New Kid on the Block: Getting Started with Alpine

New Kid on the Block: Getting started with Alpine

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 the basics of the Alpine cluster
2. Getting an account & logging in
3. Alpine Allocations
4. Navigating Research Computing
5. Alpine Software
6. Moving your data
7. Running a job (time allowing)
8. Help!

Things to take note of:

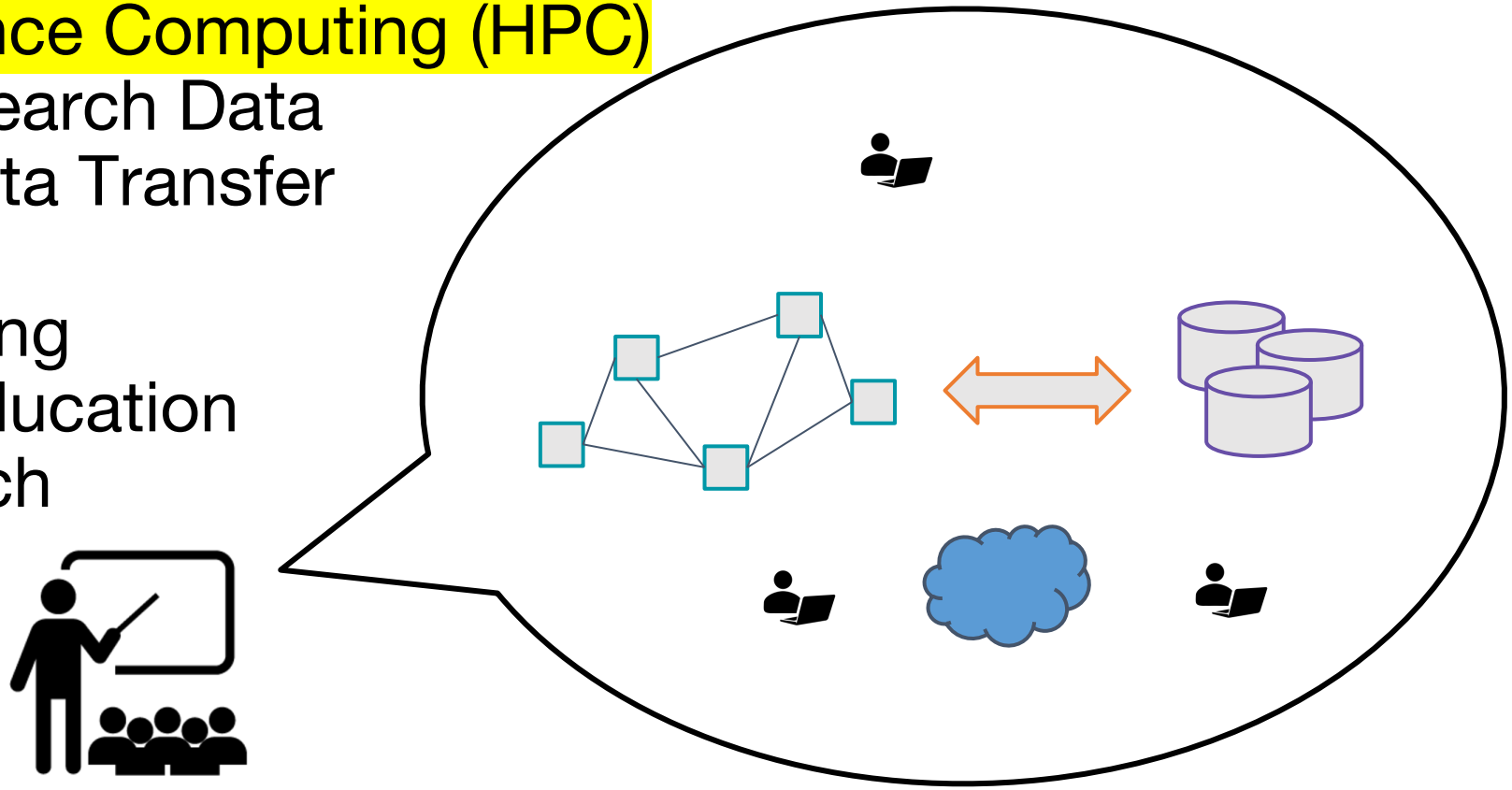
- Confusing, ambiguous, highly nuanced concepts
- Our goal is to help you avoid common mistakes, pitfalls, and frustrations

Ask Questions!

