Alpine: New User Seminar

Research Computing
UNIVERSITY OF COLORADO **BOULDER**

Be Boulder.

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.

Account Check

Does anyone ***not*** have a **CU Research Computing account** who would like to use a temporary account*?

**only available during seminar*

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!

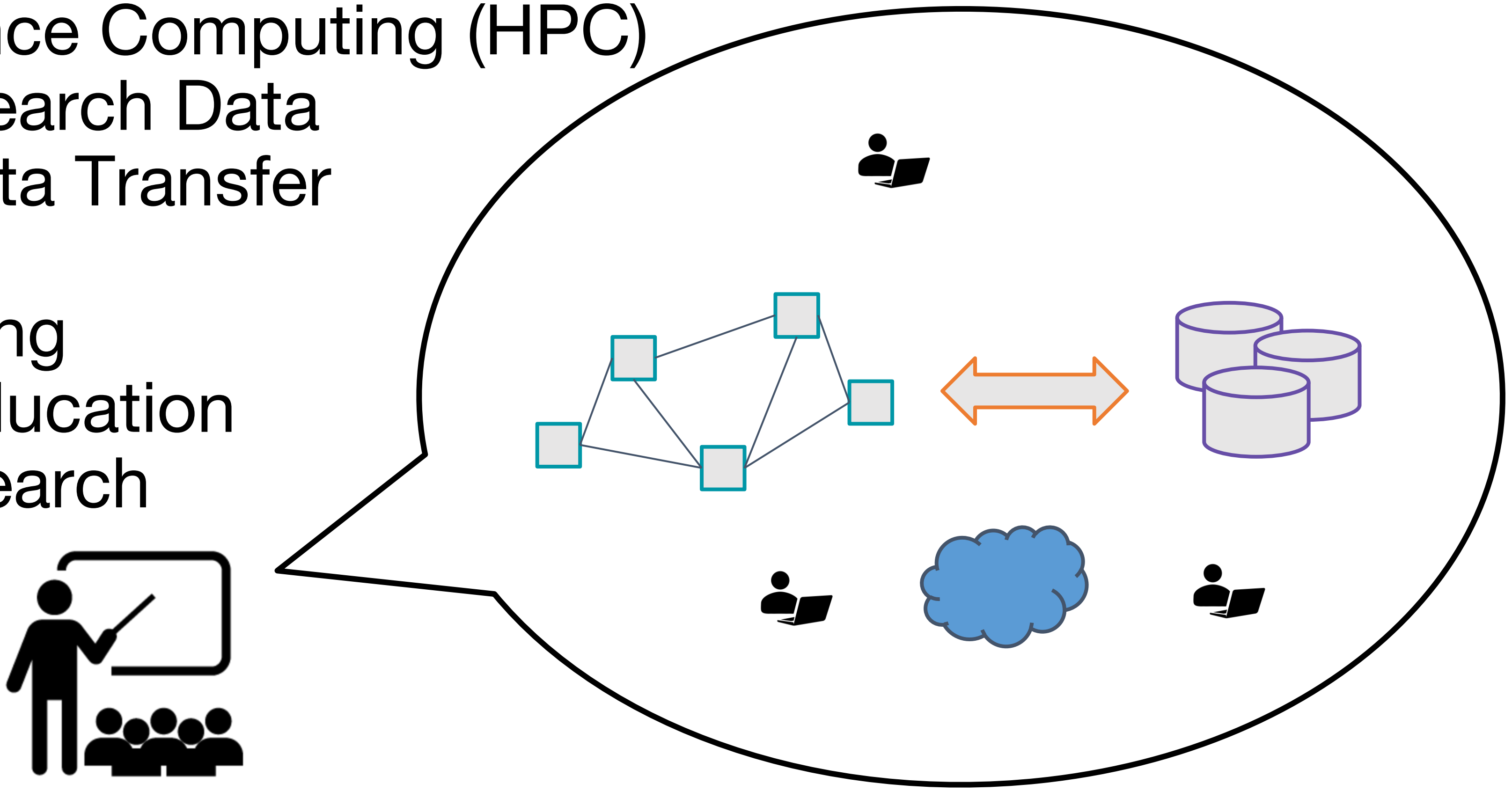
Things to take note of:

