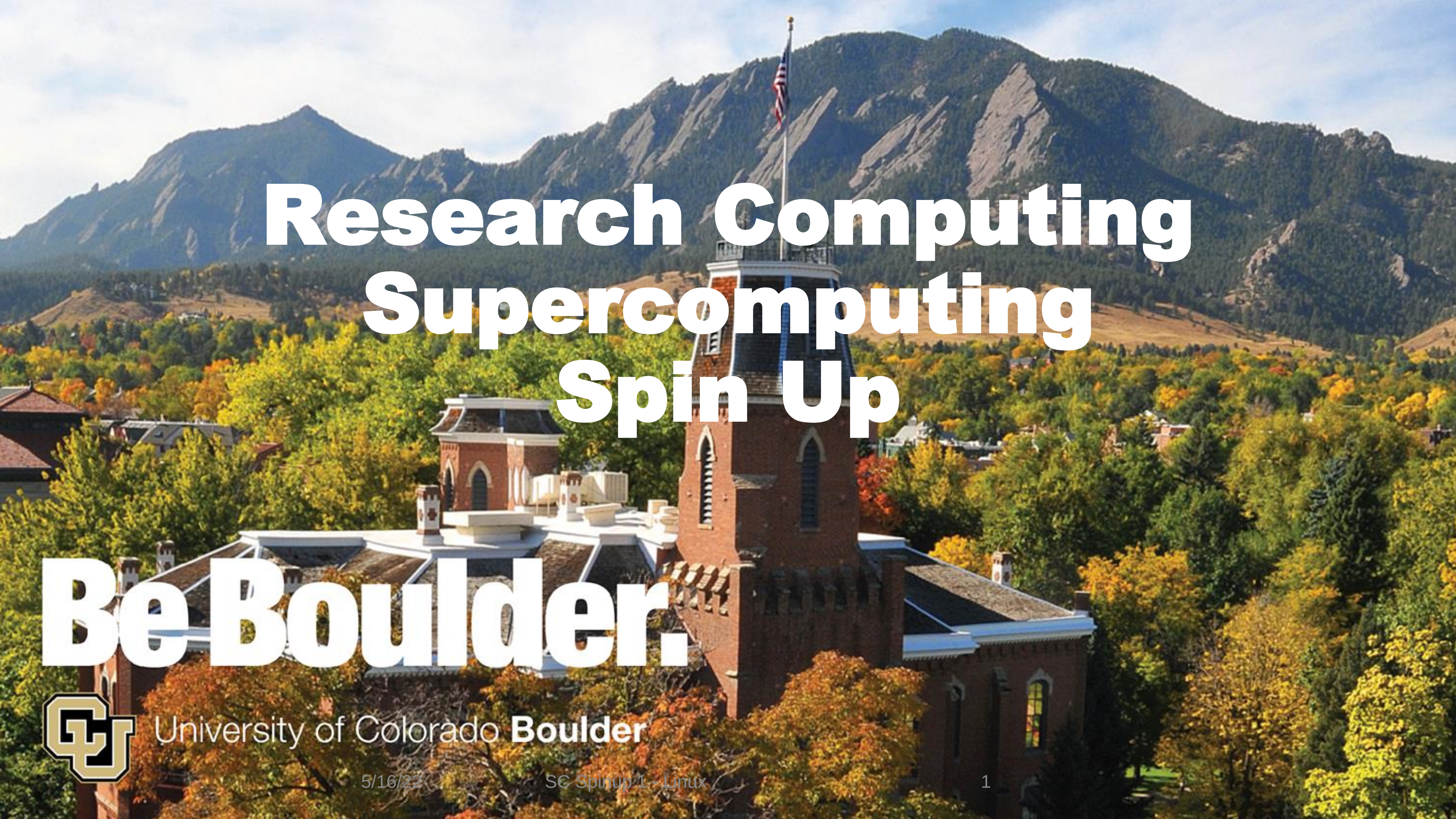


# Research Computing Supercomputing Spin Up

Be Boulder.