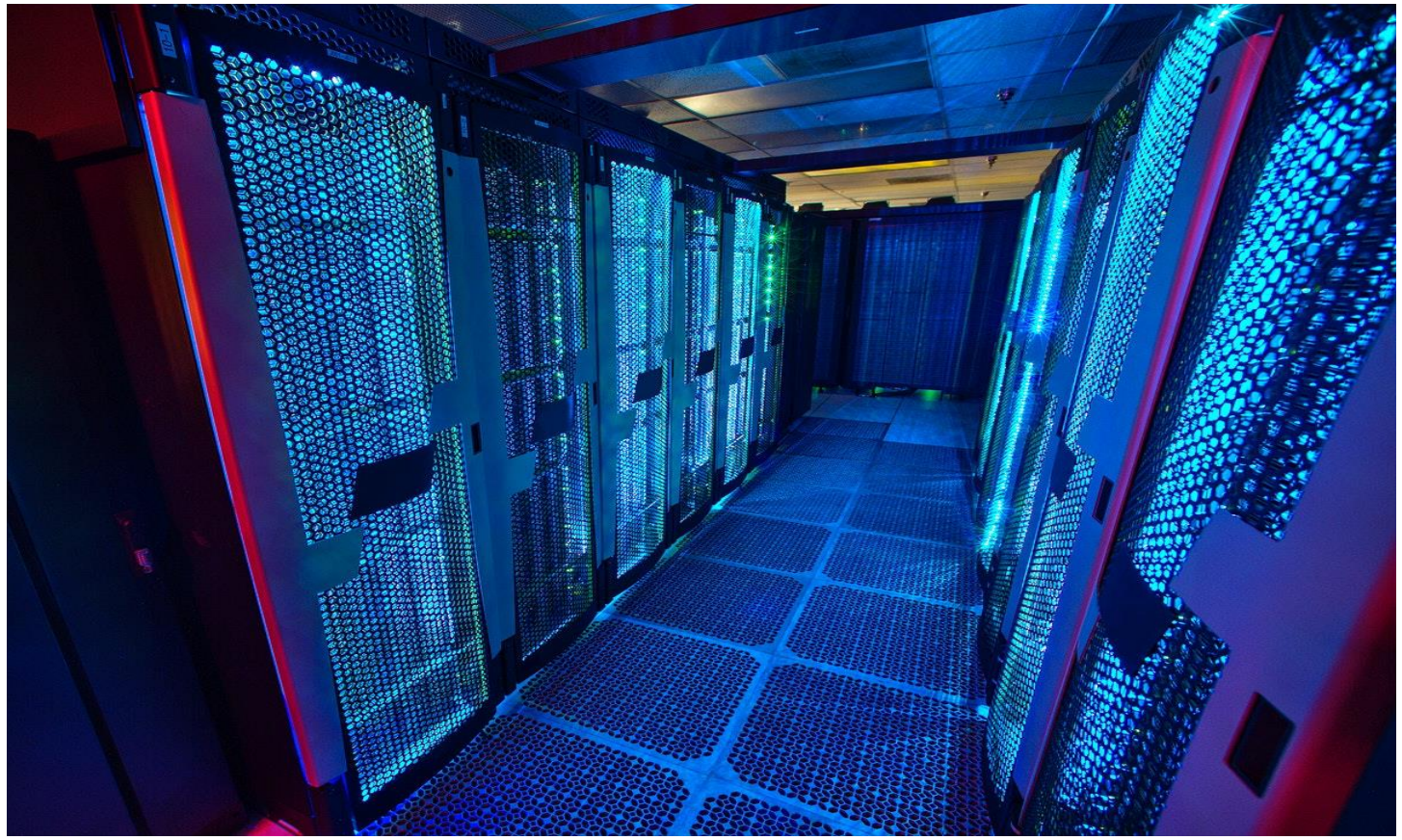
Understand the Basics of the Alpine Cluster

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

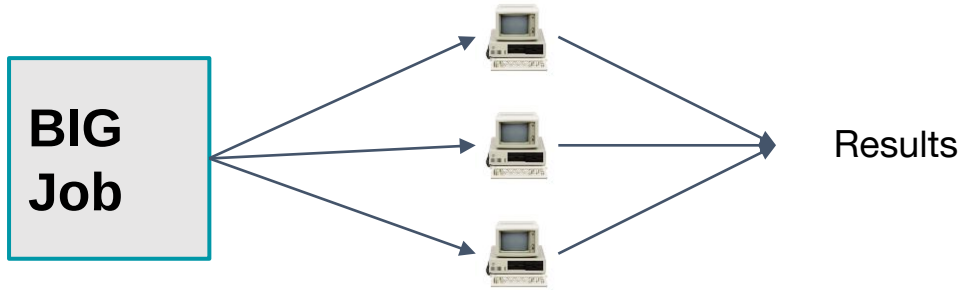
- Traditional computing *generally* has access to a single processor (perhaps multiple cores)

What can / use HPC for?

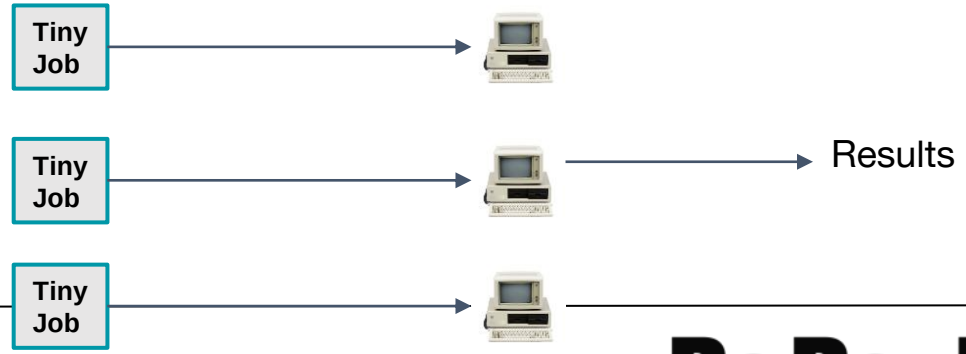
- Solving large problems that require more:
  - Memory than you have on your PC
  - cores/nodes/power thank you have on your PC
- Jobs that require hardware you may not have:
  - High Performance GPU computing
  - Specific Operating System
- Visualization rendering

What can / use HPC for?