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

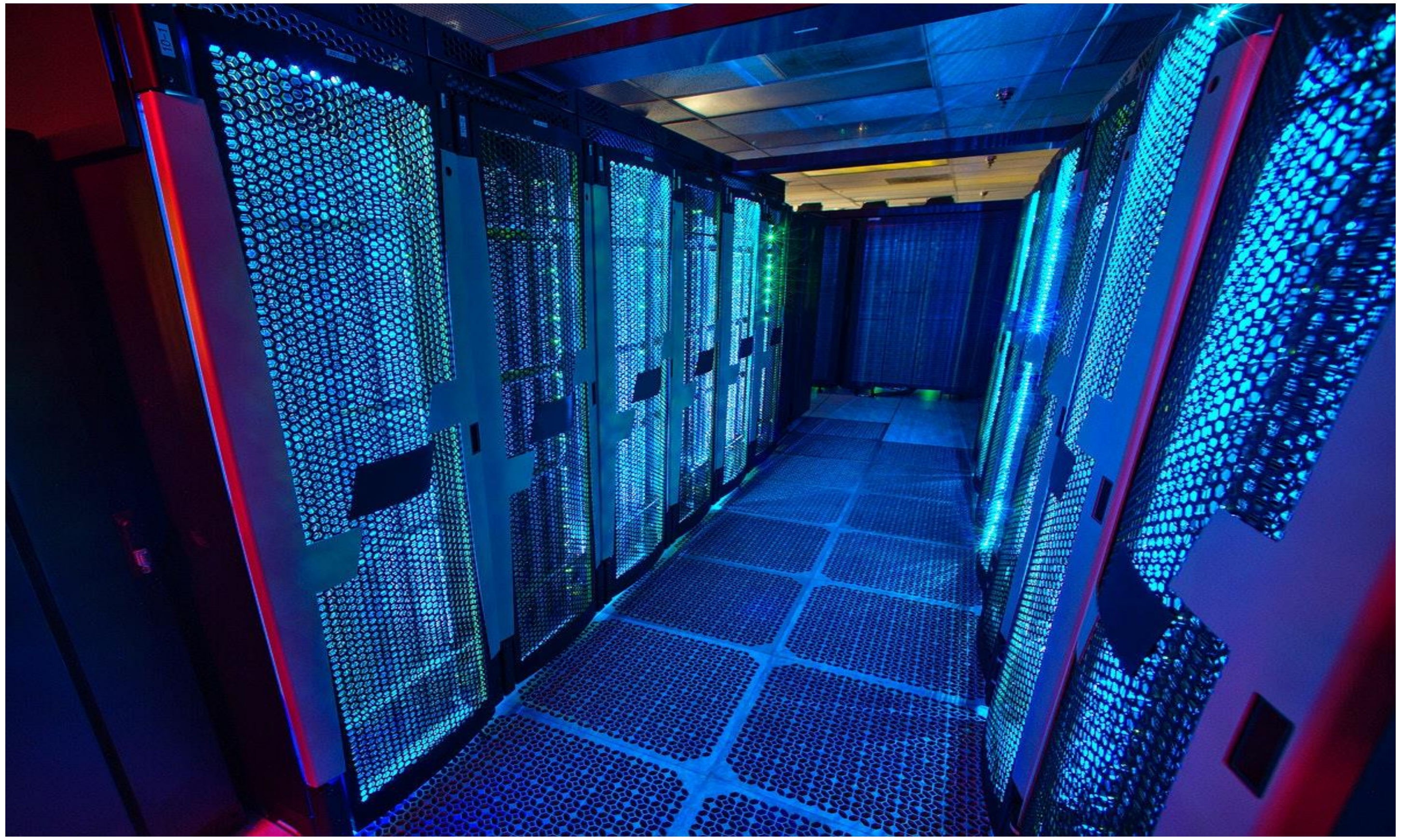
Ask Questions!

Resources Include:

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



Primarily known for:
High Performance Computing (HPC)

