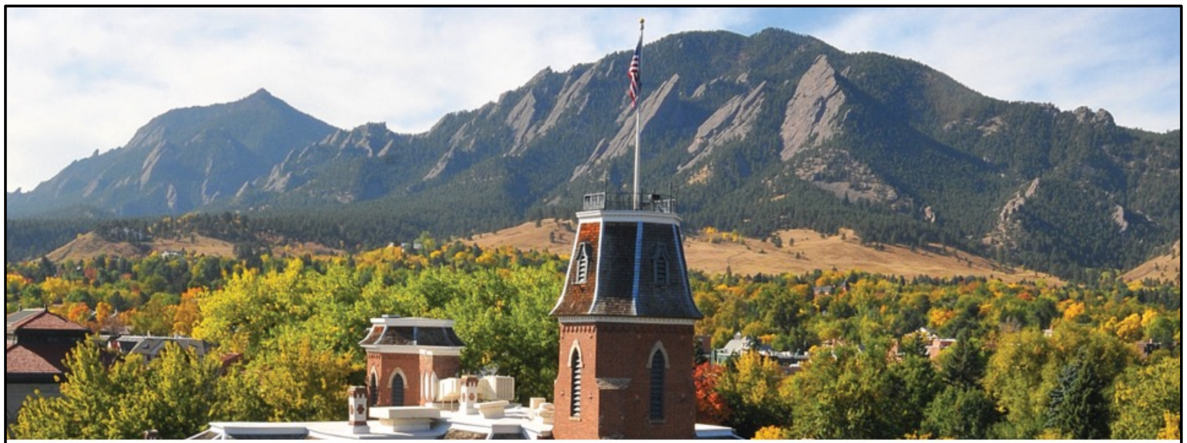

Scheduling Jobs on a Supercomputer

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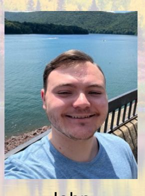
Meet the User Support Team

Layla Freeborn

Brandon Reyes

Andy Monaghan

Michael Schneider


John Reiland

Dylan Gottlieb

Mohal Khandelwal

Ragan Lee

Website: www.rc.colorado.edu

Documentation: https://curc.readthedocs.io

Helpdesk: rc-help@colorado.edu

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https://github.com/ResearchComputing/scheduling_a_job_on_a_supercomputer_rc_shortcourse

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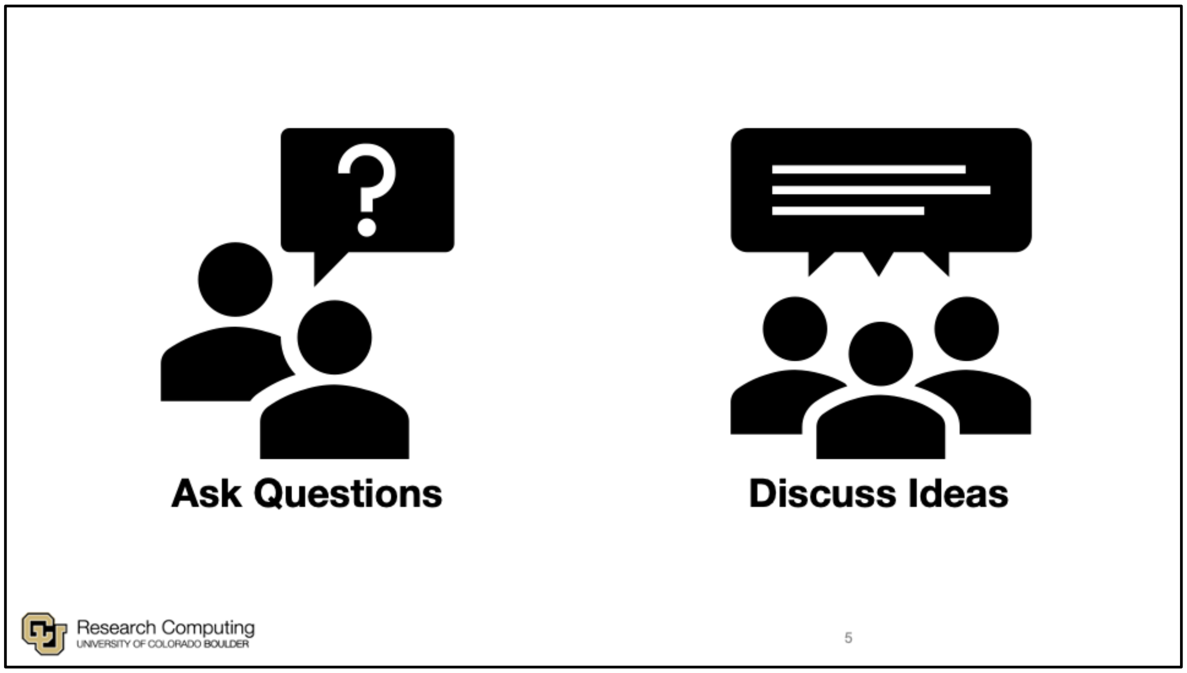
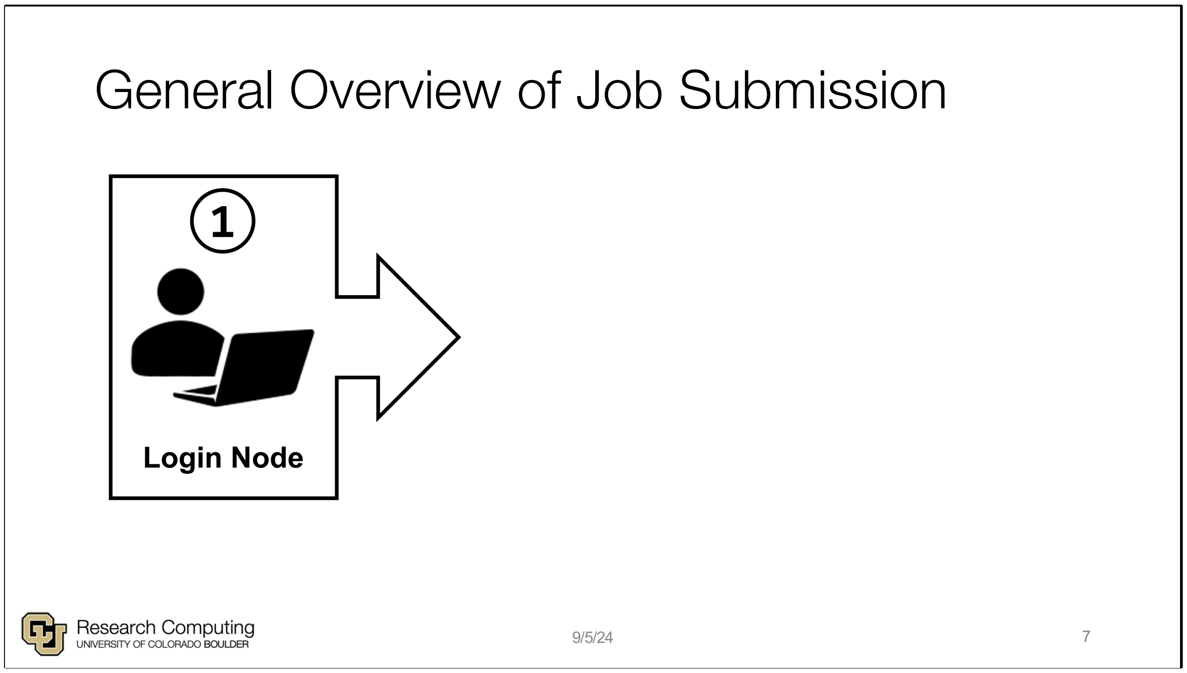


This workshop is meant to be empowering and information-rich – to help you get the most out of your HPC workflow.

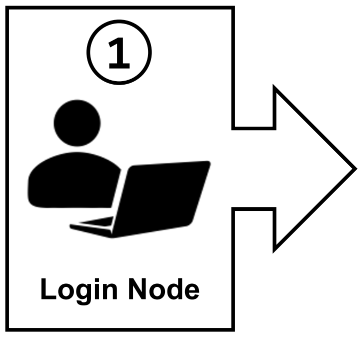
Feel free to ask questions during the presentations and to discuss ideas/thoughts during breaks and the hands-on portion of the workshop.