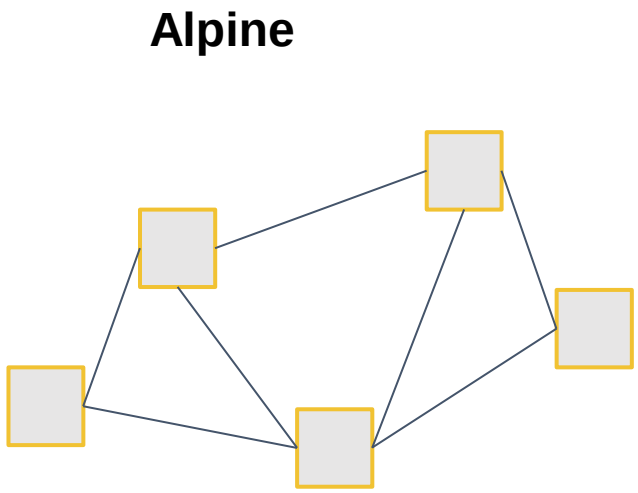
- Jobs that would take a long time on local machines can instead be distributed over hardware:
  - Parallelized to split up then joined (if software enabled)



  - Broken up into many serial jobs



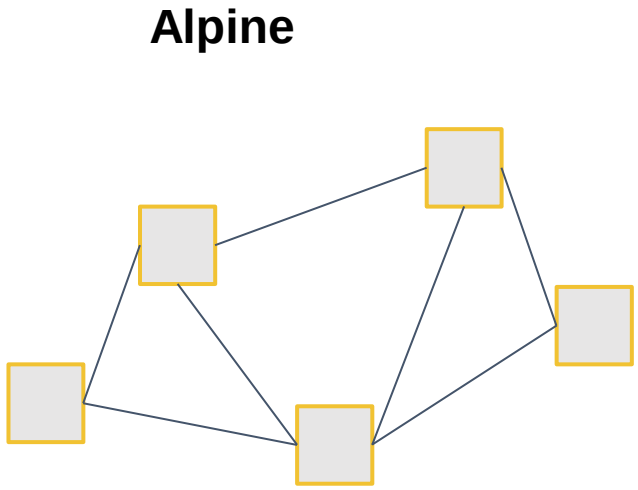
HPC Cluster: Alpine



- 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

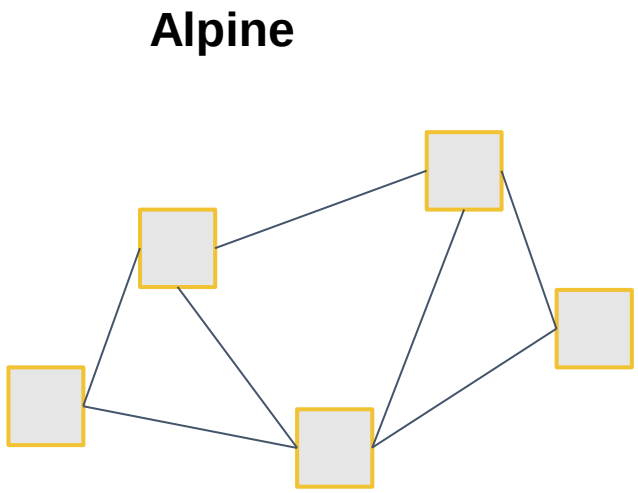
HPC Cluster: Alpine



- 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



- 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

Getting an Account & Logging in

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

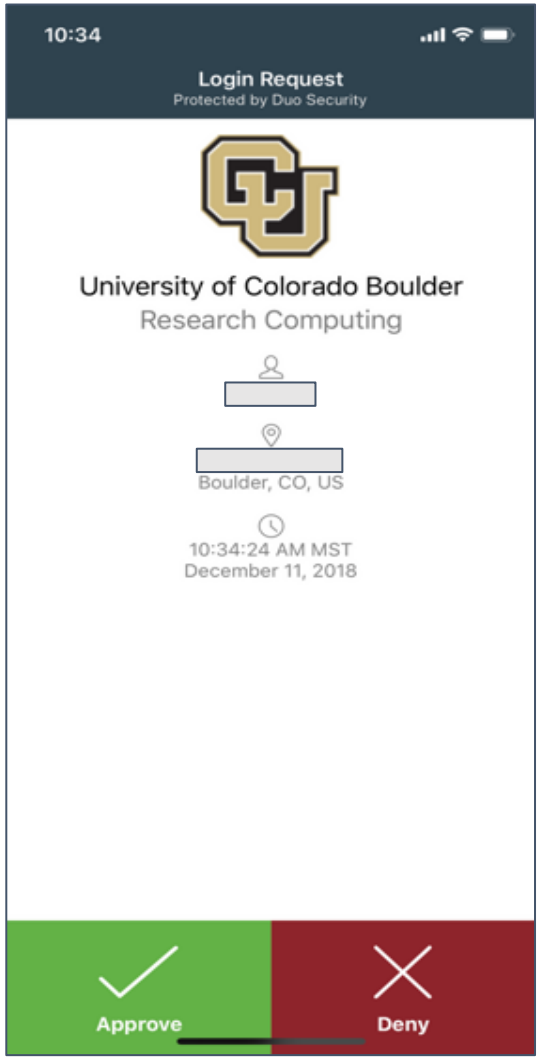
Two Factor Authentication (Duo)