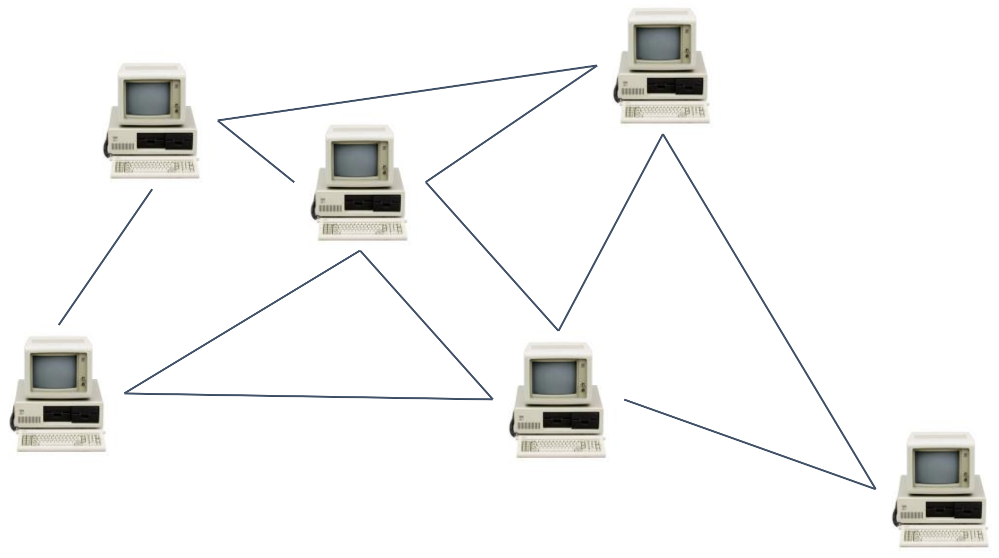


High Performance Computing (HPC) vs. Traditional Computing

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

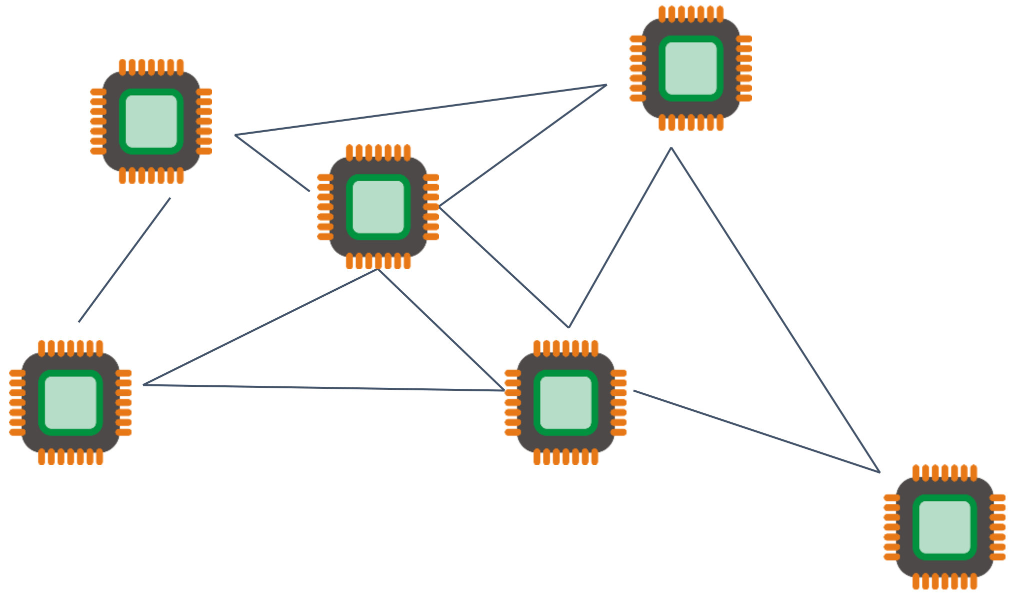
High Performance Computing (HPC) vs. Traditional Computing

- HPC is a network (or cluster) of hardware we call "nodes" linked together with high-speed interconnects



High Performance Computing (HPC) vs. Traditional Computing

- HPC is a multiprocessor environment that allows users to run jobs on several processors at once (also called parallel processing).



What can I 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

Puzzle Analogy

- Working on a puzzle by yourself (although enjoyable!) will take time, even if you're fast!

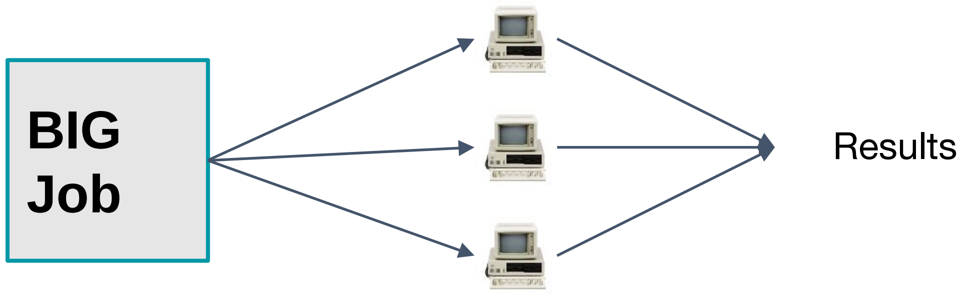
Puzzle Analogy

- You can speed it up by inviting friends over and enticing them with food!

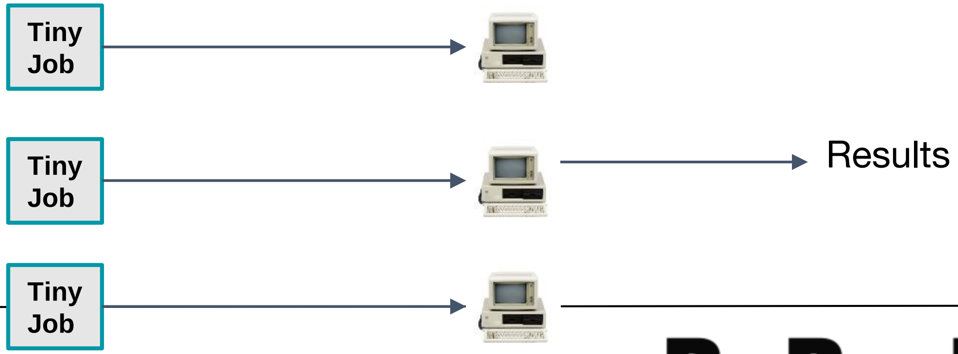
- What happens if there are too many people?

What can I 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)