Session Overview

- Overview of Jobs Submissions
- Resource Requests
- Interactive & Batch Jobs
- Monitoring jobs



General Overview of Job Submission

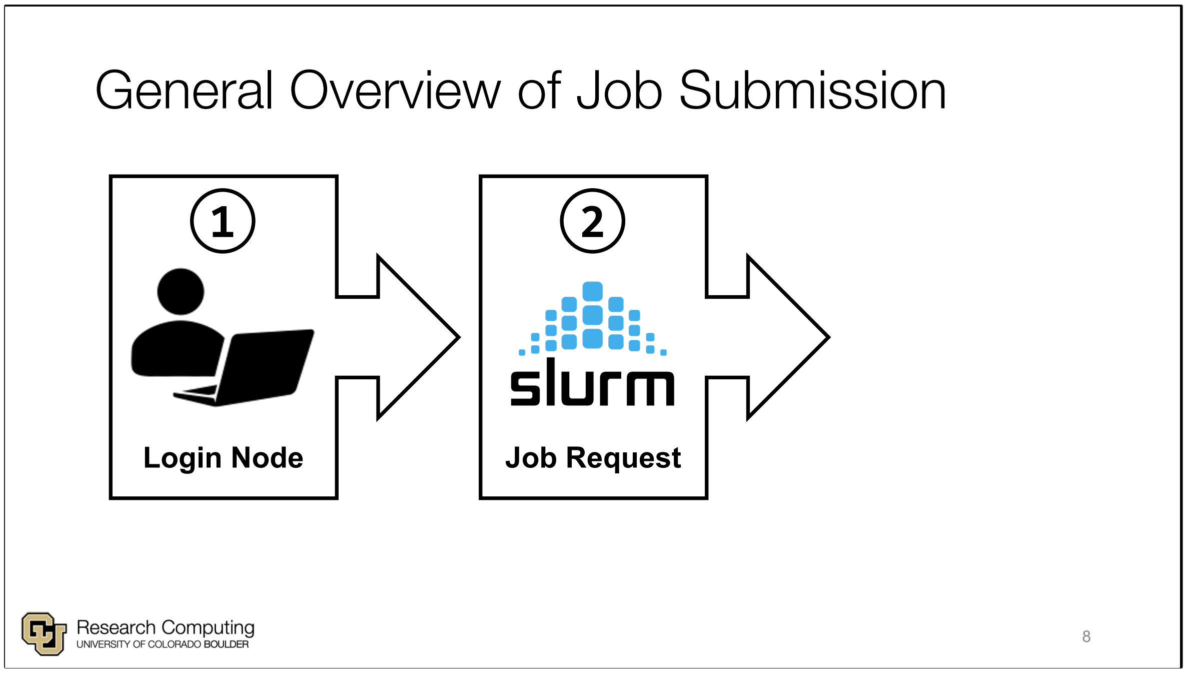


A job submission consists of three general steps:

1. Log onto a CURC Login Node (ssh, OnDemand)

Warning/Reminder

Software cannot be accessed/run from a login node. You must run your applications from a compute node. But, in order to run on a compute node, you must first request the system resources through a ”job”



General Overview of Job Submission

1
Login Node
2
slurm
Job Request

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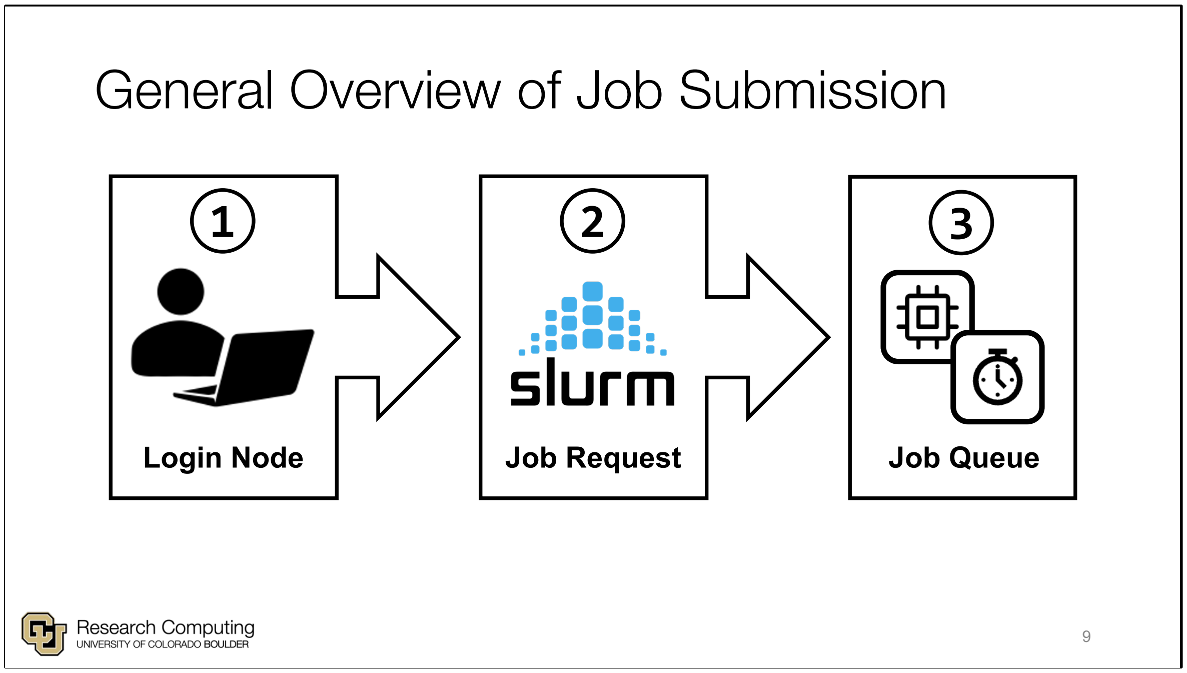
A job submission consists of three general steps:

1. Log onto a CURC Login Node (ssh, OnDemand)

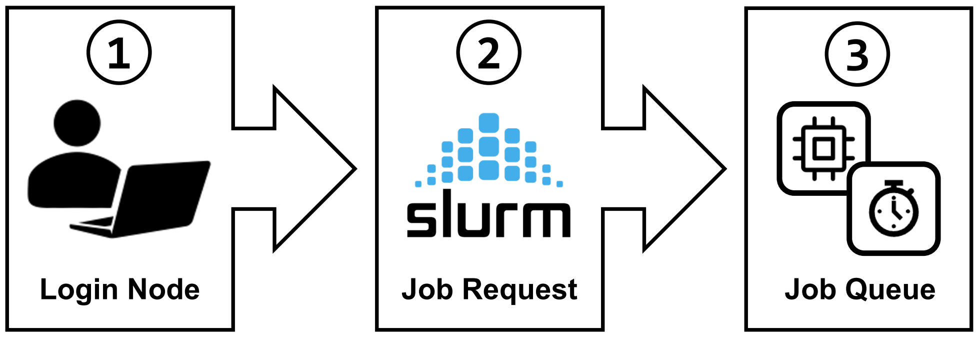
Warning/Reminder

Software cannot be accessed/run from a login node. You must run your applications from a compute node. But, in order to run on a compute node, you must first request the system resources through a ”job”

2. Job requests are submitted to SLURM, our system’s Job Scheduler which manages how and when system resources are allocated to user submitted jobs.



General Overview of Job Submission



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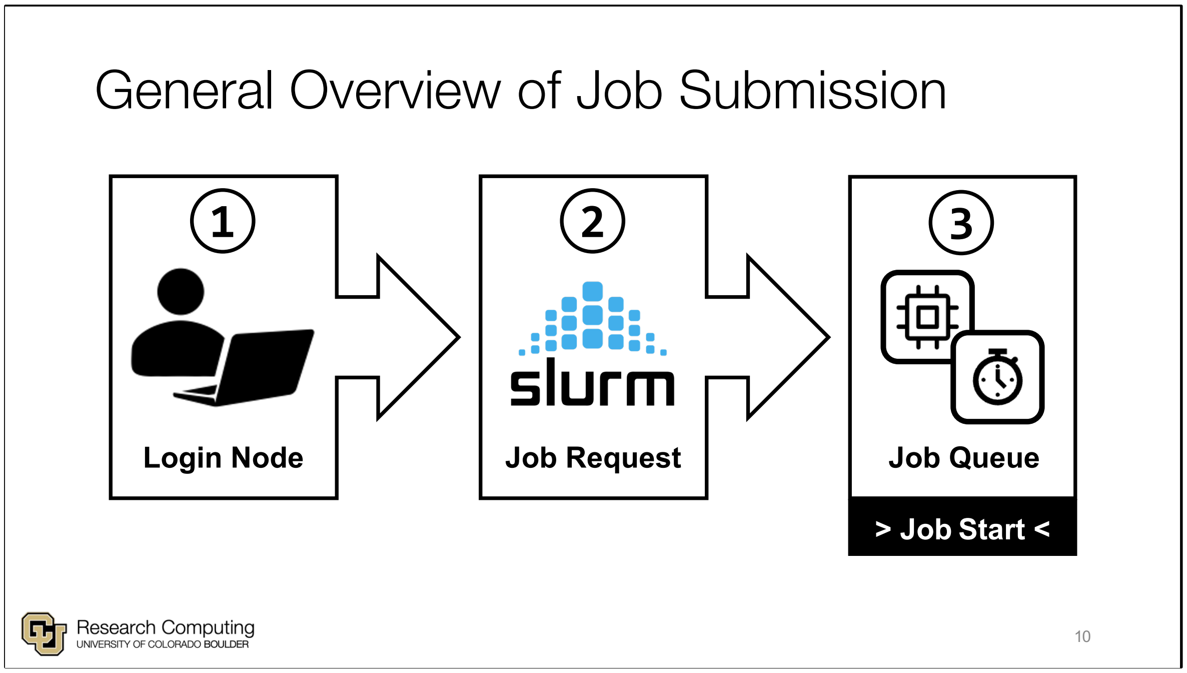
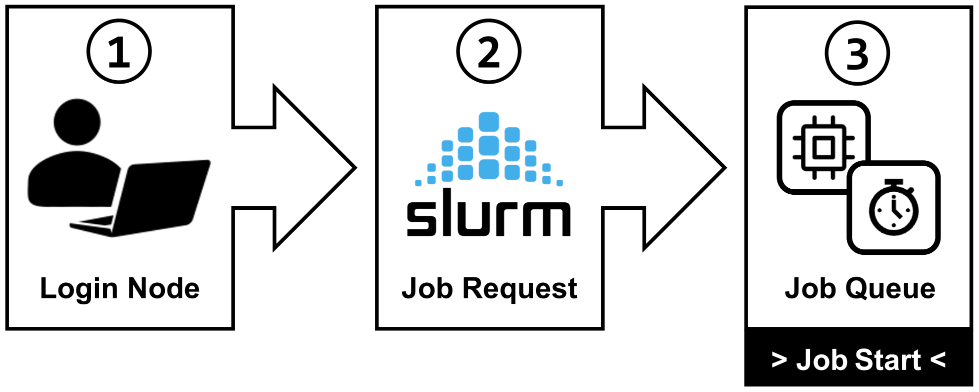
9