- 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

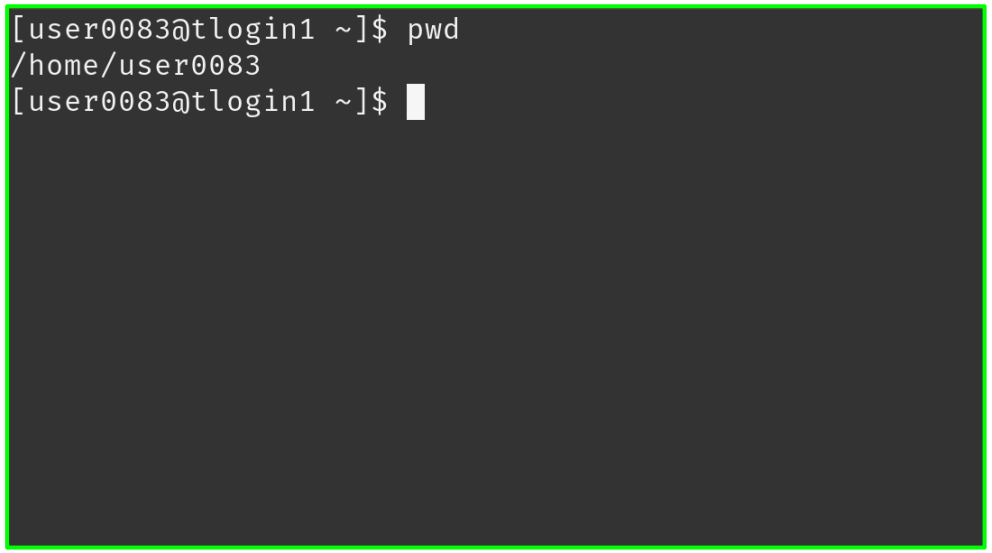
Duo Authentication

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



Accessing CURC

- 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

Alpine Allocations

Alpine Allocations

How much of the Alpine system can I use?

- Users are granted ~2,000 SUs / Month
  - SUs are roughly equivalent to CPU-hours, if you are running on a CPU node

What if I need to use more than 2,000 CPU-Hours / Month?

- Request more!

Alpine Allocations

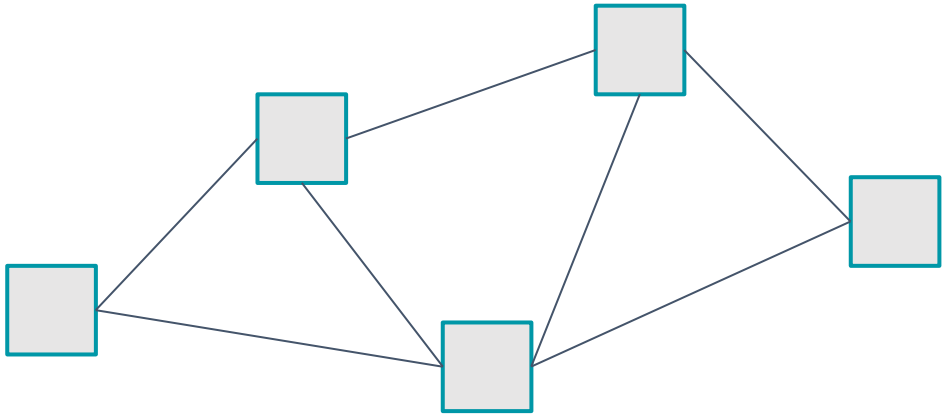
How can I use more computational time?:

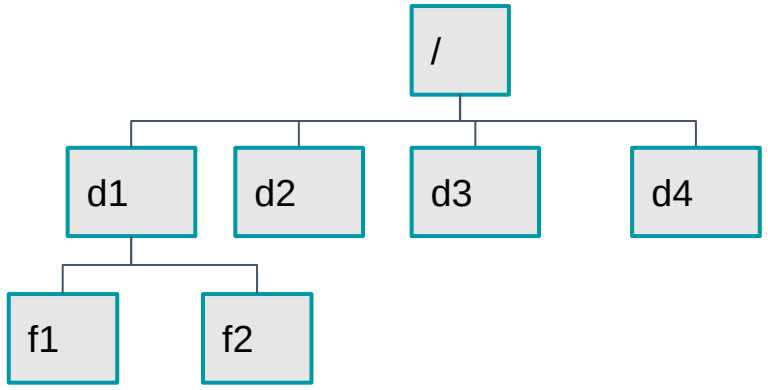
- Trailhead Allocation (Default)
  - ~2,000 SUs / Month
- Ascent Allocation
  - 250,000 SUs
- Peak Allocation
  - >250,000 SUs