University of Colorado Boulder

# HPC Job Submission

**Workshop Type:** Short Course
**Instructor:** Trevor Hall

*RC Homepage: https://www.colorado.edu/rc/*

*RC Docs: https://curc.readthedocs.io/en/latest/*

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

Course Materials:
https://github.com/ResearchComputing/Supercomputing_Spinup

Survey: http://tinyurl.com/curc-survey18

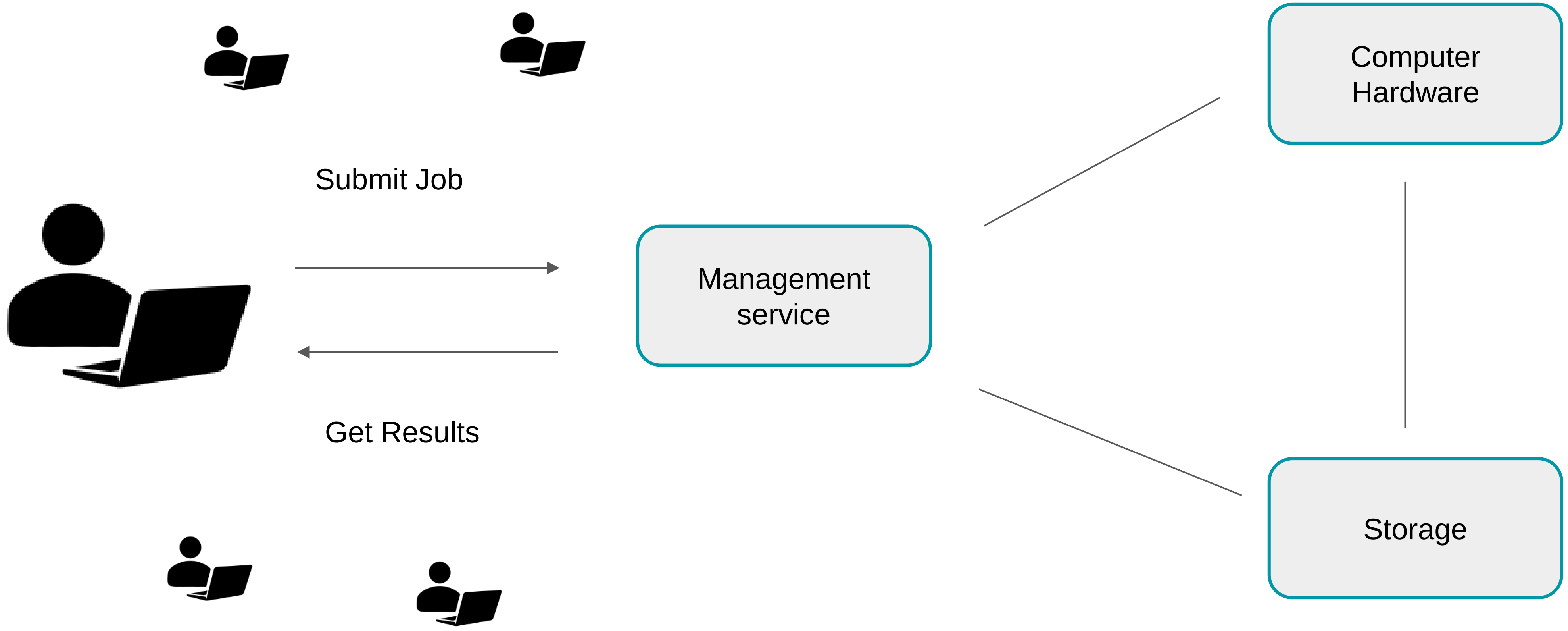
*Adapted from presentations by RC members Andrew Monaghan, Aaron Holt, John Blaas, and Mea Trehan: 1, 2, 3, 4.*