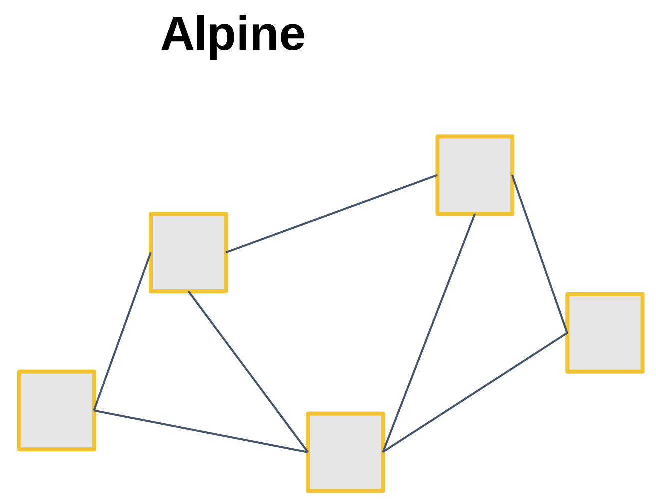


  - Broken up into many serial jobs



Research Computing Resources

HPC Cluster: Alpine

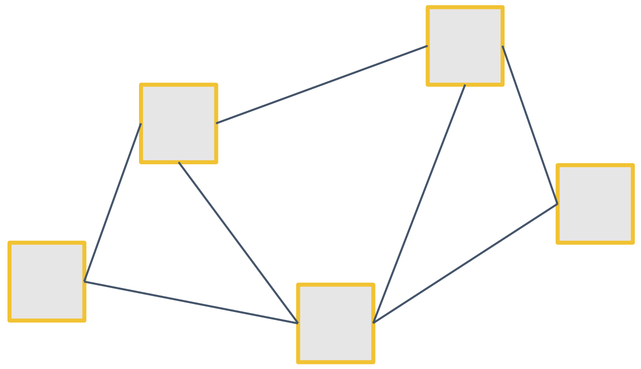


- Alpine is the 3rd-generation HPC cluster at CURC, following:
  - Janus
  - RMACC Summit

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

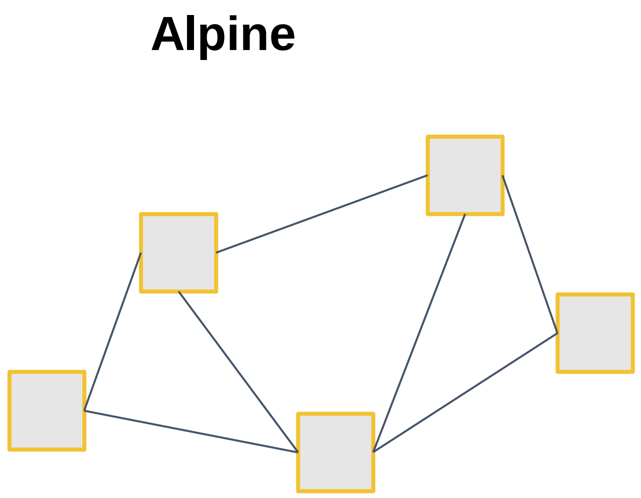
HPC Cluster: Alpine

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*

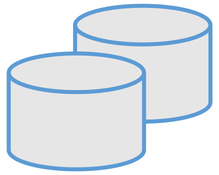
HPC Cluster: Alpine



- 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

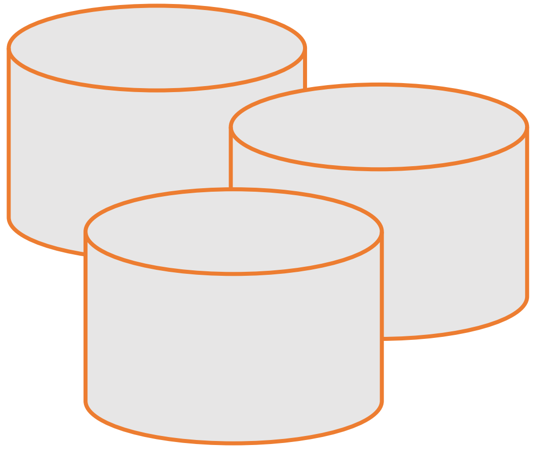
Storage at CURC

Core



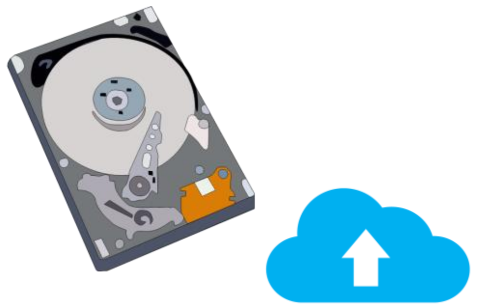
- Included with RC account
  - /home
  - /projects
  - scratch space

