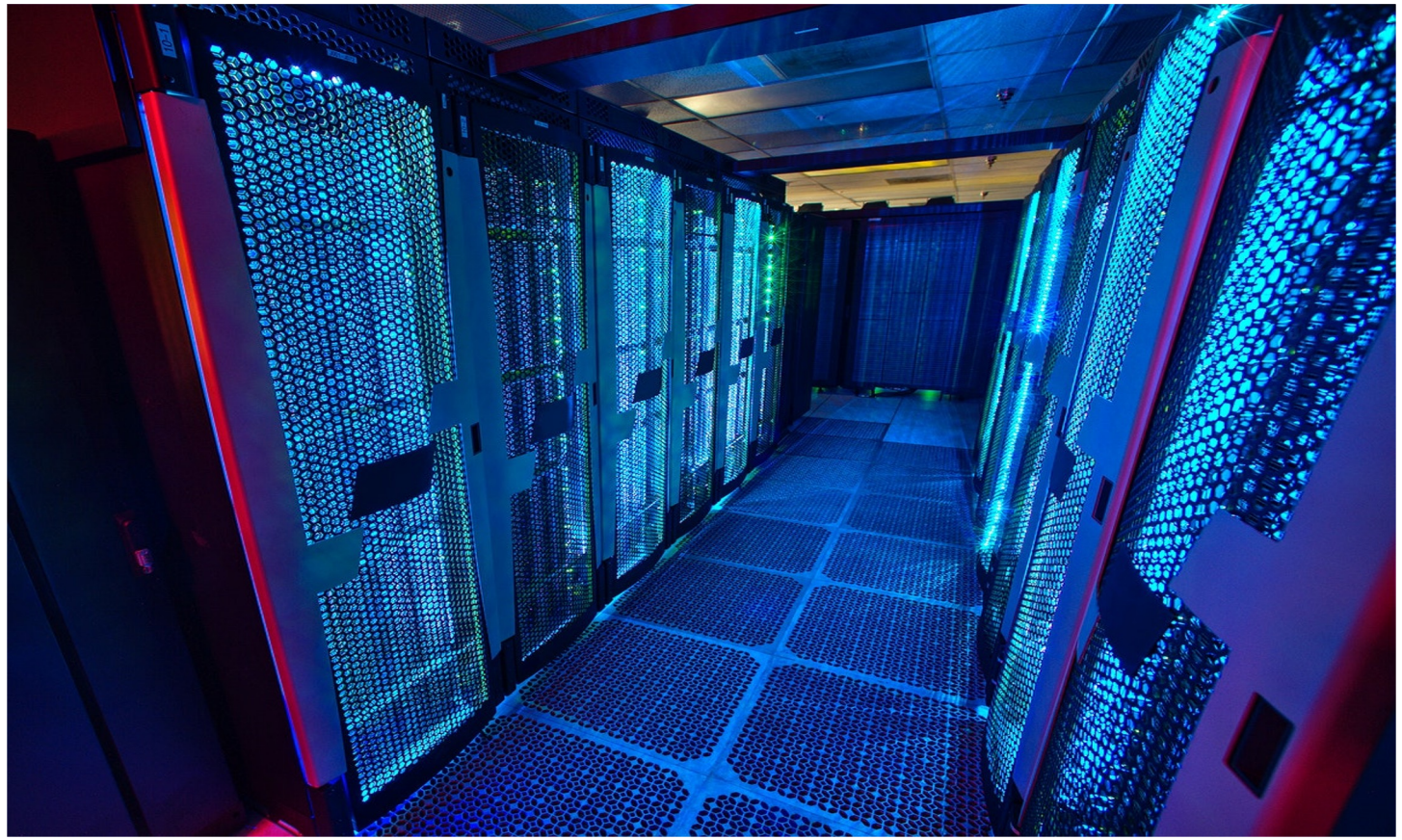
Ask Questions!

CURC Resources Include:

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



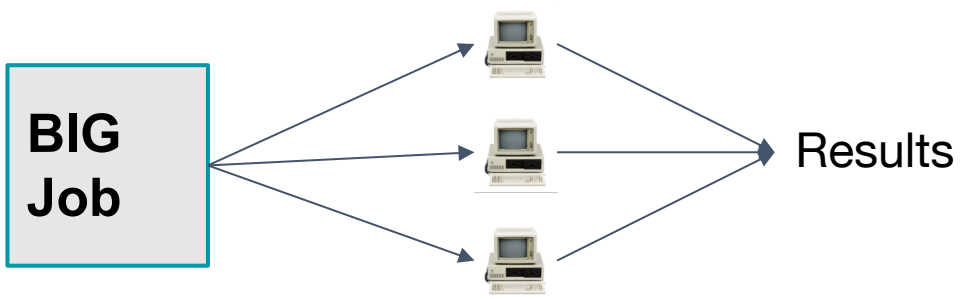
Primarily known for:
High Performance Computing (HPC)