# Outline

- General Information
  - Alpine resources

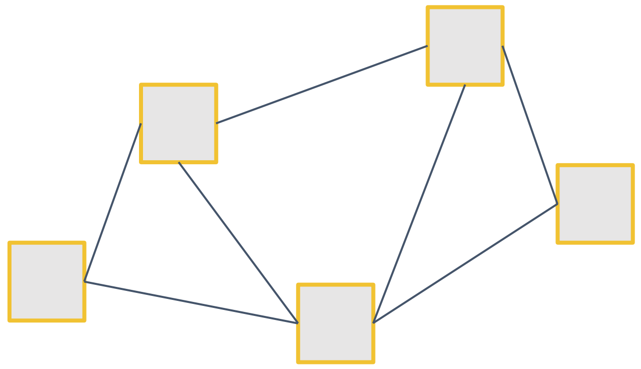
- Examples of submitting jobs to the supercomputer!
  - Traditional job submission (terminal)
    - Simple batch jobs: hello world, running programs
    - GPU Jobs
    - Advanced batch jobs: mpi, serial-parallel
    - Interactive jobs

# HPC - High Performance Computing



# HPC Cluster: Alpine

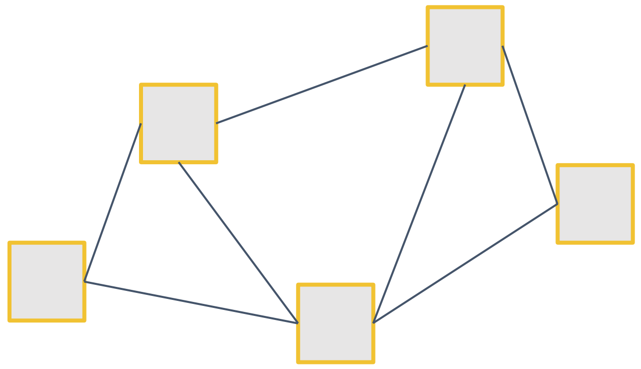
**Alpine**



- 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 Medical Campus
- Access is available to CU Boulder, CSU, AMC, and RMACC users

# HPC Cluster: Alpine

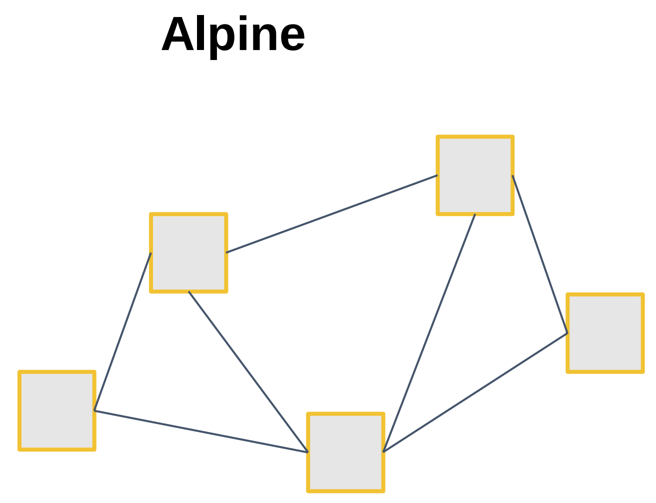
**Alpine**



- 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*
  - 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
    - nvlink compatibility in progress
  - **Scratch Storage:** 25Gb Ethernet +RoCE
- Operating System
  - RedHat Enterprise Linux version 8 operating system

## Submitting Jobs via Terminal

# RC Access: Logging in

- 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

# RC Access: Logging in

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/

## Working on RC Resources

- When you first log in, you will be on a login node. Your prompt:

```
[user@loginNN ~]$
```

- The login nodes are lightweight virtual machines primarily intended to serve as ‘gateways’ to RC resources. In order to get a better view of the software available on Alpine start a compile job.

```
[user@loginNN ~]$ acompile
```

- Navigate to a workspace of your choice (e.g. scratch) and download the material for this workshop:

```
[user@c3cpu-a5-u32-4 ~]$ git clone
https://github.com/ResearchComputing/Supercomputing_Spinup.git
[user@c3cpu-a5-u32-4 ~]$ cd Supercomputing_Spinup
[user@c3cpu-a5-u32-4 ~]$ export SPINUP_ROOT=$(pwd)
```