PetaLibrary



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

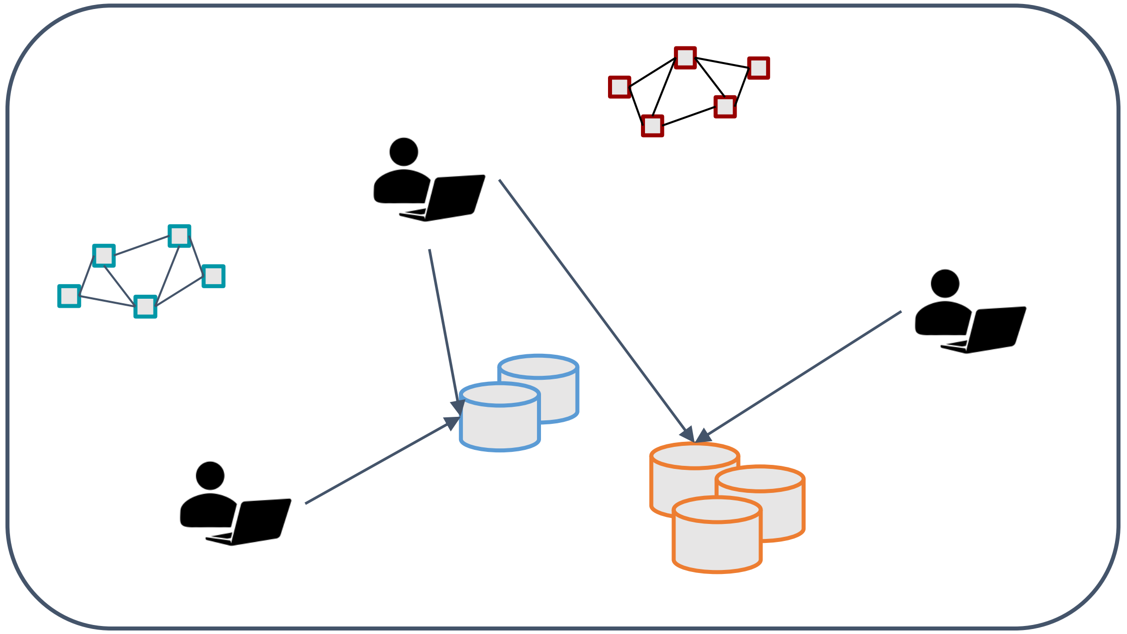
Local or Cloud



- You can download your data locally or to a variety of other cloud resources

Data Sharing: Within RC

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

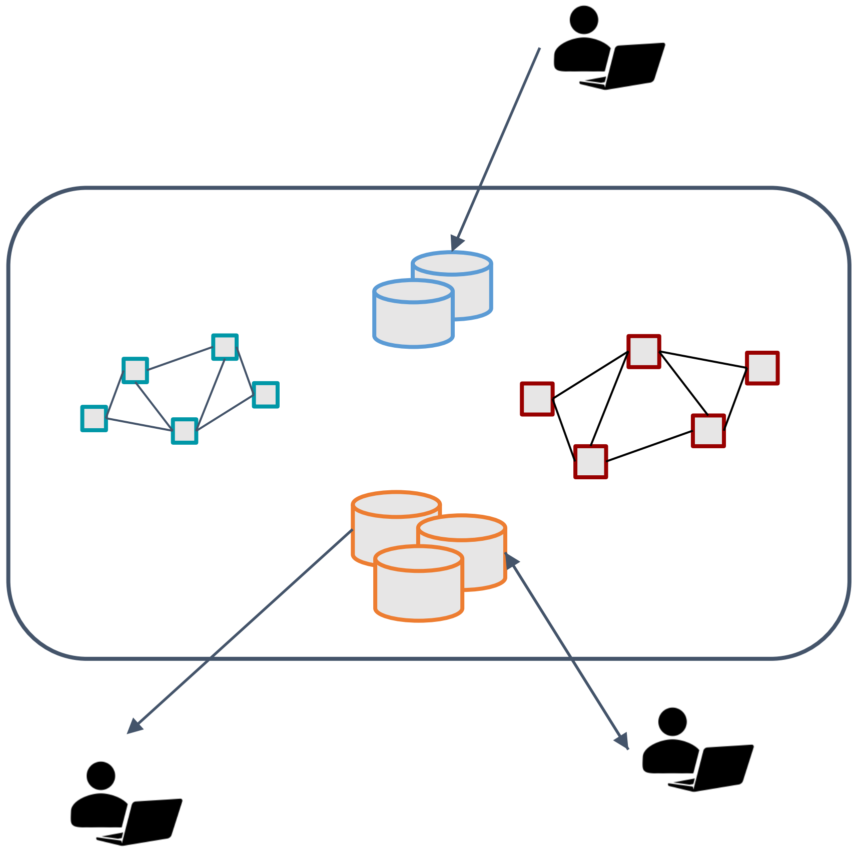


*If you have purchased PetaLibrary space

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
- Command line tools
  - scp, sftp, rsync, rclone



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

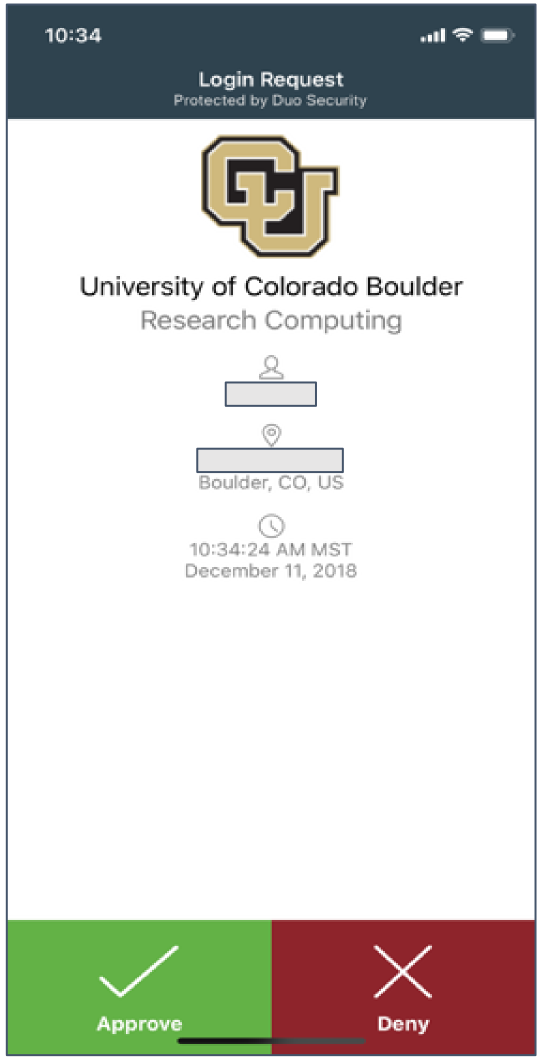
Two Factor Authentication (Duo)