High Performance Computing (HPC) vs. Traditional Computing

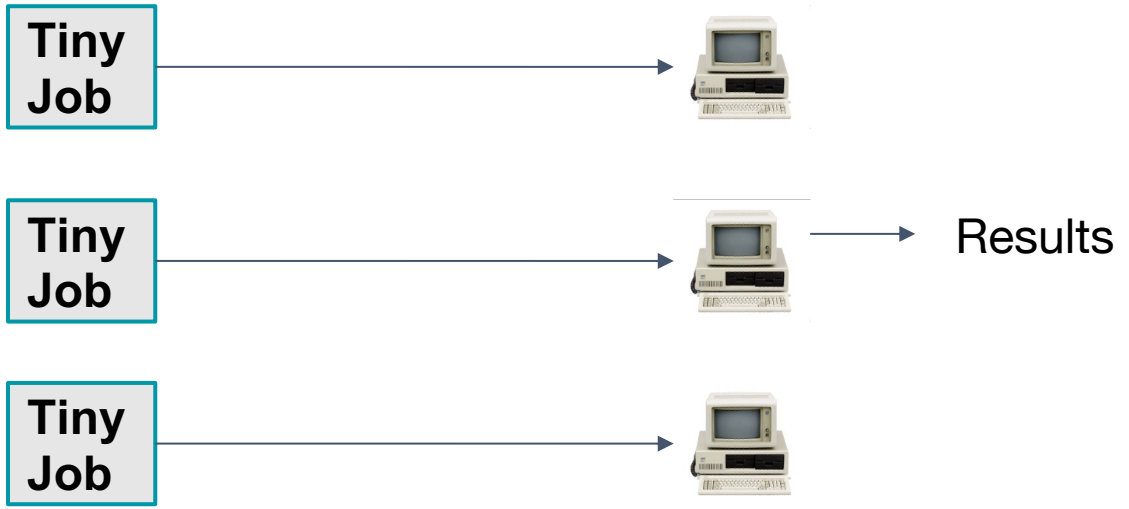
- Traditional computing *generally* has access to a single processor (perhaps multiple cores)

What can / use HPC for?



Code-Internal Parallelization

- *Example: Climate model*



Code-External Parallelization

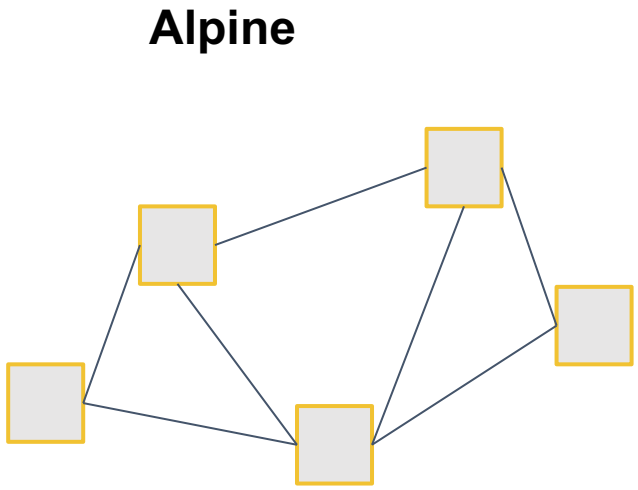
- *Example: Lots of satellite images*

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

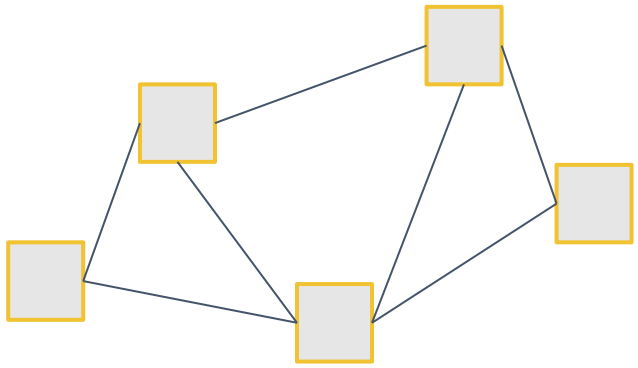


- Alpine is the 3rd-generation HPC cluster at CURC, following:
  - Janus
  - RMACC Summit