# Working Directory

- Navigate to the “job_submission_spinup” directory

```
[user@loginNN ~]$ cd $SPINUP_ROOT/job_submission_spinup
```

- This is the “working directory” we will be working with in this course/tutorial, keep in mind as we submit/create jobs

## Jobs

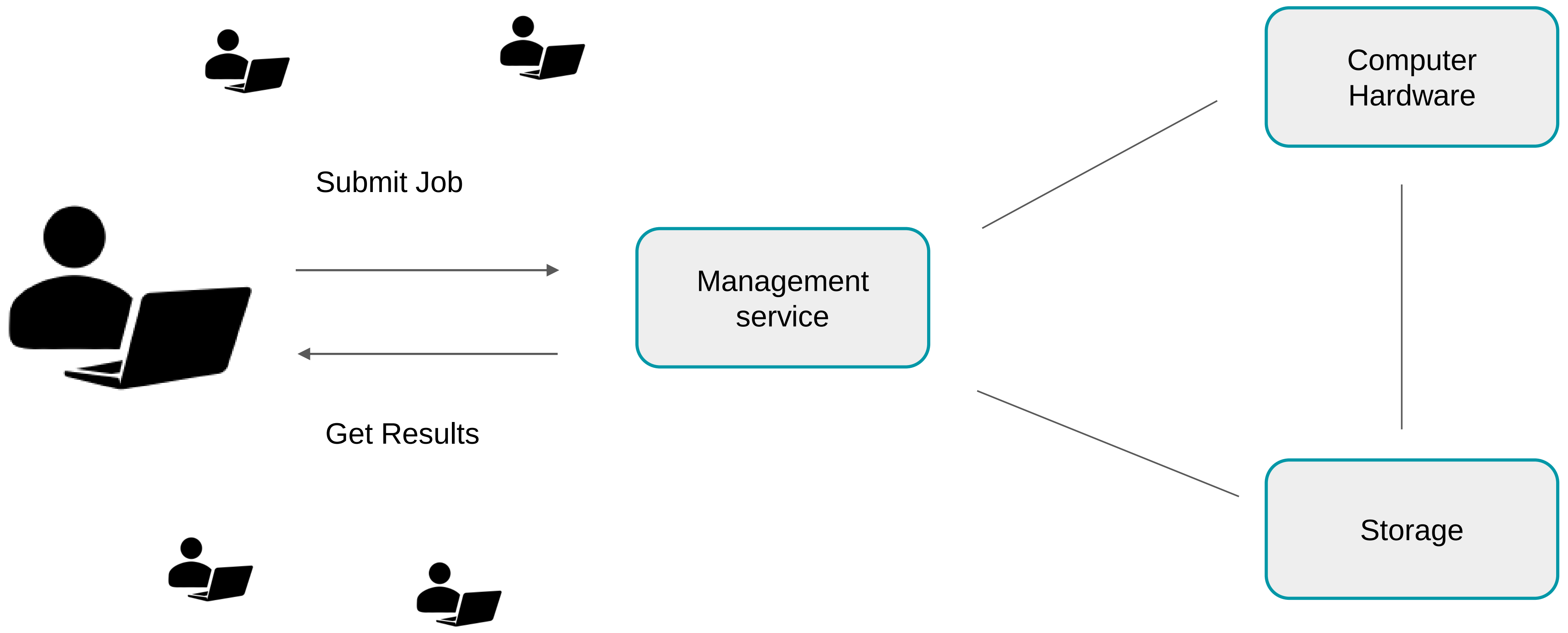
- Because our clusters are shared resources with many users trying to utilize available compute with their applications, we need a system to divide compute in a simple and fair system.