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

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





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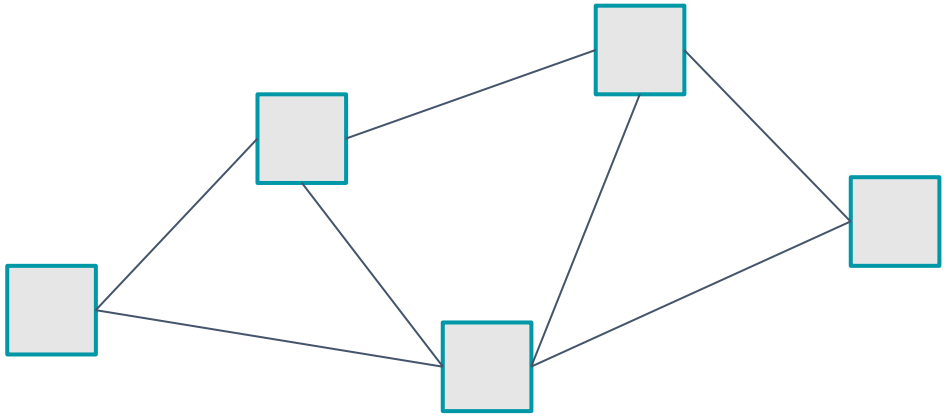
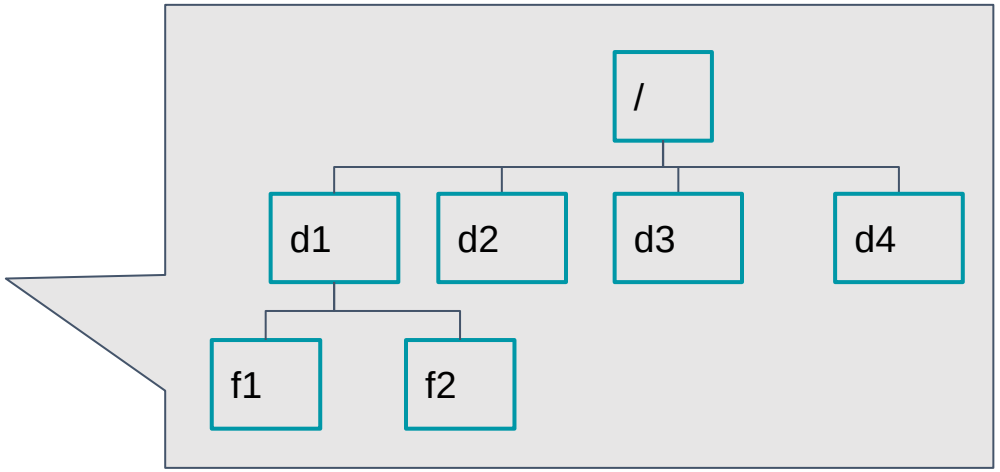




Node Types

Login	Compile	Compute
• Where you log in to • For editing code, job submission • No heavy computation	• Where you compile code, install packages • Explore the Alpine software environment • Edit code, submit jobs • No heavy computation	• Where scheduled jobs run • 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

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

Alpine Software

Demo: Exploring Software

- Once logged in, type:

  ```
  $ acompile
  ```

  To start an Alpine compile job.