3. Jobs do not run immediately but instead wait in a SLURM managed queue. A job's placement in the queue is dependent on multiple factors. We will discuss a few of the most common factors, but a general rule to follow is that the more resources a job requests the longer it will wait in the queue.



General Overview of Job Submission



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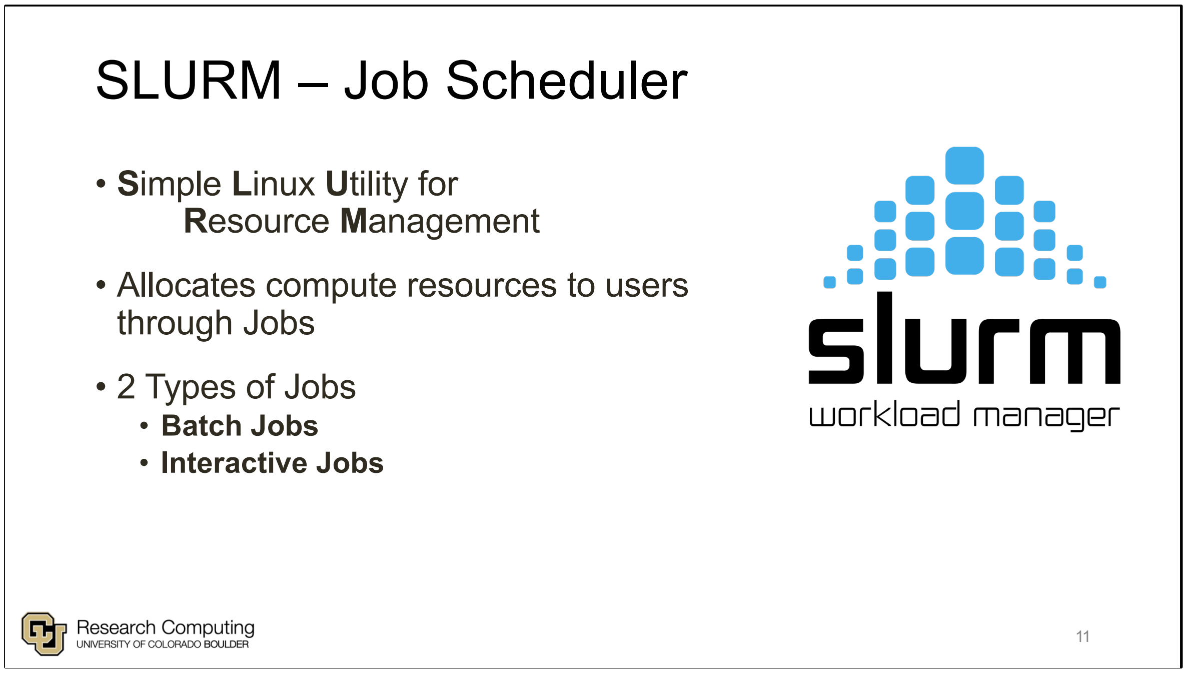
10

Once SLURM determines they system is ready, it will start the job. As we will discuss, quite a few factors influence how long a submitted job waits on the queue. But, in general, the more resources you request the longer your job will have to wait in the queue.



SLURM – Job Scheduler

- **S**imple **L**inux **U**tility for **R**esource **M**anagement
- Allocates compute resources to users through Jobs
- 2 Types of Jobs
  - **Batch Jobs**
  - **Interactive Jobs**

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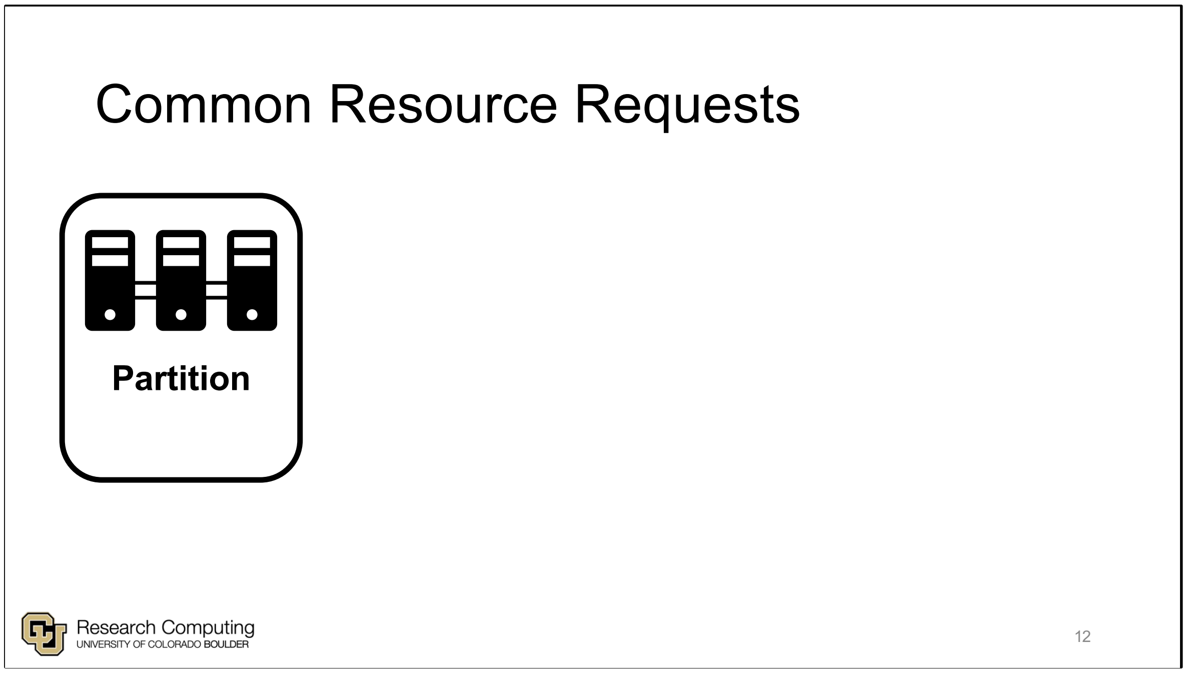
Slurm manages our system's shared resources and ensures they are equitably shared amongst CURC users.

In the next section we will discuss common resources a job can request and then cover the two types of jobs we support (Batch and Interactive).