- SLURM
  - **S**imple **L**inux **U**tility for **R**esource **M**anagement

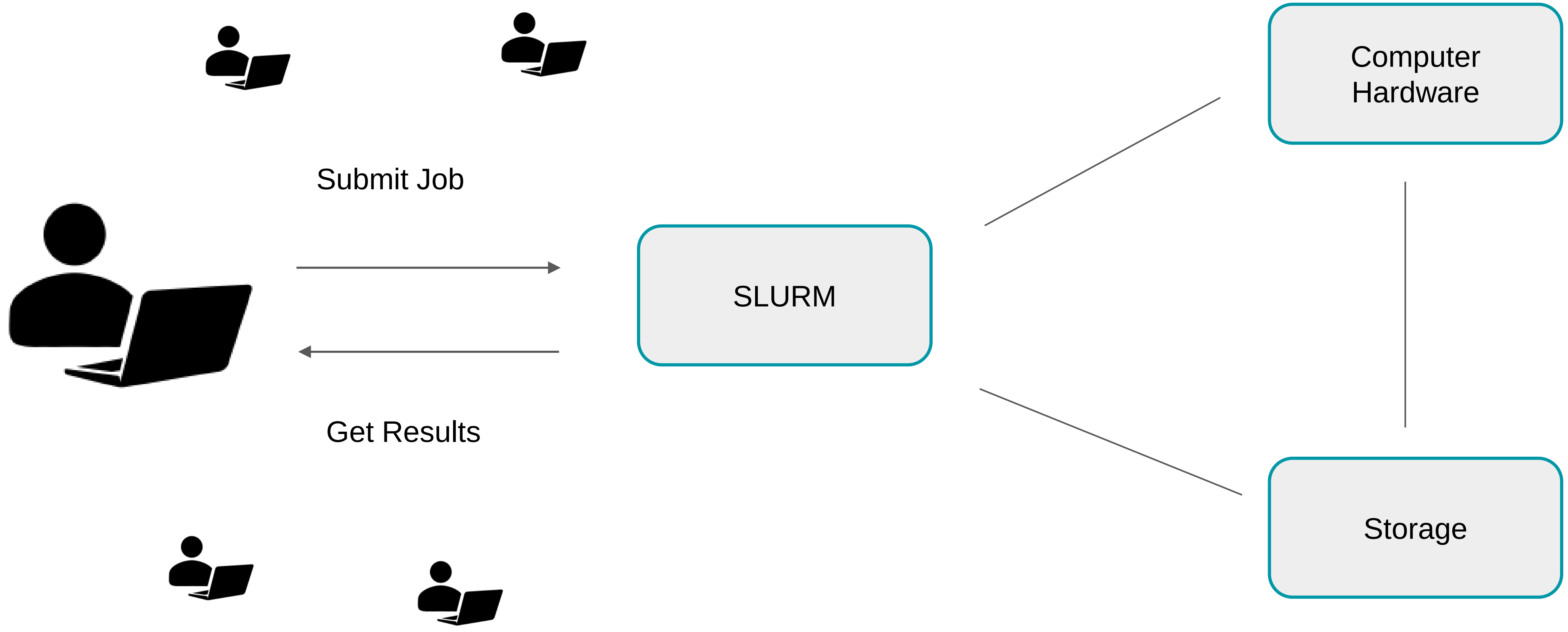
- Through SLURM, users can grab allotments of compute resources called Jobs

- 2 Types of Jobs
  - **Batch Jobs**
  - **Interactive Jobs**

# HPC - High Performance Computing



# HPC - High Performance Computing



## Batch Jobs

- **Batch Jobs** are jobs you submit to the scheduler where they are run later without supervision.
  - By far the most common job on Alpine
  - Requires a job script

- A job script is simply a script that includes **SLURM directives** (resource specifics) ahead of any commands.

# Submit your first batch job

- First, load up the **slurm Alpine module**

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

- sbatch: command to submit a batch job
- Submit your first job! :

```
$ cd $SPINUP_ROOT/job_submission_spinup
$ sbatch alpine_scripts/submit_test.sh
```

- The SLURM Script contains the parameters needed to define a job but additional flags can be used to temporarily replace any set parameters.

```
$ sbatch --partition=atesting --qos=testing alpine_scripts/submit_test.sh
```

# Anatomy of a job script

```
#!/bin/bash

## Directives (HPC Resources)
#SBATCH --<resource>=<amount>

## Software
module load <software>

## User scripting
<command>
```