- Once on a compile node, type:

  ```
  $ module avail
  ```

  To list currently available software

- Alternatively, type:

  ```
  $ module spider <software>
  ```

  To search for a specific software

Moving your Data

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

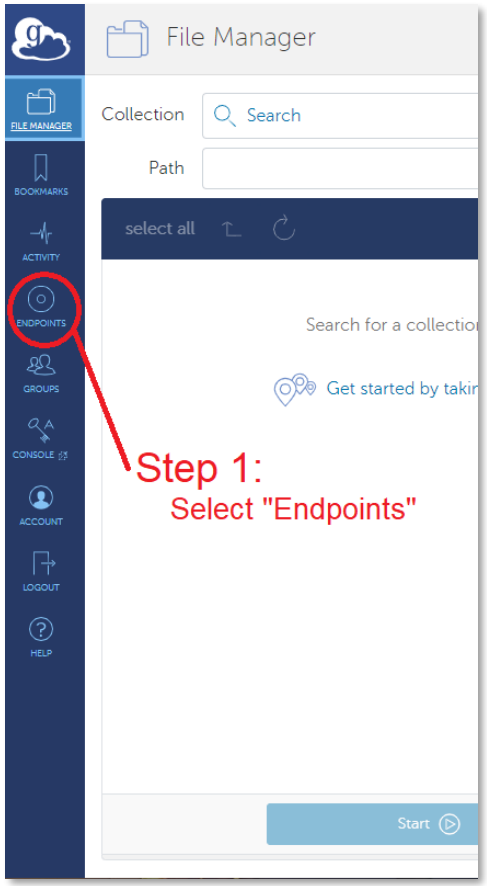
Exploring the Filesystem

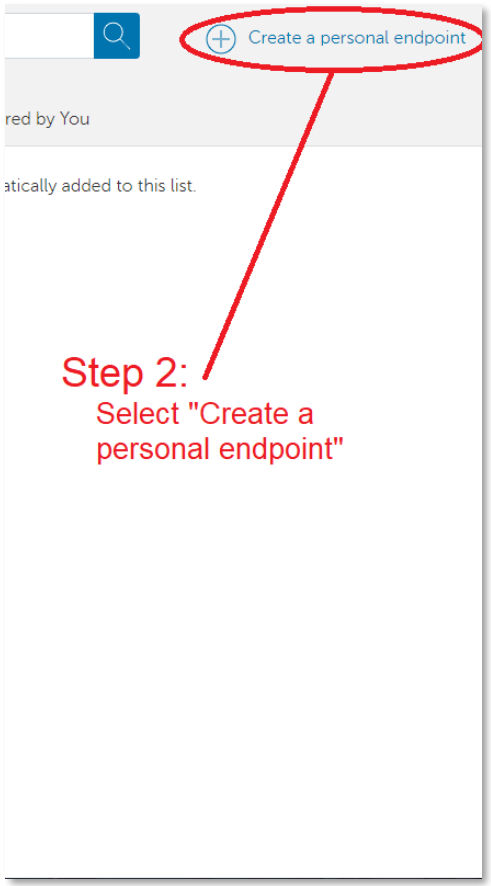
- Once logged in use the following commands to navigate to your different workspaces

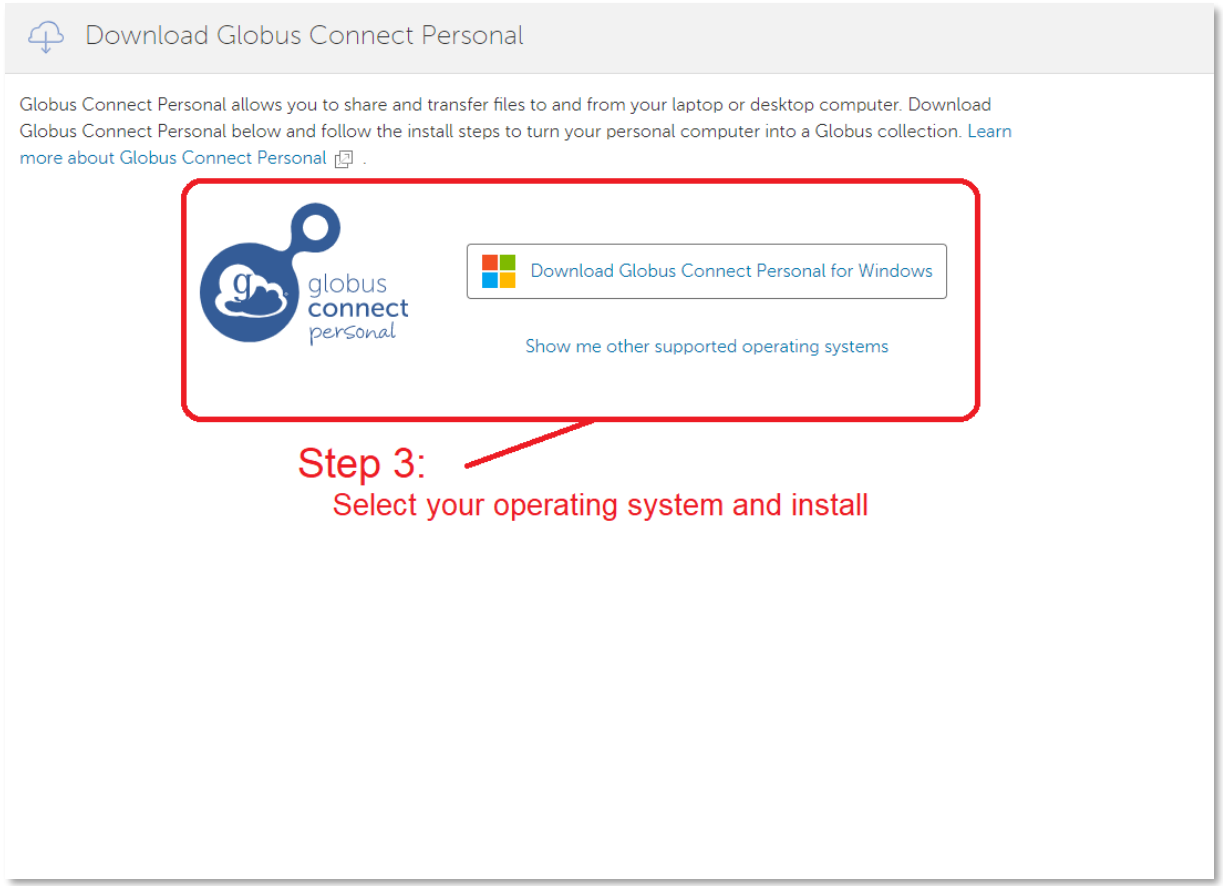
```
$ cd  /home/<user>
$ cd  /projects/<user>
$ cd  /scratch/alpine/<user>
```

How do I store my data on Research Computing resources?