- 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

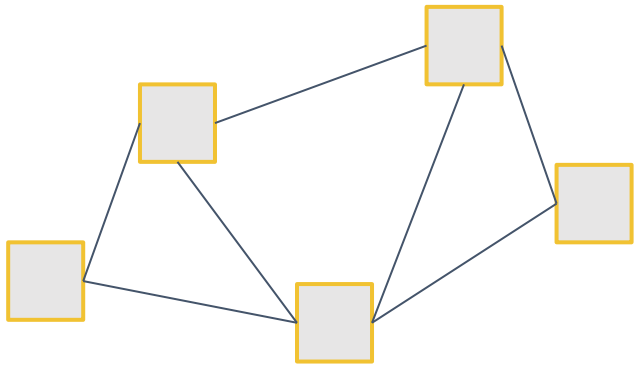


- Hardware on Alpine will continue to be purchased and released in stages:

- Alpine (stage 4):
  - 347 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

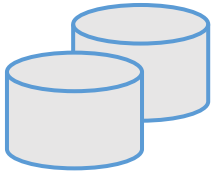
Alpine



- 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

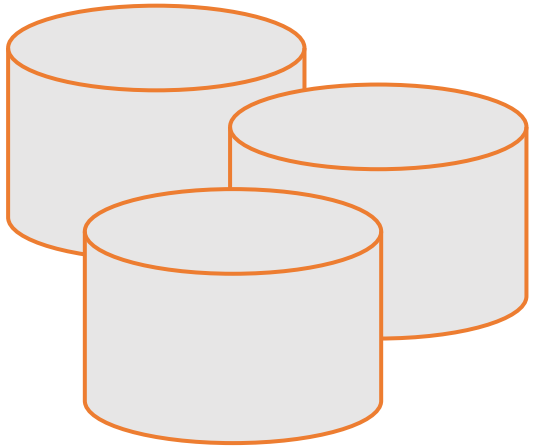
Storage at CURC

Core



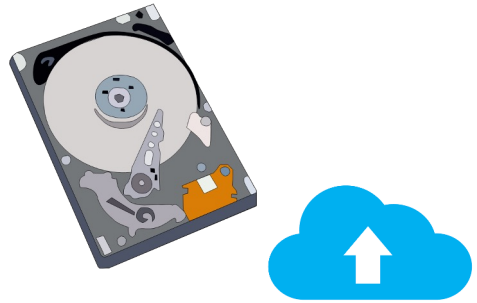
- Included with RC account
  - /home
  - /projects
  - scratch space