## Anatomy of a job script

- open `alpine_scripts/submit_test.sh` (nano or vim)

```
#!/bin/bash

## Directives
#SBATCH --ntasks=1                      # Number of requested tasks/cores
#SBATCH --time=0:01:00                  # Max run time
#SBATCH --partition=amilan              # Specify Alpine CPU node
#SBATCH --output=test_%j.out            # Rename standard output file

## Software
module purge                           # Purge all existing modules

## User commands
echo "This is a test of user $USER"
```

# Job Options

Specified at command line or in job script as…
`#SBATCH <options>` …where options include:

|  |  |
|---|---|
| • **Partition:** | `--partition=<partition_name>` |
| • Sending emails: | `--mail-type=<type>` |
| • Email address: | `--mail-user=<user>` |
| • **Number of nodes:** | `--nodes=<nodes>` |
| • **Number of cores:** | `--ntasks=<number-of-tasks>` |
| • Quality of service: | `--qos=<qos>` |
| • Allocation: | `--account=<account_name>` |
| • Wall time: | `--time=<wall time>` |
| • Job Name: | `--job-name=<jobname>` |
| • **Output:** | `--output=<name>` |

*More on slurm commands: https://slurm.schedmd.com/quickstart.html*

*FYI: You do NOT actually type <> above – this designates something specific you as a user must enter about your job*

# 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 | 48 | 0 |

# Quality of Service

- Quality of Service specifies additional constraints Job
  - On Alpine, this means if your job needs to run longer than 1 day
  - Specify with the `--qos` flag
  - Doesn't need to be set otherwise

```
#SBATCH --qos=long
```

| QoS | Description | Max wall time | Max jobs/user | Max nodes/user |
|---|---|---|---|---|
| normal | Default QoS | 24 H | 1000 | 128 |
| long | For jobs needing longer wall times | 7 D | 200 | 20 |
| mem | High-memory jobs | 7 D | n/a | 12 |

## Writing your first job script

## Your turn!

- Create a job script and submit it as a batch job with the following instructions:

  1. Navigate back to the job_submission_spinup directory
  2. Create file alpine_scripts/sleep.sh
  3. The job should contain the following commands:

```
echo "Running on host" `hostname`
echo "Starting Sleep"
sleep 30
echo "Ending Sleep. Exiting Job!"
```

*Details on job script parameters are in the next slide*

# Job details of sleep.sh

1. The job will run on **1 core on 1 node**
2. We will request a **1 minute wall time**
3. Run on the **atesting partition**
4. Set the output file to be named **“sleep_%j.out”**
5. Contains the following **commands** ->

```
echo "Running on host" `hostname`
echo "Starting Sleep"
sleep 30
echo "Ending Sleep. Exiting Job!"
```

* Bonus: Email yourself when the job ends

```
$ sbatch alpine_scripts/sleep.sh
```

# Job Output

- Once a job completes its execution, the standard output of the script will be redirected to an output file.
  - Great for debugging!
  - Could be different from output generated by your application
  - File is created in directory job was run unless specified in your --output directive.
  - If the directive --output is not provided then a generic file name will be used (slurm_xxxxxx.out).

```
$ cat output/sleep.xxxxxx.out  # where xxxxxx is your Job Id
```

*Solution can be found in "./solutions" subdirectory*

# Checking your jobs (1)

- `squeue`: Monitor your jobs status **in queue and while running**:
  - By Default shows all jobs in queue
  - Narrow this down with:

```
$ squeue –u <username>
$ squeue –p <partition>
```

- sacct: Check back on usage statistics of **previous Jobs**
  - By default only checks all jobs from the start of the current day.
  - Narrow this down with:

```
$ sacct –u <username>
$ sacct --start=MM/DD/YY –u <username>
$ sacct –j <job-id>
```

# Checking your jobs (2)

- Another method of checking details of your job while running is with `scontrol`
- Advanced command usually used by system administrators, but you can use it too!

```
$ scontrol show job <job number>
```

- seff: Utility to **check efficiency post-job**

```
$ module load slurmtools
$ seff <job number>
```

# Software and Jobs

- Okay so running a job is easy, but how do I run a job with my software?