Common Resource Requests

Partition

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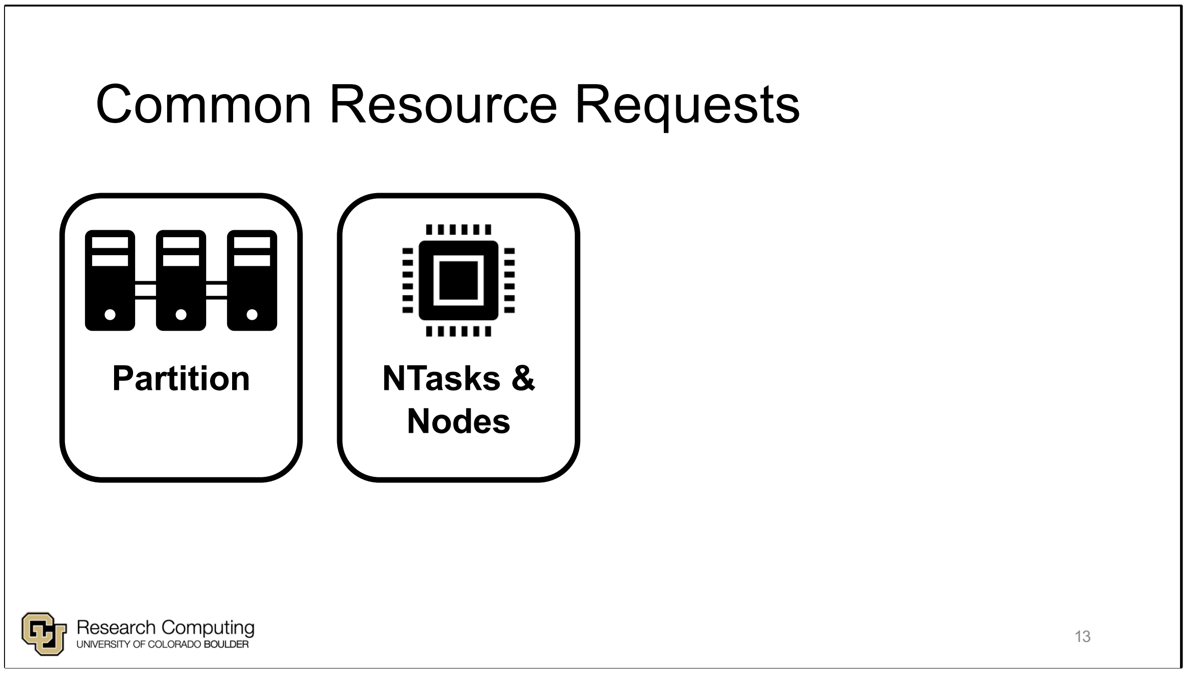
12

Partition – Defines what type of hardware your job has access to.



Common Resource Requests

Partition

NTasks & Nodes

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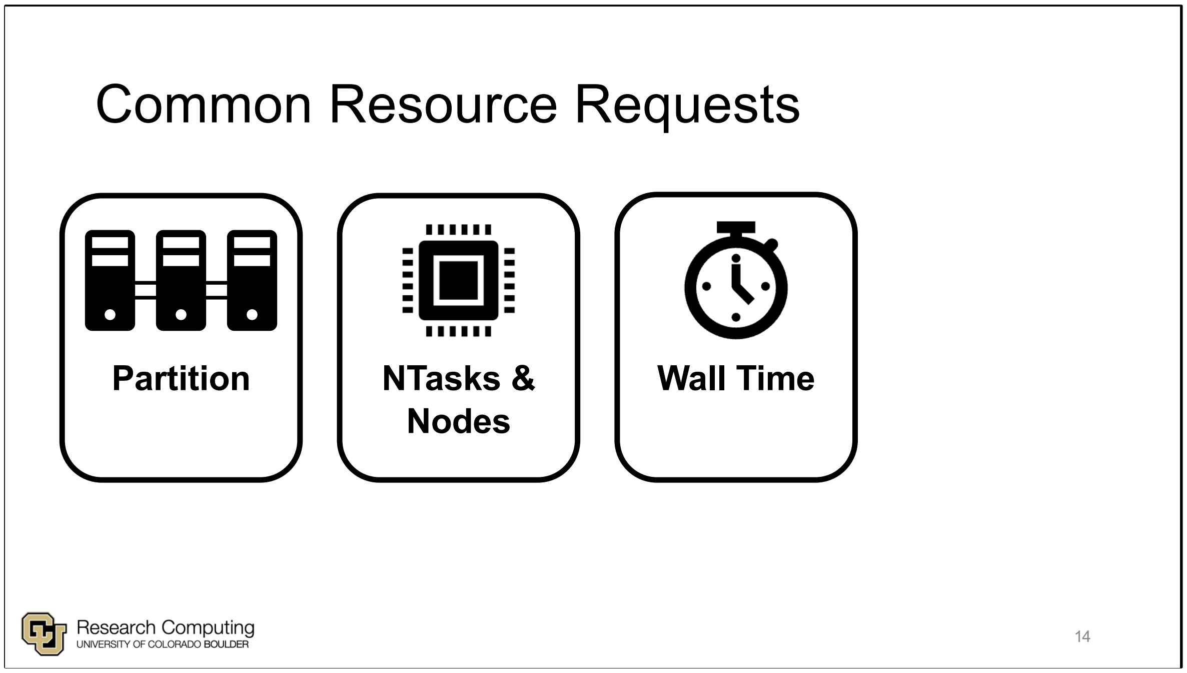
13

Partition – Defines what type of hardware your job has access to.

Ntasks – How many CPU cores your job is requesting

Nodes – How many nodes your job will run across (typically 1, but can be more)



Common Resource Requests

Partition

NTasks & Nodes

Wall Time

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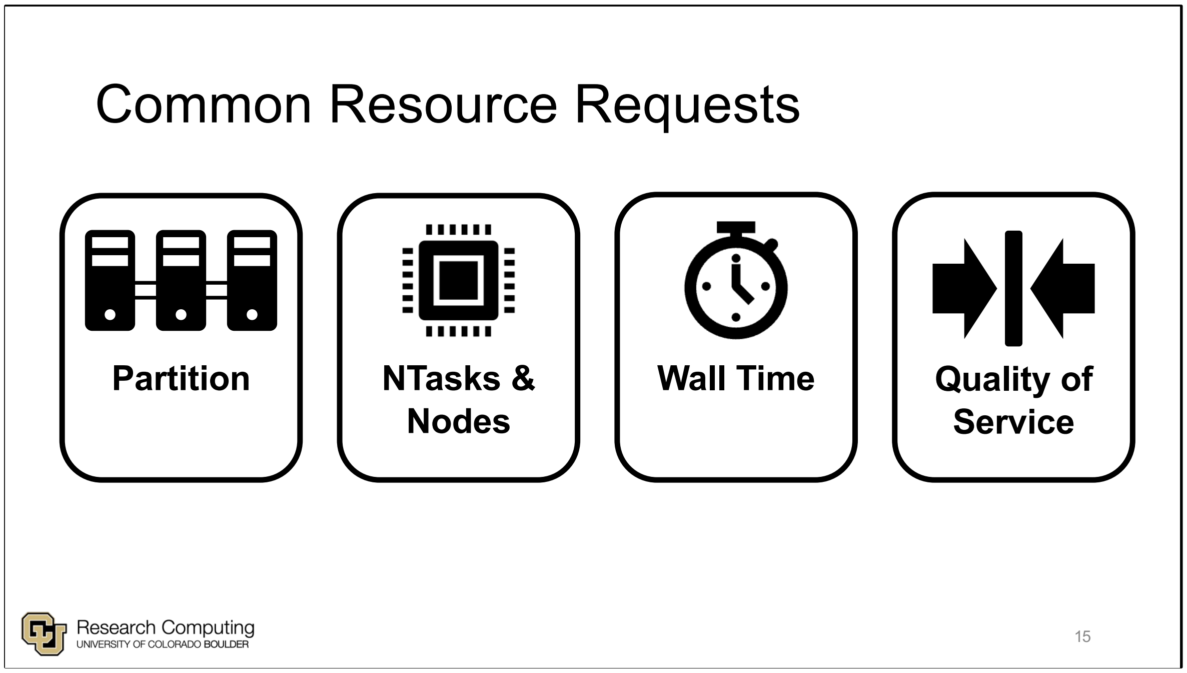
14

Partition – Defines what type of hardware your job has access to.