PetaLibrary



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

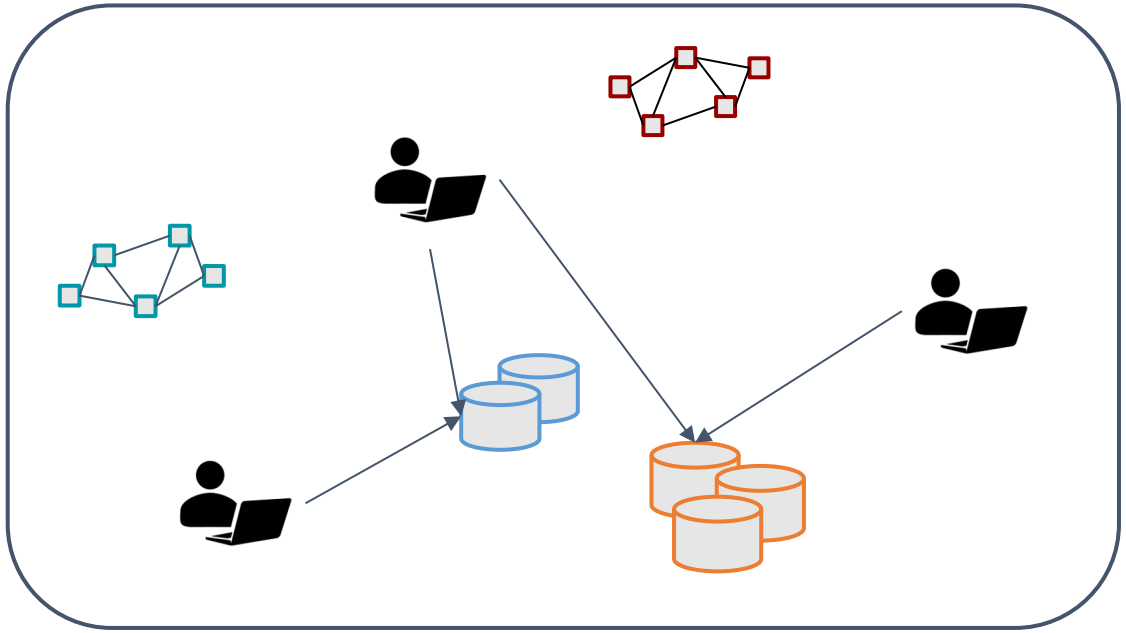
Local or Cloud



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

Data Sharing: Within RC

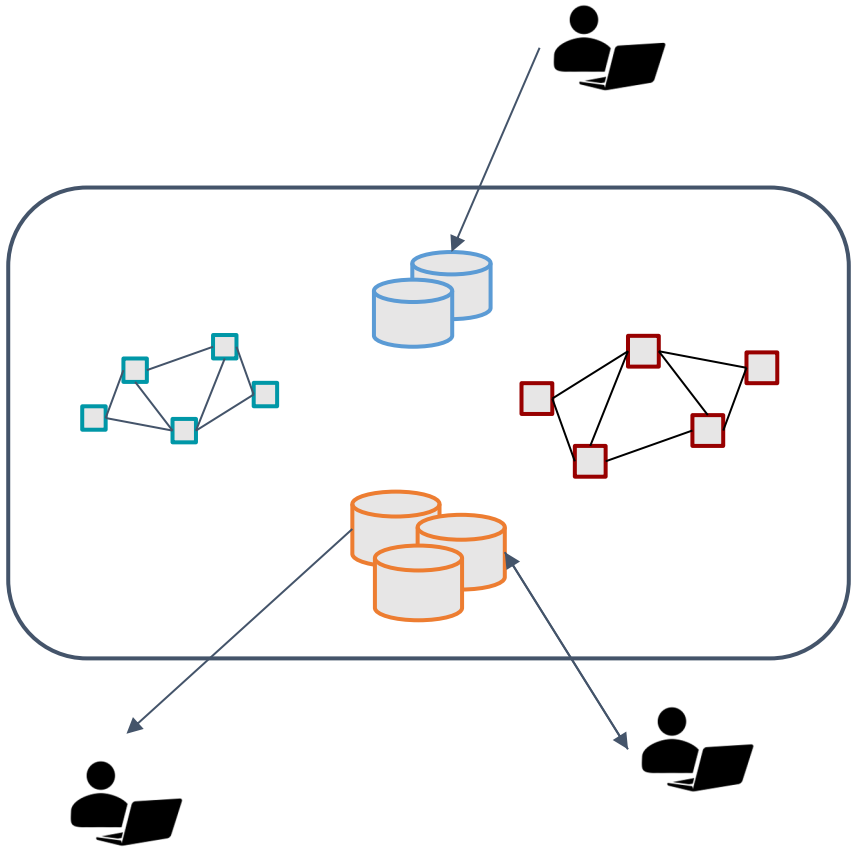
- Sharing workspaces
  - Project space
  - Scratch Space
  - PetaLibrary Space*



**If you have purchased PetaLibrary space; RMACC members may purchase PetaLibrary active space at an external user rate (institutional agreement required).*

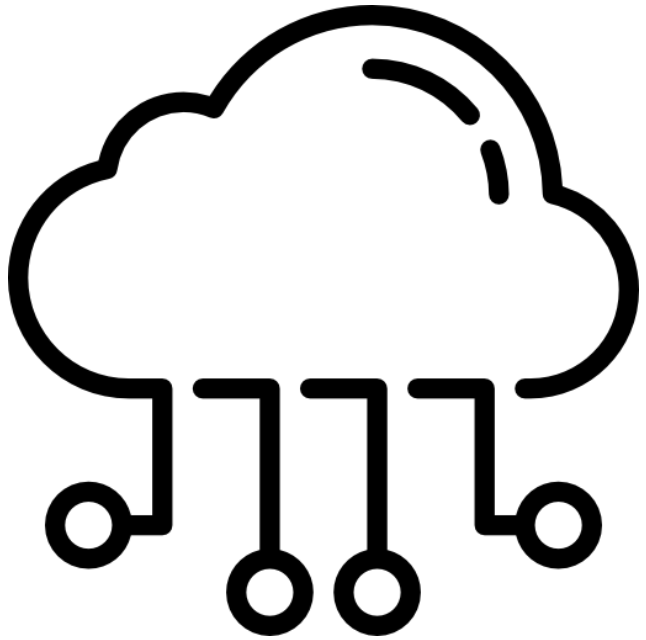
Data Sharing: Outside RC

- Globus (recommended):
  - GUI Web Application
  - Automates large transfers
  - Resumes failed transfers
  - Distributes large transfers across data transfer nodes (DTNs)
  - Endpoints that can shared
- Command line tools
  - scp, sftp, rsync, rclone
  - Note: not available to all RMACC members



Cloud Computing

- CURC supports AWS, Azure, and GCP
  - For use cases not well-supported by HPC
  - *Note: RMACC users are not eligible for CURC's commercial cloud support (use Jetstream2!)*
- Can be used as an alternative to HPC
- Can be used to enhance HPC
  - Automatic job submission, high availability, etc.



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 (1)

- **University of Colorado, Boulder users and CU Boulder 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/

If you do not have an account yet, we would be happy to assist after this lecture if time allows!

Getting an RC Account (2)

- **CU Anschutz Users:**
  - Create an ACCESS-CI Account in the ACCESS user portal
  - Reach out to hpcsupport@cuanschutz.edu to receive and sign the End-User Agreement

- **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

If you do not have an account yet, we would be happy to assist after this lecture if time allows!