- LMOD
  - Module system on CURC systems
  - Modifies your environment to make your desired software visible to your terminal.

```
$ module load matlab
$ ml matlab #shorthand version!
```

# Software and Jobs (2)

- More LMOD commands:

```
$ module purge                #Unloads all current modules
$ module unload matlab        #Unloads matlab
$ module spider matlab        #Searches for matlab in module tree
```

- What if my software isn't available through LMOD?
  - Software must be installed locally if not available through LMOD
  - RC User support is happy to assist,*installs are best effort*
  - For more assistance contact rc-help@colorado.edu

# Example: Serial R Code

# Running an external program

- Let’s run R on an R script
- Batch script calls and runs programs/R_program.R
    - Let’s take a look at the R program

- Let’s examine the batch script scripts/submit_R.sh
    - Note how R is loaded
    - R program can be run with “Rscript <script>”

- Go ahead and submit the batch script:

```
$ sbatch scripts/submit_R.sh
```

## Interactive Jobs

## Interactive jobs

- Sometimes we want our job to run in the background
- Sometimes we want to work on program in real time
    - Great for testing, debugging

- We can get access to a compute node interactively with `sinteractive`

- For example, let’s run the R job we previously ran as a batch job, but this time let’s do it interactively

# Running an interactive job

- To work with R interactively, we request time from Alpine
- When the resources become available the job starts
- Commands to run:

```
$ sinteractive --time=00:10:00
```

- Once we receive a prompt, then:

```
$ module load R
$ cd programs
$ Rscript R_program.R
```

- Once we finish, we must exit! (job will time out eventually)

```
$ exit
```

# Thank you!

- Survey: http://tinyurl.com/curc-survey18
- Documentation: curc.readthedocs.io/
- Trainings with Center for Research Data and Digital Scholarship (CRDDS): https://www.colorado.edu/crdds/
    - Coming up:
        - Increasing Your Priority with Alpine Allocations (2/5)
        - Alpine in Your Browser with Open OnDemand (2/6)
        - Introduction to the Commercial Cloud (2/7)
- Helpdesk: rc-help@colorado.edu
- Consult Hours (Tuesday 12:00-1:00 in-person, Thursday 1:00-2:00 virtually)

## Extra Materials: GPU Jobs

# GPU Jobs

- On Alpine the `--gres` slurm directive is ***required*** to use GPU accelerators on a GPU node.

- At a minimum, one would specify:
  - A GPU partition (e.g. `--partition=aa100` for an nvidia GPU node)
  - `--gres=gpu` in a job to specify that they would like to use a single gpu on their specified partition
    - You can request up to 3 accelerators on Alpine (e.g. `--gres=gpu:3` )

## GPU Job Script Example

```
 #!/bin/bash

 ## Directives
 #SBATCH --ntasks=1                     # Number of requested tasks/cores
 #SBATCH --time=0:01:00                 # Max run time
 #SBATCH --partition=aa100              # Specify Alpine NVIDIA A100 node
 #SBATCH --gres=gpu:2                                     # Request 2 GPUs
from the node
```

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## Extra Materials: Advanced Job Scripts

## Running an mpi job

- For cases where you have a code that is parallelized, meaning it can run across multiple cores.
- Number of tasks always > 1. E.g.,

```
#SBATCH --ntasks=4
```

- Will always need to load a compiler and mpi. E.g.,

```
module load intel impi
```

- Executable preceded with mpirun, srun, or mpiexec. E.g.,

```
mpirun –np 4 python yourscript.py
```

- Examine and run the example ‘submit_python_mpi.sh’

```
$ sbatch scripts/submit_python_mpi.sh
```

## Running serial jobs in parallel

- Not all code is designed to run with MPI (nor always makes sense to do so)

- RC has a couple different tools that lets users run serial programs in parallel
  - RC LoadBalancer
  - GNU Parallel

- Example in: `scripts/python_loadbalance.sh`