- Globus
  - By far the most stable and recommended way for data transfers
  - Fast transfers
  - Transfers continue if a user disconnects
  - Web GUI option or Globus Connect Personal


File Manager
FILE MANAGER
BOOKMARKS
ACTIVITY
ENDPOINTS
GROUPS
CONSOLE
ACCOUNT
LOGOUT
HELP
Collection
Search
Path
select all
Search for a collectio
Get started by takir
Start
Step 1:
Select "Endpoints"


Create a personal endpoint
red by You
atically added to this list.
Step 2:
Select "Create a
personal endpoint"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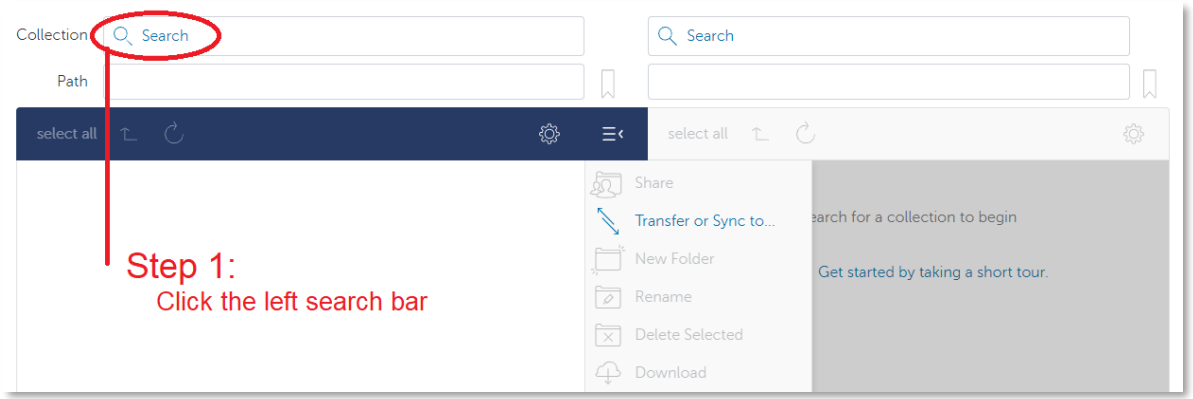
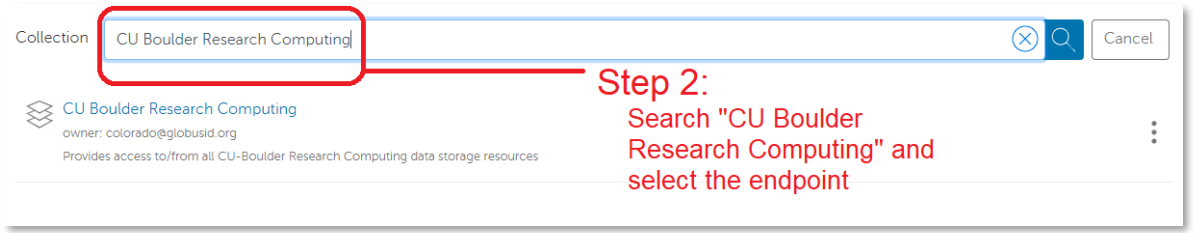
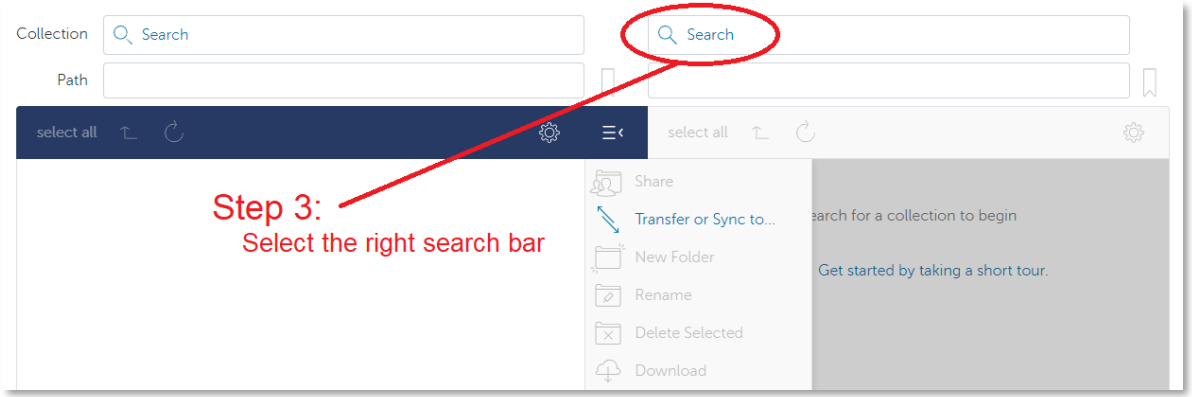
Globus Connect Personal allows you to share and transfer files to and from your laptop or desktop computer. Download Globus Connect Personal below and follow the install steps to turn your personal computer into a Globus collection. Learn more about Globus Connect Personal .
globus
connect
personal
Download Globus Connect Personal for Windows
Show me other supported operating systems
Step 3:
Select your operating system and install