Demo: Getting an Account

- CU Boulder, CSU users and affiliates:
  - Request an account through the RC Account request portal:
    https://rcamp.rc.colorado.edu/accounts/account-request/create/organization
- AMC, RMACC users and affiliates:
  - Request an account through the ACCESS-CI User Registration Portal:
    https://identity.access-ci.org/new-user.html

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 for all users)
  - ~2,000 SUs / Month
- Ascent Allocation
  - 350,000 SUs. (100,000 SUs for RMACC members; variable for AMC, CSU)
- Peak Allocation
  - >350,000 SUs (not available to RMACC members; variable for AMC, CSU)

Request an allocation at https://curc.readthedocs.io/en/latest/clusters/alpine/allocations.html

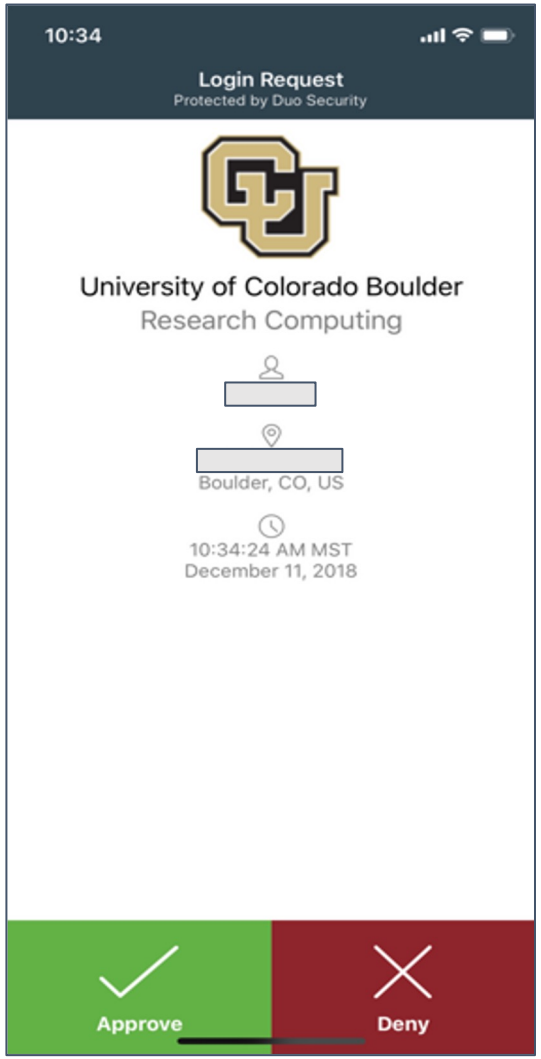
Two Factor Authentication (Duo)

- Provides an extra level of authentication
  - We are outside the firewall!
  - Valuable resources
  - Inviting, high-profile target

- Duo
  - You will receive information on setting up Duo when your account is established.
  - The Duo instance you use depends on your institutional affiliation.

Duo Authentication

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

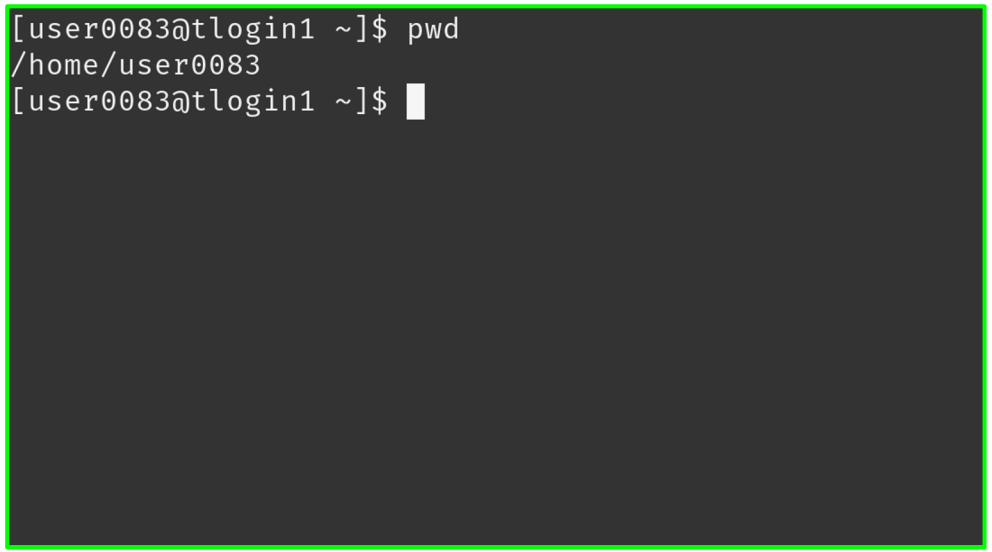


Linux comfort level check

- 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
  - For CU Boulder users: ondemand.rc.colorado.edu/
  - For AMC, CSU and RMACC users: ondemand-rmacc.rc.colorado.edu/