- 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


10:34

Login Request
Protected by Duo Security

University of Colorado Boulder
Research Computing

[redacted]

[redacted]
Boulder, CO, US

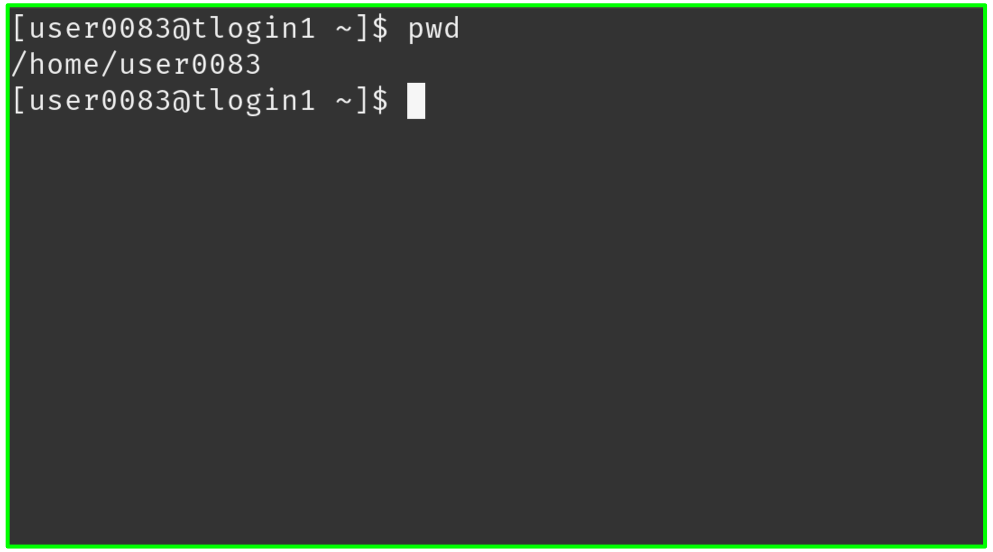
10:34:24 AM MST
December 11, 2018

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

---

If you're using a tutorial account (we provide password):

```
$ ssh <tutorial_user>@tlogin1.rc.colorado.edu
```

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

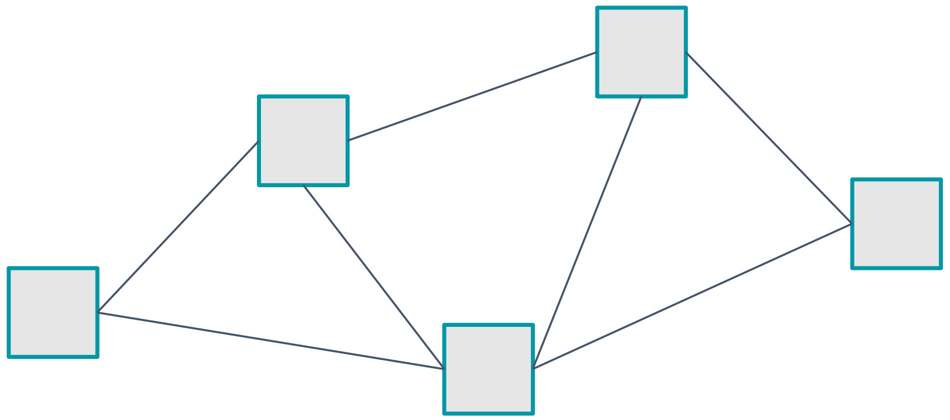
- It's important to note that you are ***NOT*** logging into any specific resource, Alpine, Blanca, etc.

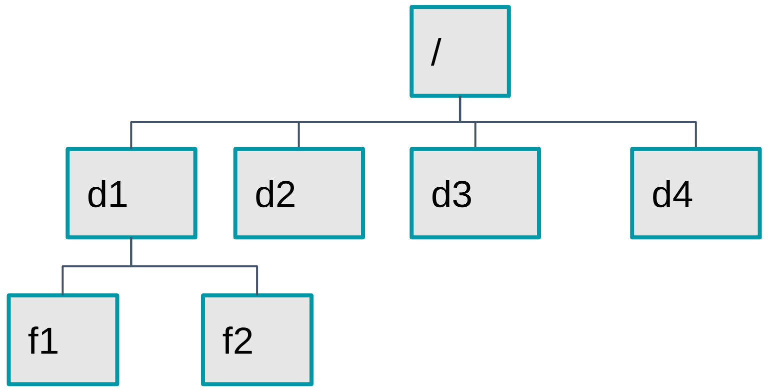
- When you log in, you land on our ***login nodes***