Ntasks – How many CPU cores your job is requesting

Nodes – How many nodes your job will run across (typically 1, but can be more)

Wall Time – How much time your job needs to run on the system (can be a few minutes, a few hours, to multiple days)



Common Resource Requests

Partition
NTasks & Nodes
Wall Time
Quality of Service
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15

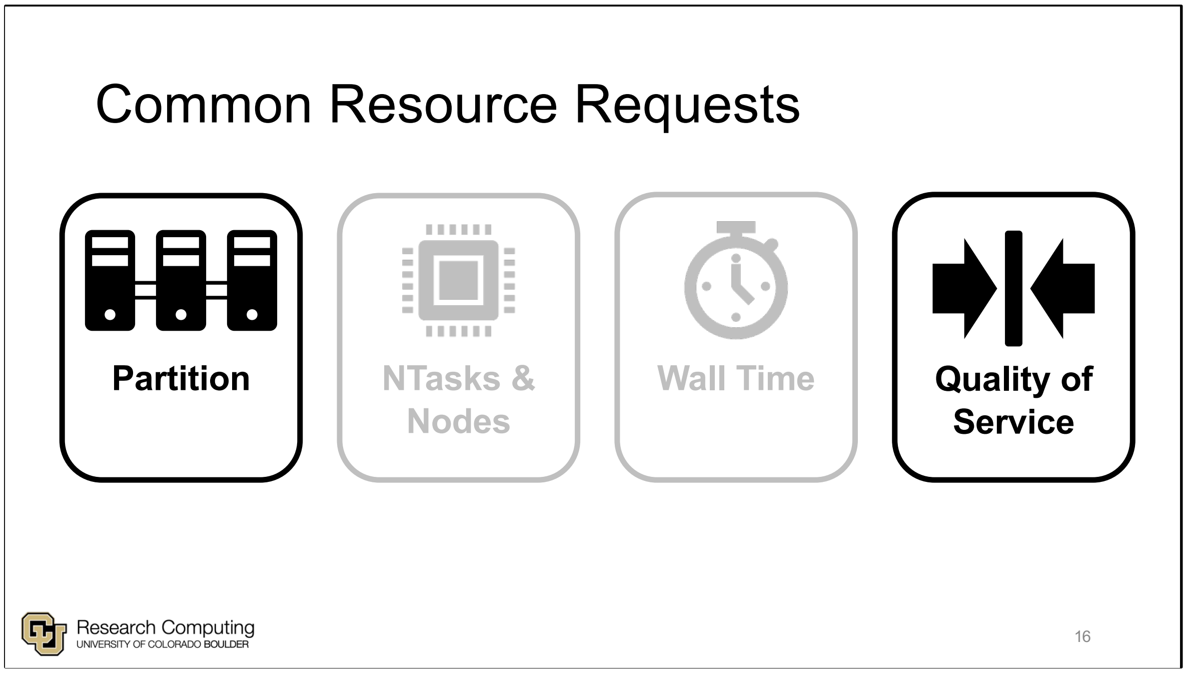
Partition – Defines what type of hardware your job has access to.

Ntasks – How many CPU cores your job is requesting

Nodes – How many nodes your job will run across (typically 1, but can be more)

Wall Time – How much time your job needs to run on the system (can be a few minutes, a few hours, to multiple days)

Quality of Service (QOS) – Defines additional job constraints – i.e. limits to how much your job can request.



Common Resource Requests

Partition
NTasks & Nodes
Wall Time
Quality of Service

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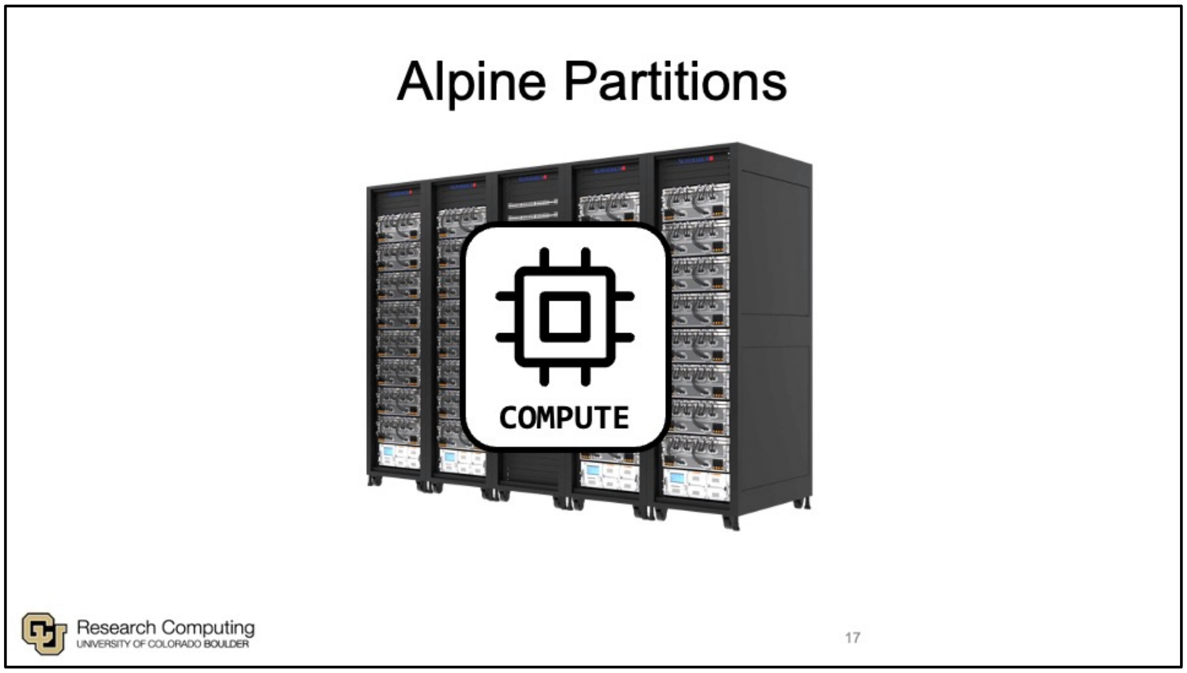
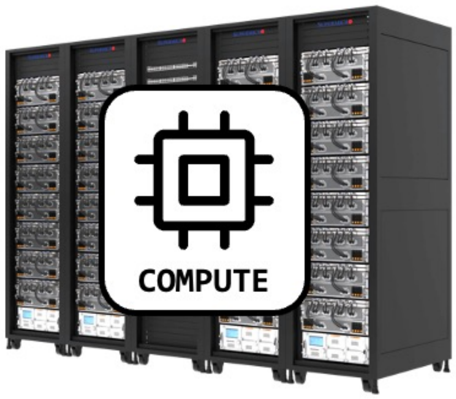
What resources and how many you can request is heavily dependent on what partition and qos you select. We will now provide a general overview of our primary partitions and qos's.



Alpine Partitions



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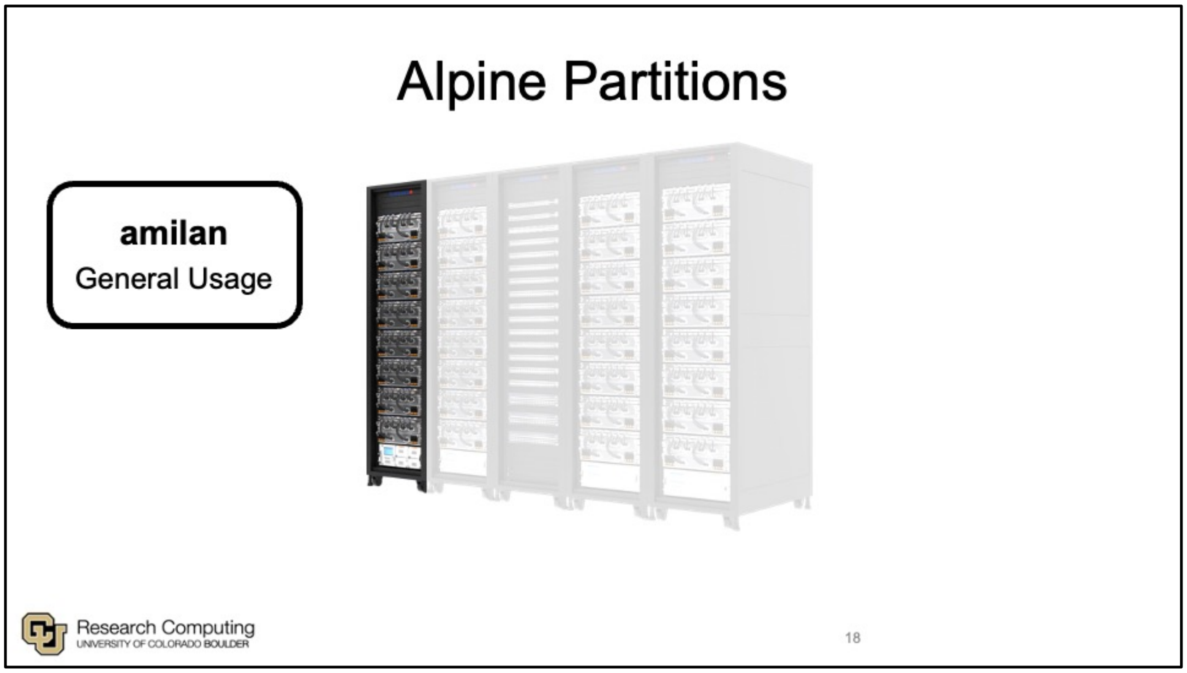
Compute nodes are organized into partitions – logical groups of similarly spec'd hardware.

Partitions make it easier to request specific resources and ensure a more consistent user experience.

The Alpine Cluster has four primary partitions.