Demo: Logging in via Terminal*

- To login to an RC login node (CU or CSU users):

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

- To login to an RC login node (AMC users):

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

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

**ssh-based login is not available to RMACC users at this time – use OnDemand!*

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: https://ondemand.rc.colorado.edu.
- Other RMACC Institutions: https://ondemand-rmacc.rc.colorado.edu/

Logging In

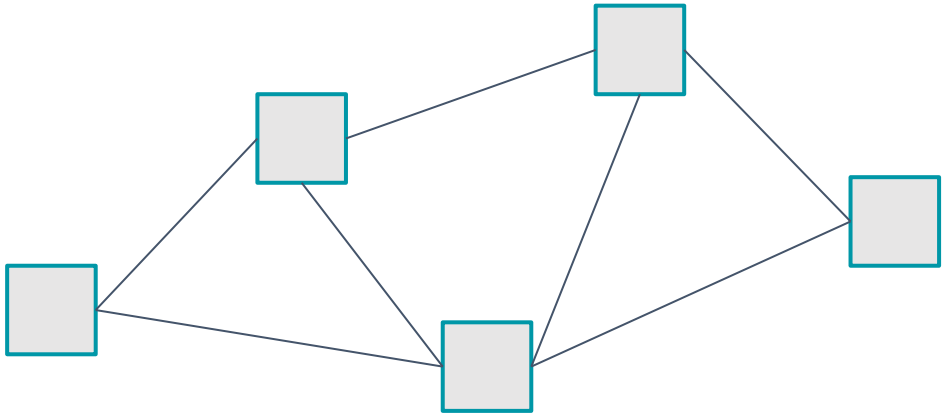
- It's important to note that you are ***NOT*** logging into any specific resource, Alpine, Blanca, etc.

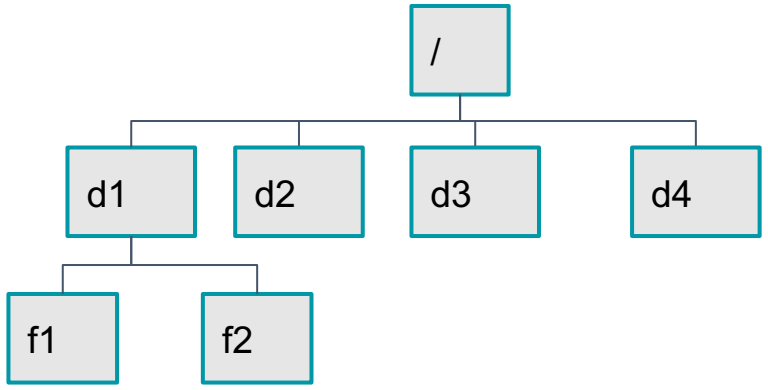
- When you log in, you land on our ***login nodes***

- From ***there***, you can access our other resources:
  - Alpine
  - Blanca
  - Petalibrary