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

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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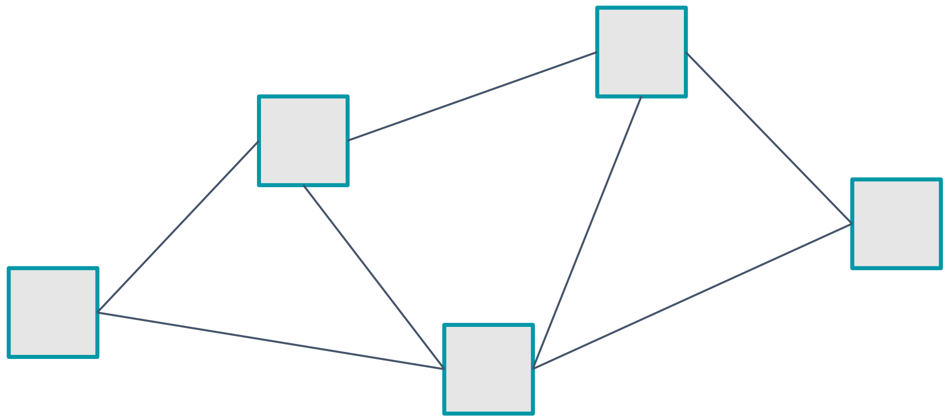
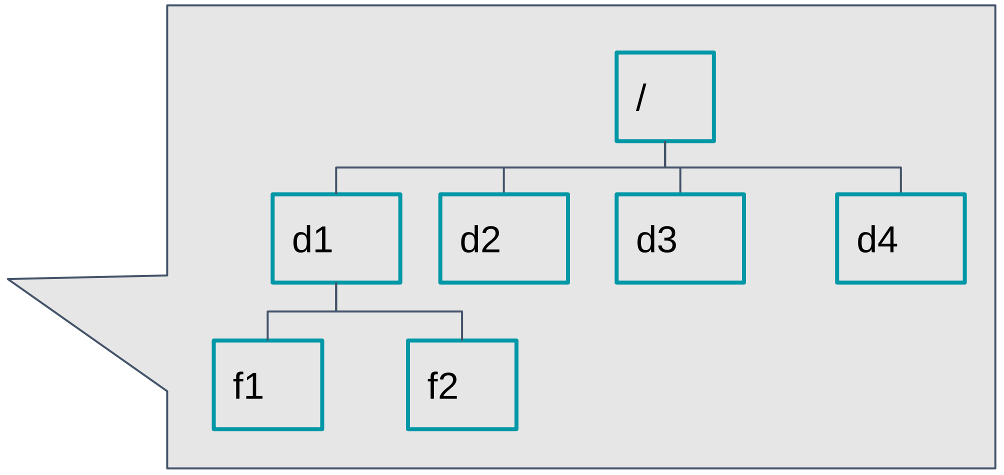




Node Types

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
    - 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)	/projects (250GB)	Scratch (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

Demo: 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

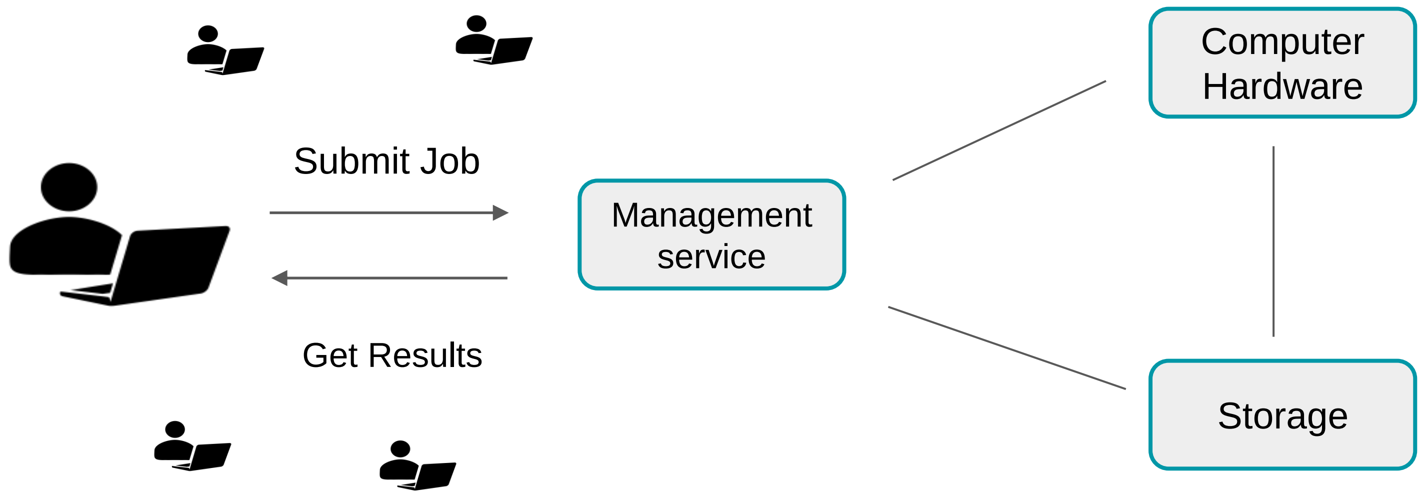
What is a "***job***"?