Detailed Information on Alpine Hardware:
https://curc.readthedocs.io/en/latest/clusters/alpine/alpine-hardware.html



Alpine Partitions

amilan
General Usage

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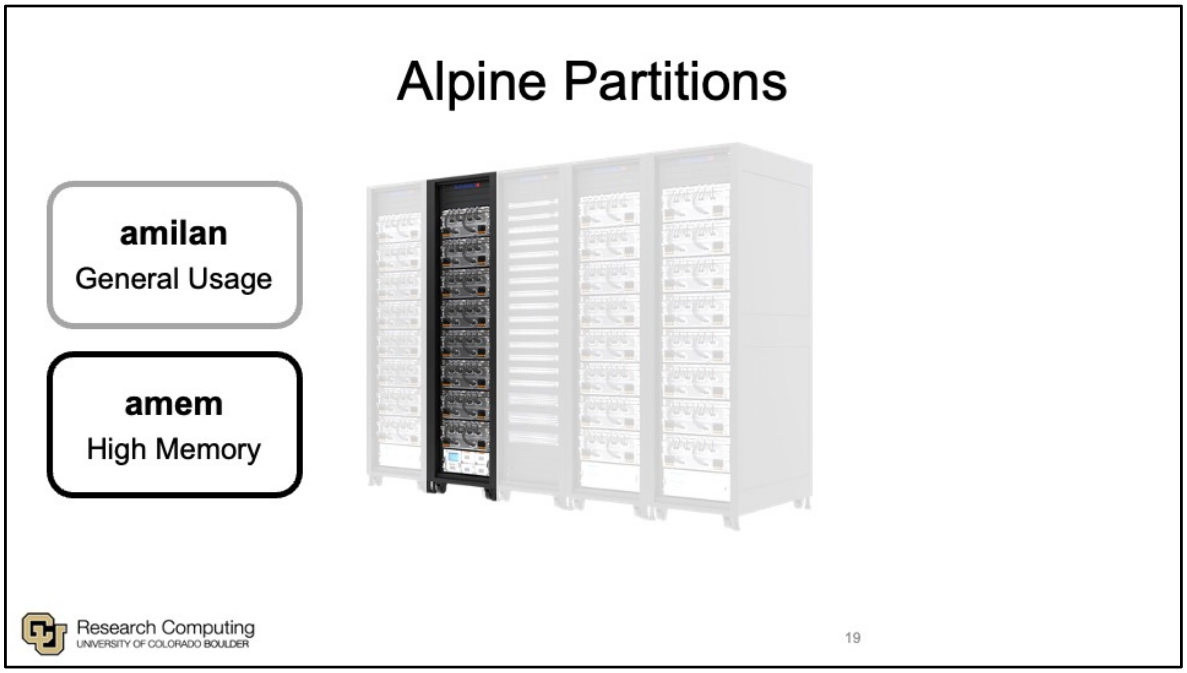
amilan:
285 Nodes
64 CPU Cores per Node
3.75 GB of RAM per CPU (240 GB total)

Detailed Information on Alpine Hardware:
https://curc.readthedocs.io/en/latest/clusters/alpine/alpine-hardware.html



Alpine Partitions

amilan
General Usage

amem
High Memory

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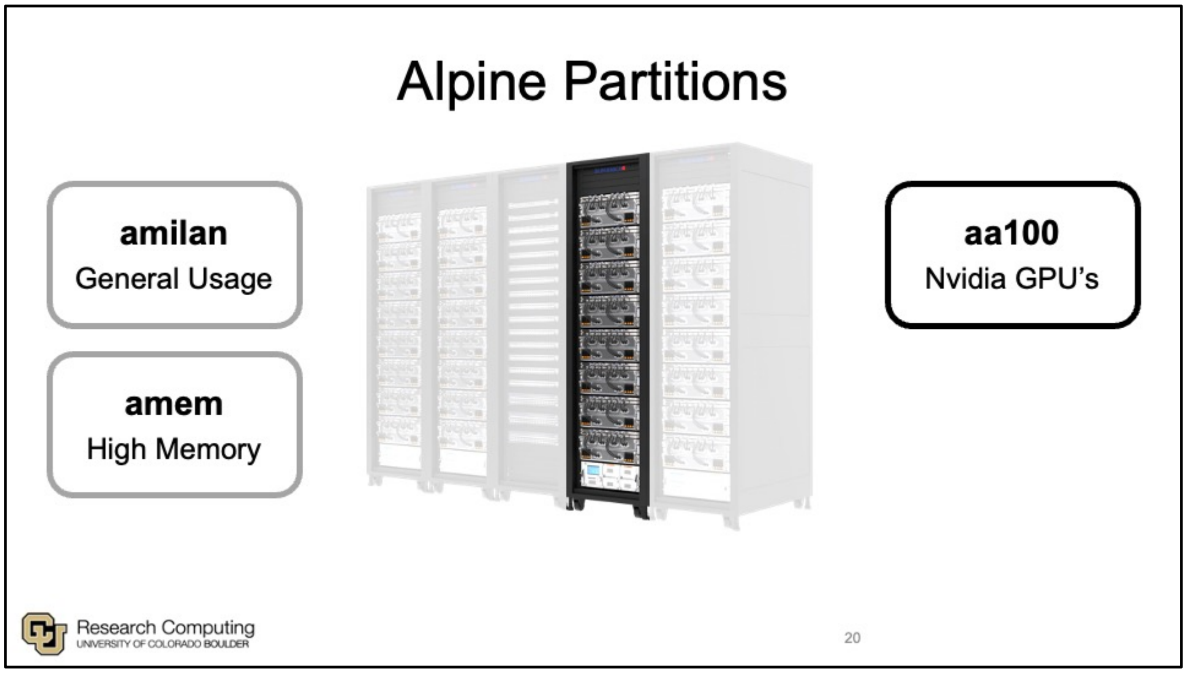
amem:
22 Nodes
48 CPU Cores per node (12)
64 CPU Cores per node (10)
21.5 GB of RAM per CPU (1 TB total)

Detailed Information on Alpine Hardware:
https://curc.readthedocs.io/en/latest/clusters/alpine/alpine-hardware.html



Alpine Partitions

amilan
General Usage

amem
High Memory

aa100
Nvidia GPU's

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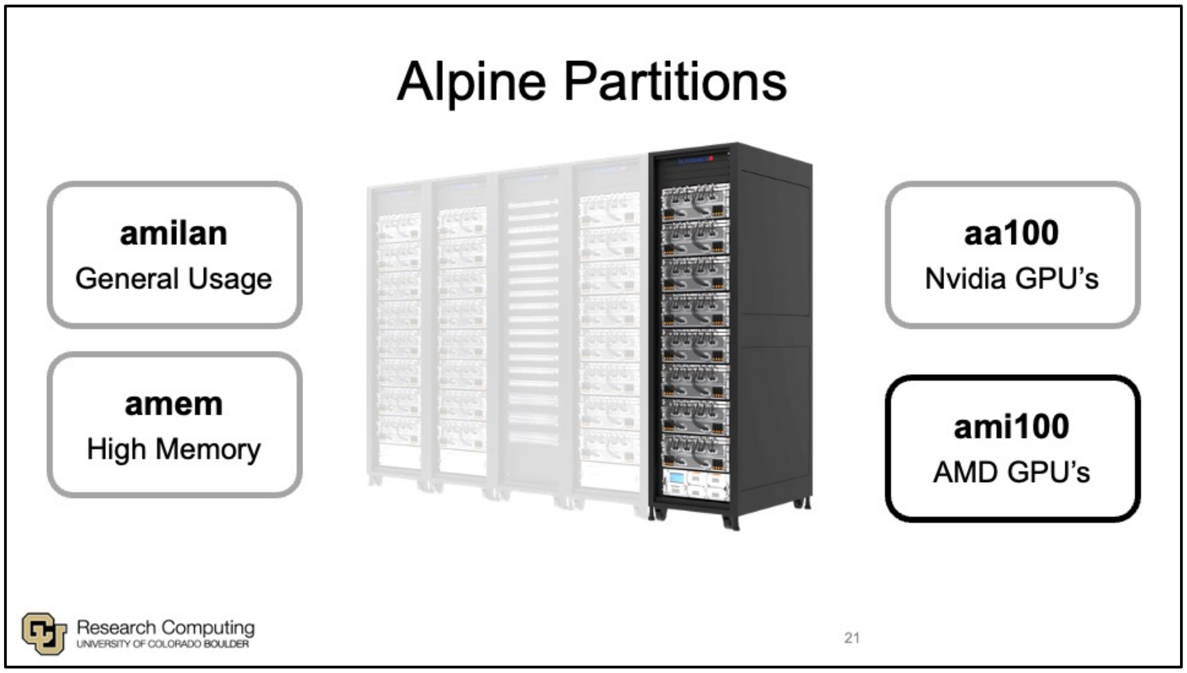
aa100
12 Nodes
64 CPU Cores per Node
3.75 GB of RAM per CPU (240 GB total)
3 GPU's per Node (Nvidia A100)