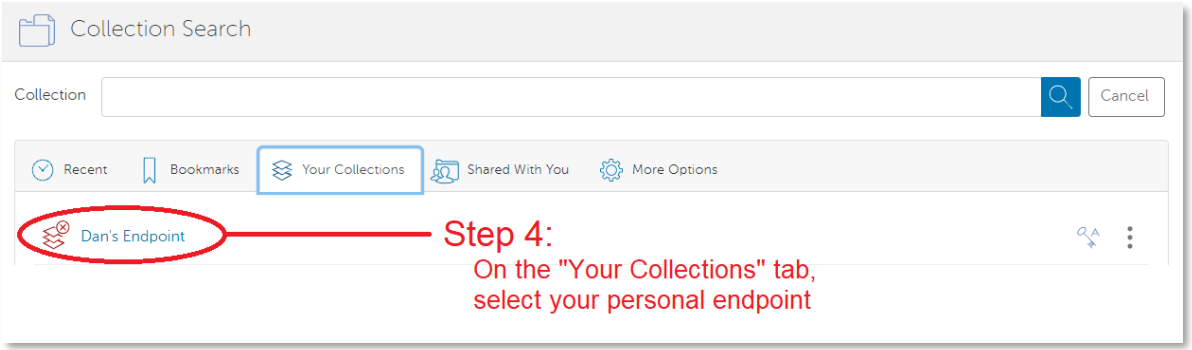
Step 1:
Click the left search bar



Step 2:
Search "CU Boulder Research Computing" and select the endpoint



Step 3:
Select the right search bar



Step 4:
On the "Your Collections" tab, select your personal endpoint

Are there other ways to move data?

- FileZilla
  - File transfer GUI application that can be used on Windows, Mac, and Linux.
- Secure Copy (scp)
  - Can send data to and fetch data from a remote server.
- Rsync
  - Can be used to synchronize files and directories across two locations, which can often lead to efficiencies in repeat-transfer scenarios.
- SFTP
  - An interactive alternative to scp that allows multiple, bi-directional transfer operations in a single session.
- Rclone
  - Command line program to manage files on cloud storage.

Check out our documentation on File Transfer for guides to using each of these tools:
https://curc.readthedocs.io/en/latest/compute/data-transfer.html

Running a Job

Jobs

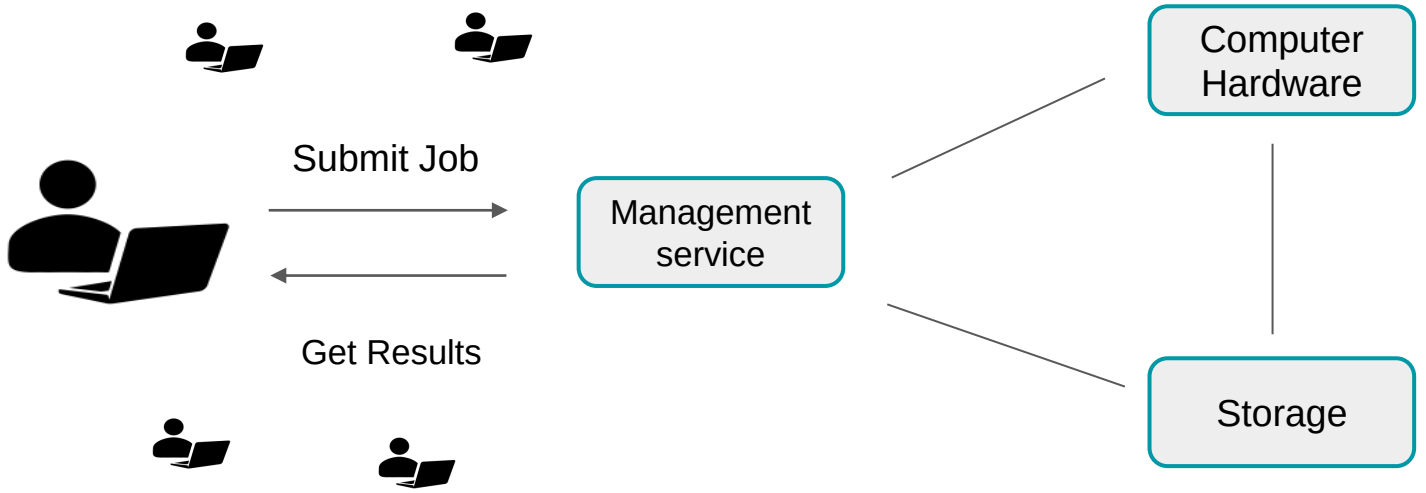
What is a "***job***"?

- 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

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 the basics of the Alpine cluster ☑
2. Getting an account & logging in ☑
3. Alpine Allocations ☑
4. Navigating Research Computing ☑
5. Alpine Software ☑
6. Moving your data ☑
7. Running a job ☑
8. 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 (4/11)
    - Supercomputing Spin Up: Part 2 – Job Scheduling (4/12)
- **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 partition 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