- 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



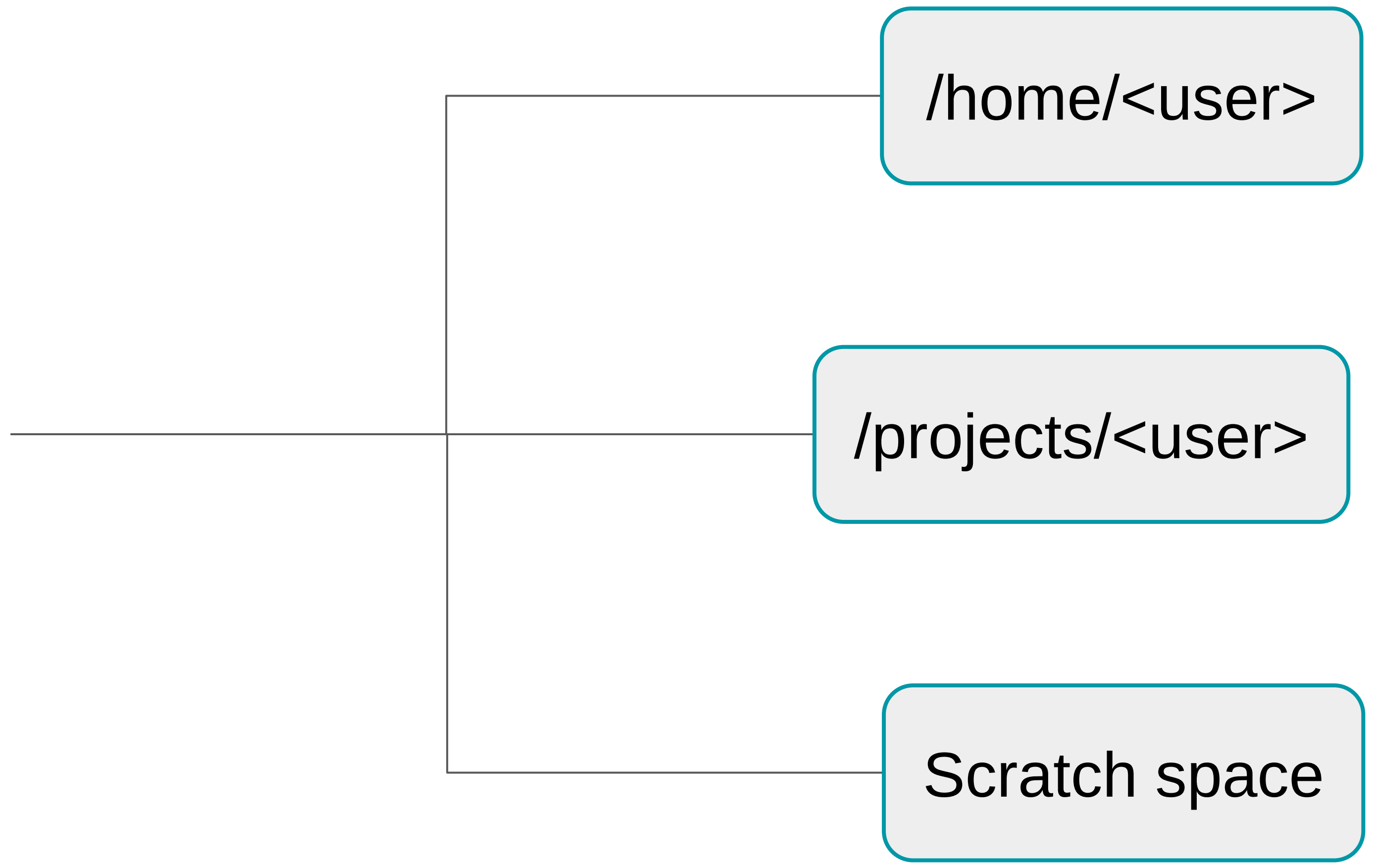
SLURM

- **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

Demo: Writing a simple job `hostname.sh`

- Submit a slurm job with the following instructions:

1. The job will be submitted from a bash script named **hostname.sh**
2. The job will run on **1 node**
3. We will request **1 minute of wall time**
4. Run on the **amilan-ucb partition**
5. Output should **contain job id**
6. The job should run the **Unix "`hostname`" command**

Demo: Writing a simple job (hostname)

- Set up batch job boilerplate
- Using text editor (vim or nano), create a file called **hostname.sh** with the following text:

```
#!/bin/bash

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

## Software
module purge

## User Scripting
```

Demo: Writing a simple job (hostname)

- Directives:
  - 1 node
  - 1 minute wall time
  - “amilan-ucb” partition
  - Output should contain job id

- Number of nodes:
  `--nodes=<nodes>`
- Wall time:
  `--time=<wall time>`
- Partition:
  `--partition=<partition_name>`
- Output file:
  `--output=<file name>`
  `(%j gives you job id)`

Demo: Writing a simple job (hostname)

- Software:
  - Do we need any software? (modules)
- User script:
  - What command do we want to run?

Demo: Writing a simple job (hostname)

```
#!/bin/bash
#SBATCH --nodes=1                       # Number of requested nodes
#SBATCH --time=0:01:00                  # Max wall time
#SBATCH --partition=amilan-ucb          # Specify Summit haswell nodes
#SBATCH --output=hostname_%j.out        # Rename standard output file

# purge all existing modules
module purge

hostname
```

Submitting a Job

1. Load up the slurm Alpine module

```
$ module load slurm/alpine
```

1. Submit the job:

```
$ sbatch <script-name>.sh
```

1. Check output

```
$ cat <output-name>.out
```

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/
- **Helpdesk**: rc-help@colorado.edu

Questions

Survey and feedback

http://tinyurl.com/curc-survey18