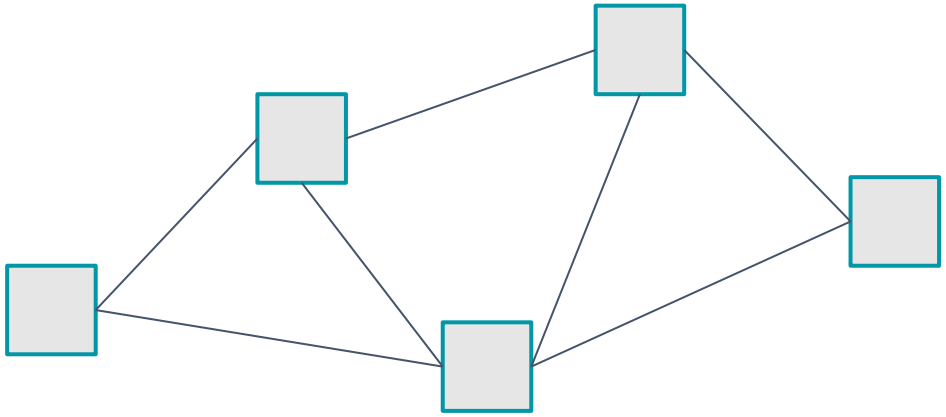
Navigating Research Computing

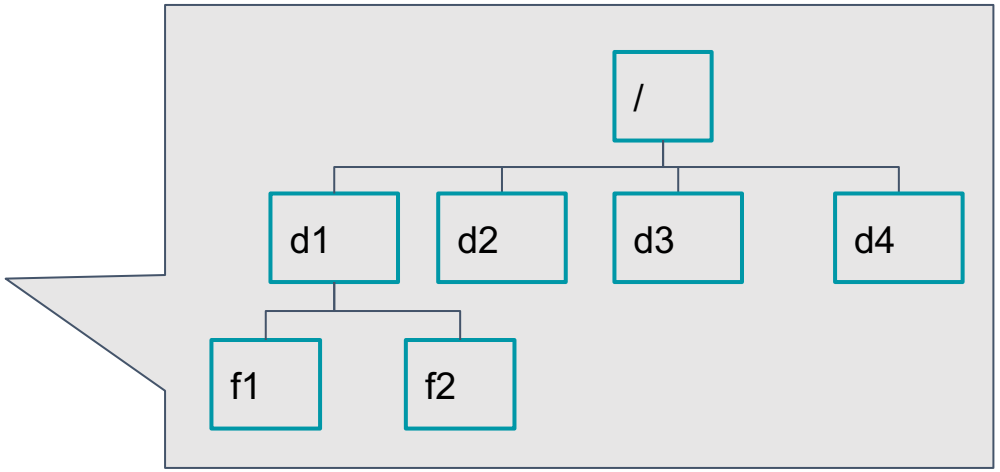
Node	File System
• One computing server • Physical hardware • Work together in parallel	• The basic tree-like layout • From most nodes* you have access to most file systems





Node	File System
• One computing server • Physical hardware • Work together in parallel	• The basic tree-like layout • From most nodes* you have access to most file systems





Node Types

Login	Compile	Compute
This is where you are when you login via a shell For editing code; job scheduling **No heavy computation**	This is where you compile code, install packages For exploring the Alpine software environment; editing compiling, and installing code; scheduling jobs **No heavy computation**	This is where scheduled jobs run For any type of research computation
Ex. edit job script	*Ex. Install python libs*	*Ex. Running Matlab*

Alpine Compile Nodes

- Alpine's `acompile` command starts an interactive job in which users can explore the compute environment and compile code.
  - 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