Alpine Partitions

amilan
General Usage

amem
High Memory

aa100
Nvidia GPU's

ami100
AMD GPU's

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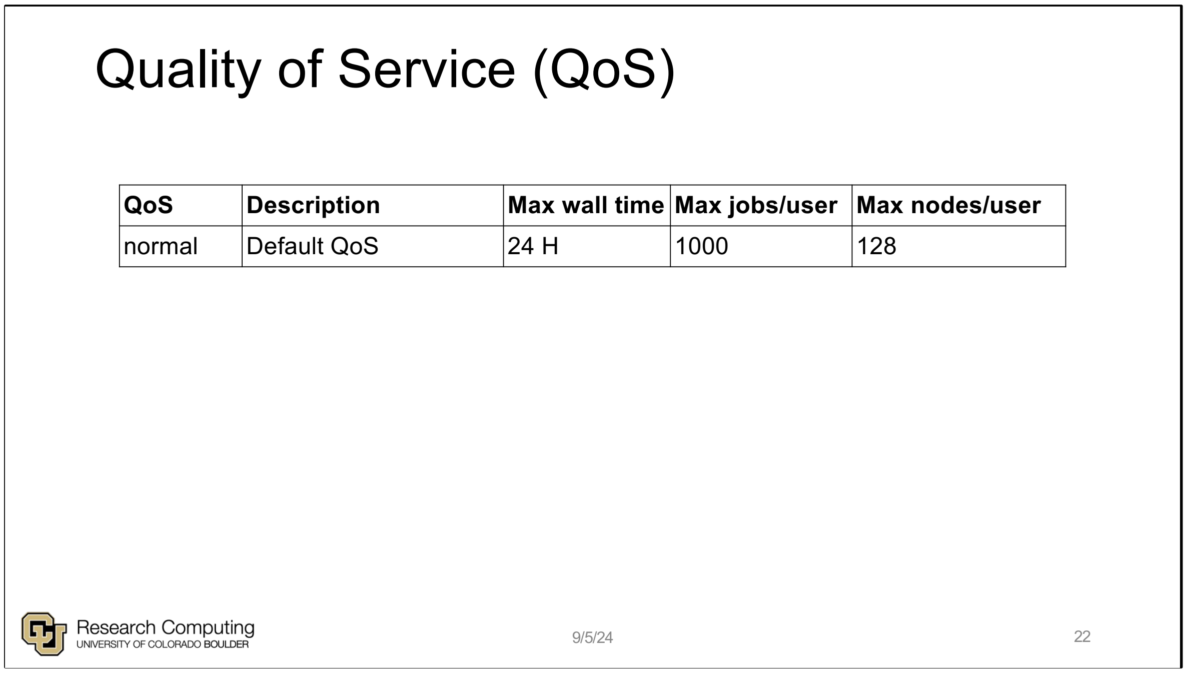
ami100
8 Nodes
64 CPU Cores per Node
3.75 GB of RAM per CPU (240 GB total)
3 GPU's per Node (AMD MI100)

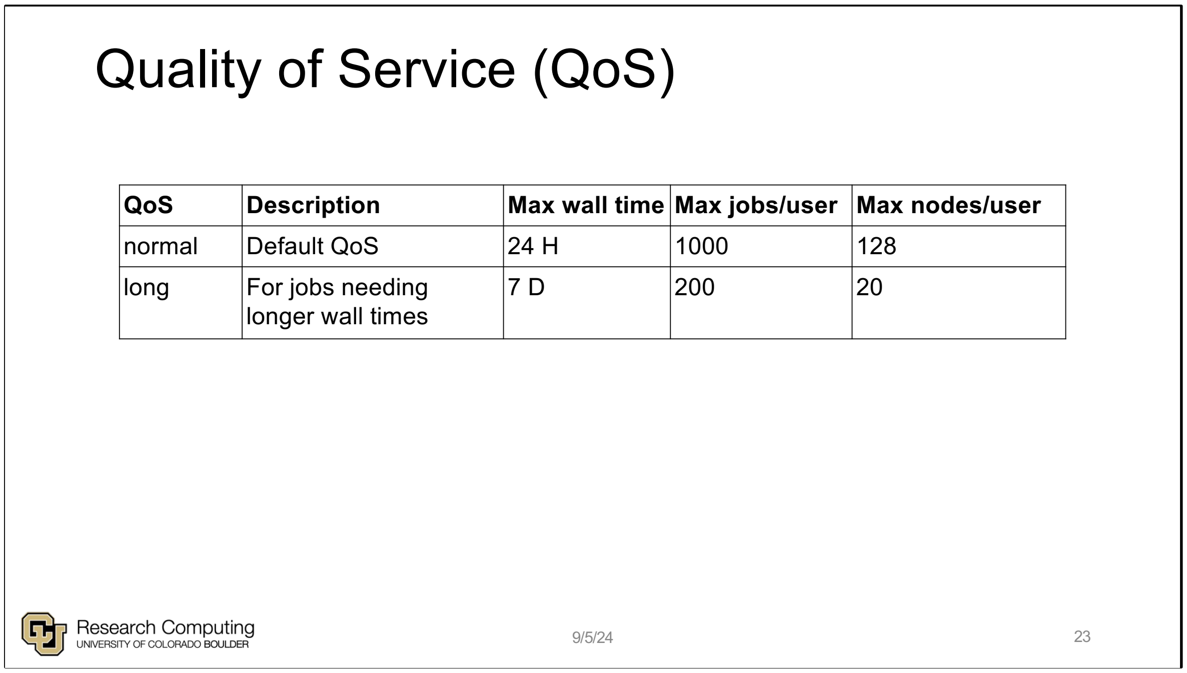
Detailed Information on Alpine Hardware:
https://curc.readthedocs.io/en/latest/clusters/alpine/alpine-hardware.html



Quality of Service (QoS)

QoS	Description	Max wall time	Max jobs/user	Max nodes/user
normal	Default QoS	24 H	1000	128

The normal qos is the default qos for all submitted jobs



Quality of Service (QoS)

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

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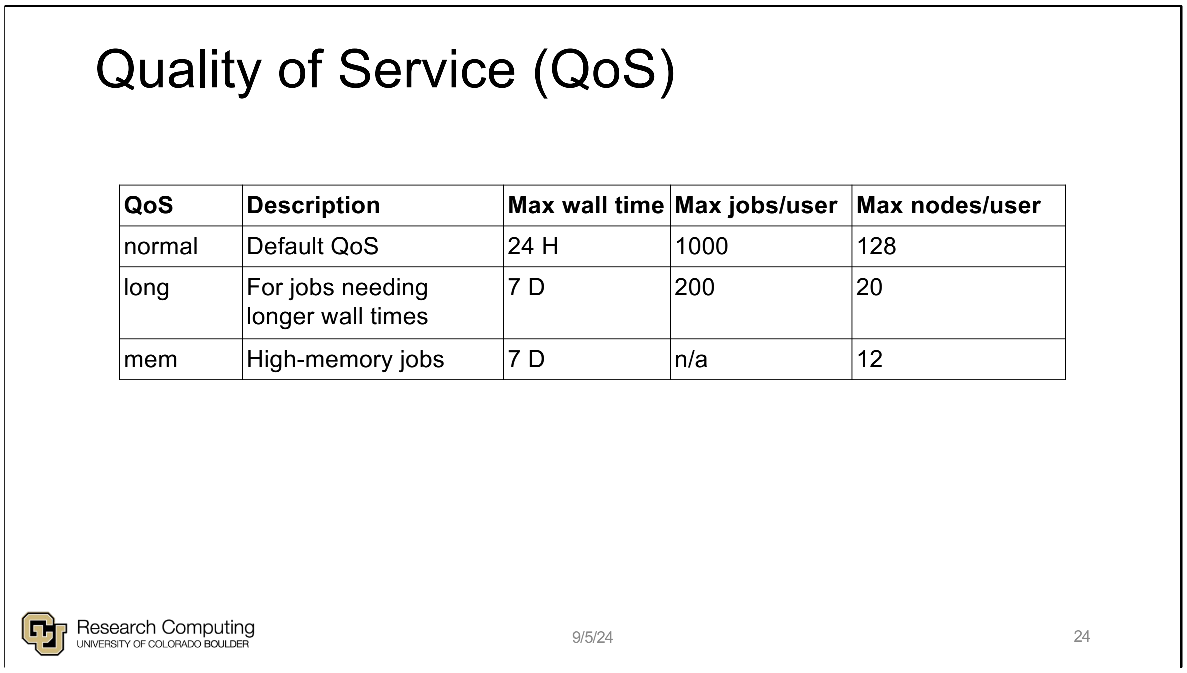
The long qos provides a subset of amilan nodes to run longer jobs.

Please note! The long qos has fewer resources than normal and may have a longer wait time in the queue.