- **`$ 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
```

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

- So far we have:
  - Logged in
  - Explored nodes
  - Explored filesystem

- How do we actually *use* the computing resources?

Running a Job

Jobs

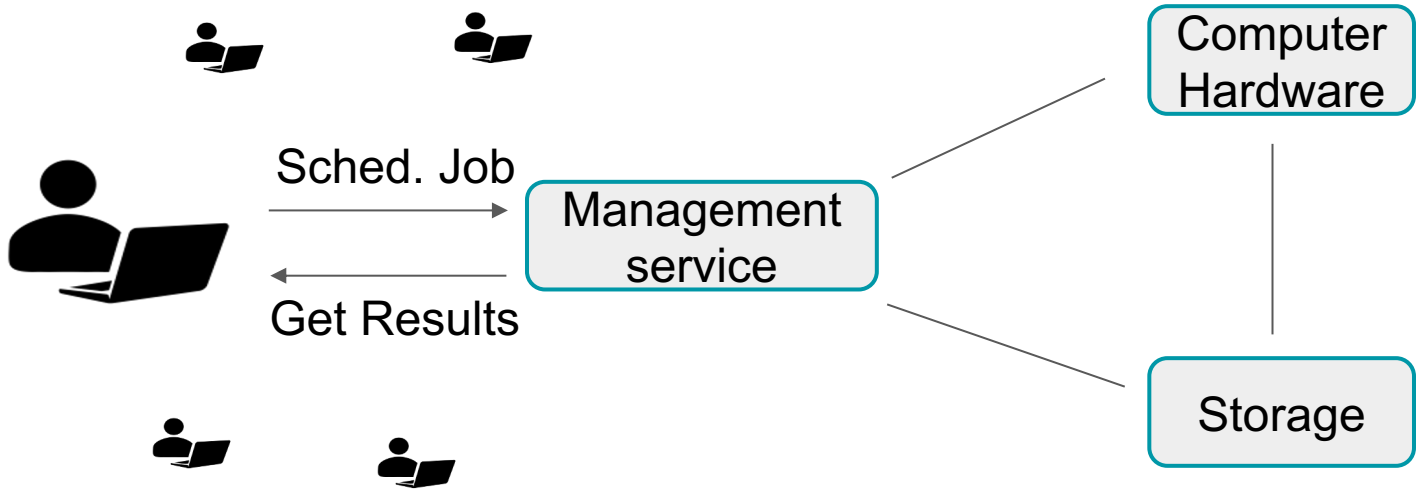
What is a "***job***"?

- 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:
  - Scheduled to a queue
  - When the required resources become available, the scheduler determines which set of nodes to use
  - Executes your job



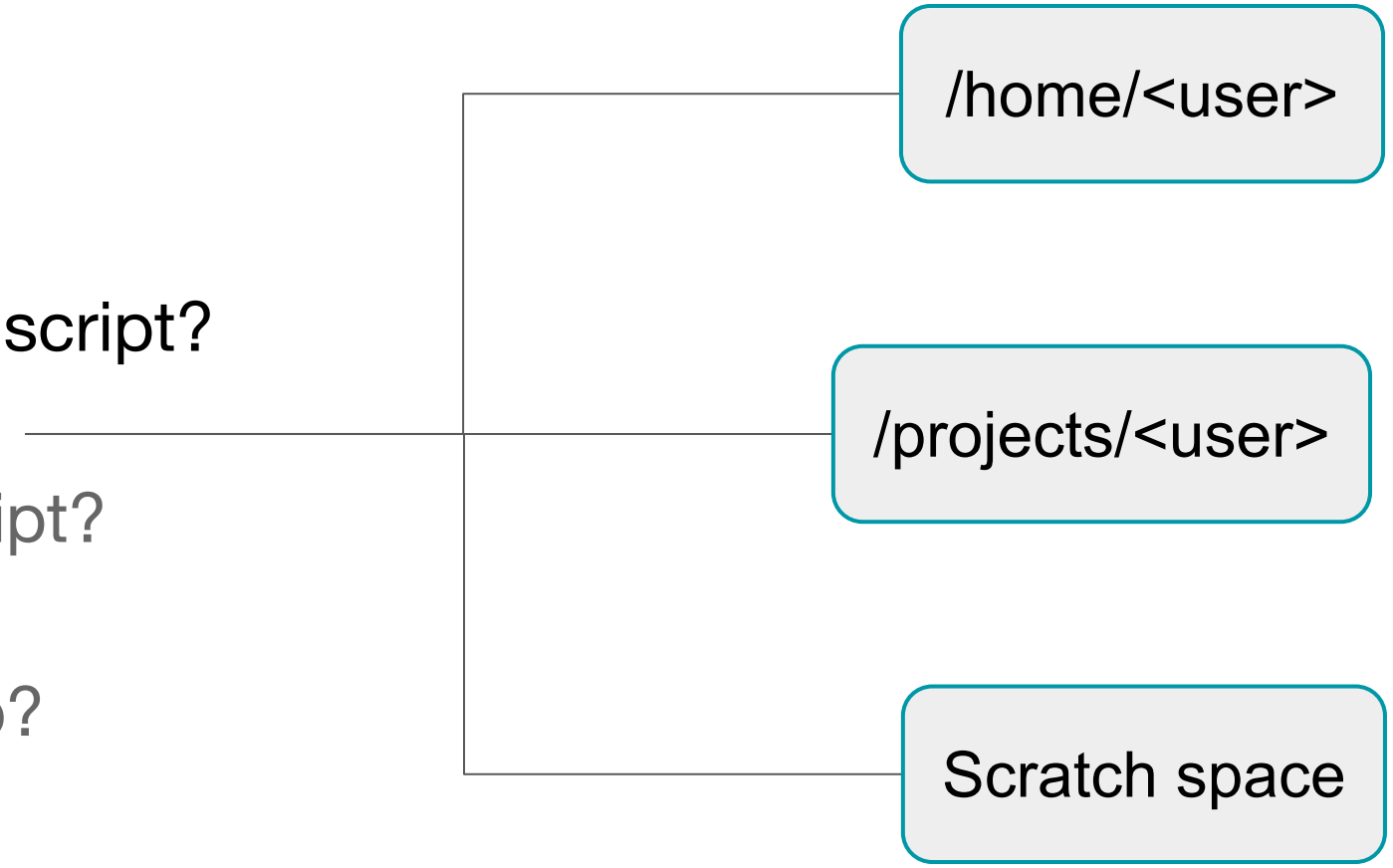
SLURM

- **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/save job script?
- How to write the job script?
- How to schedule the job?



Job Script: 3 main parts

1. Directives
   - Specify resource requirements
2. Software
   - Because jobs run on a different node than from where you scheduled…
   - …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>`
- 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 similar hardware configuration
  - **Wall time**: Max time your job will run for
  - **Node count**: Number of nodes requested
  - **Core count**: Number 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	347	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

Job scheduling Demo

- There are several example job scripts in the “examples” subdirectory of the slide repository.
- Feel free to download and adapt these for your workflow!

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/
  - **What should I do next?:**
    - Supercomputing Spin Up: Part 1 – Working with Linux
    - Supercomputing Spin Up: Part 2 – Submitting Jobs
- **Helpdesk**: rc-help@colorado.edu
- **Consultations:**
  - **Drop-in: Tuesday (12-1p) and Thursday (1-2p; virtual) during Fall/Spring semesters**
  - **Or schedule a 1:1 consultation by emailing the Helpdesk.**

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