Quality of Service (QoS)

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

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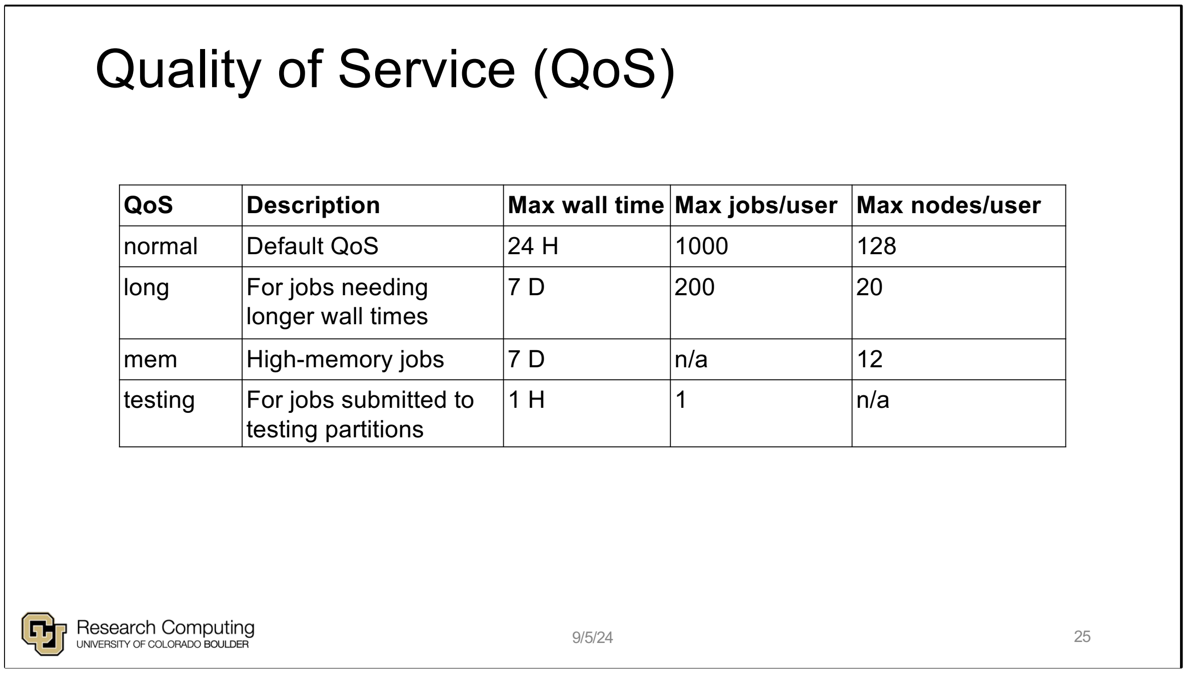
The mem qos is specifically for jobs that run on the amem partition.



Quality of Service (QoS)

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
testing	For jobs submitted to testing partitions	1 H	1	n/a

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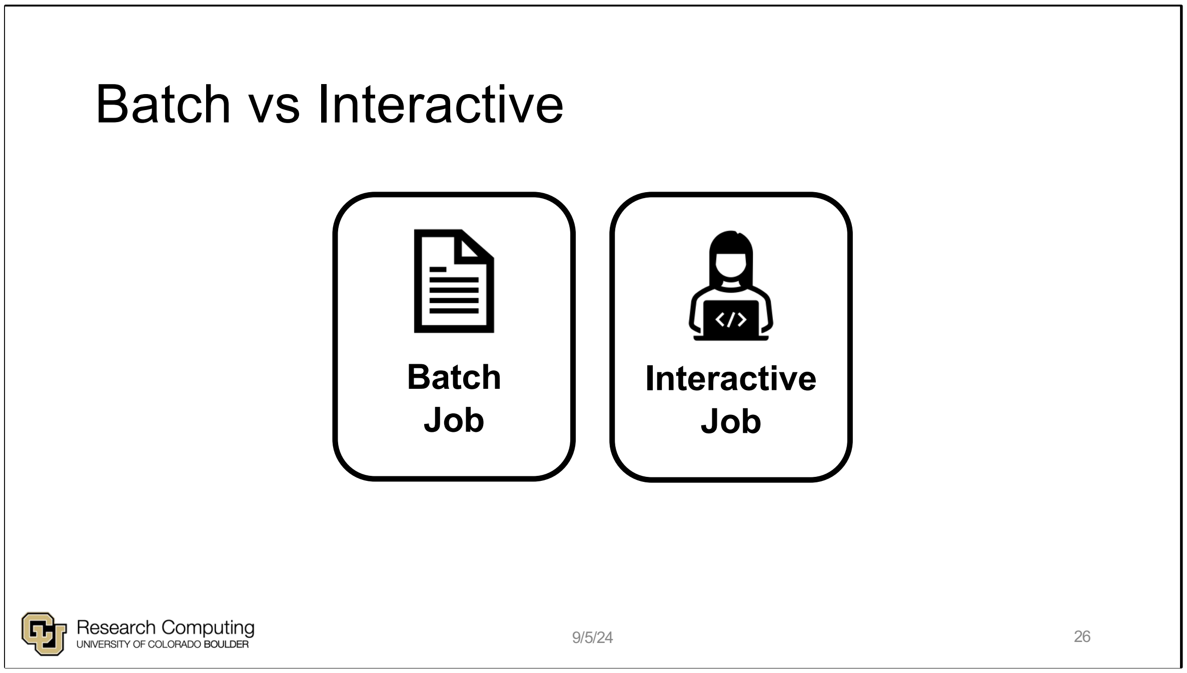
The testing qos supports the different testing partitions, ensuring that users can quickly access resources for testing their workflows. Keep in mind the stringent constraints – this partition is not intended for running regular jobs.



Batch vs Interactive

Batch Job

Interactive Job

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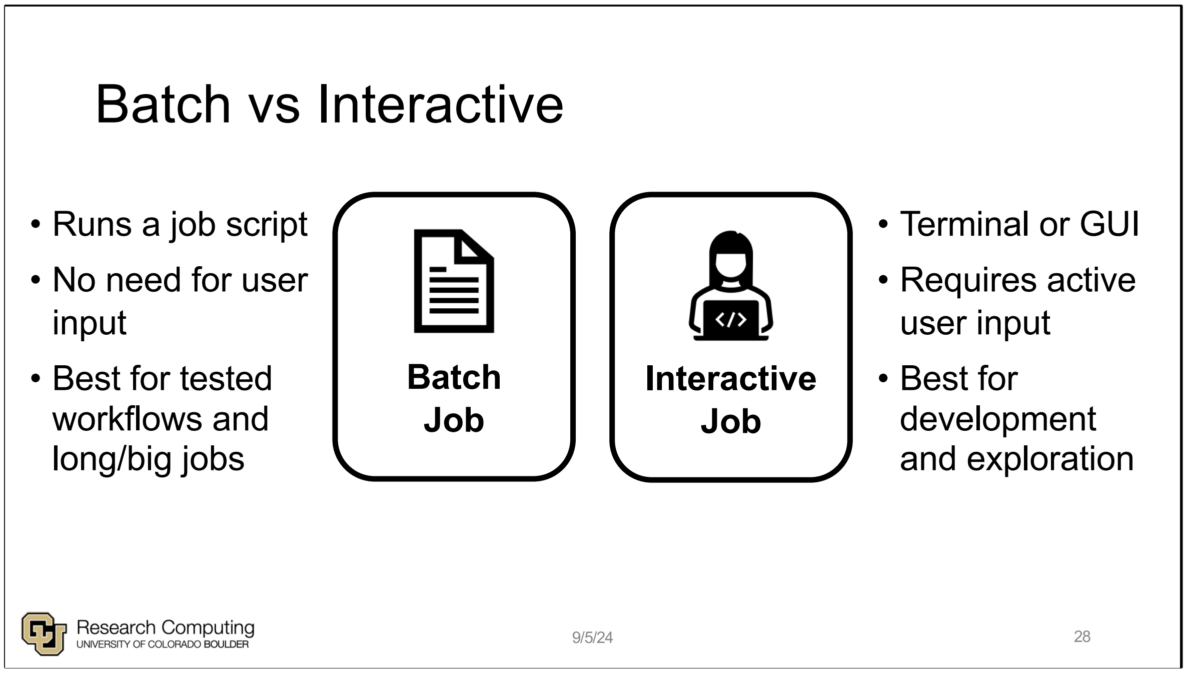
Now that you have a general idea of what resources you plan to request, you will need to consider the type of job you are wanting to schedule. A batch job or an interactive job.

Batch vs Interactive

- Runs a job script
- No need for user input
- Best for tested workflows and long/big jobs

Batch Job

Interactive Job



Batch vs Interactive

- Runs a job script
- No need for user input
- Best for tested workflows and long/big jobs

Batch Job

Interactive Job

- Terminal or GUI
- Requires active user input
- Best for development and exploration

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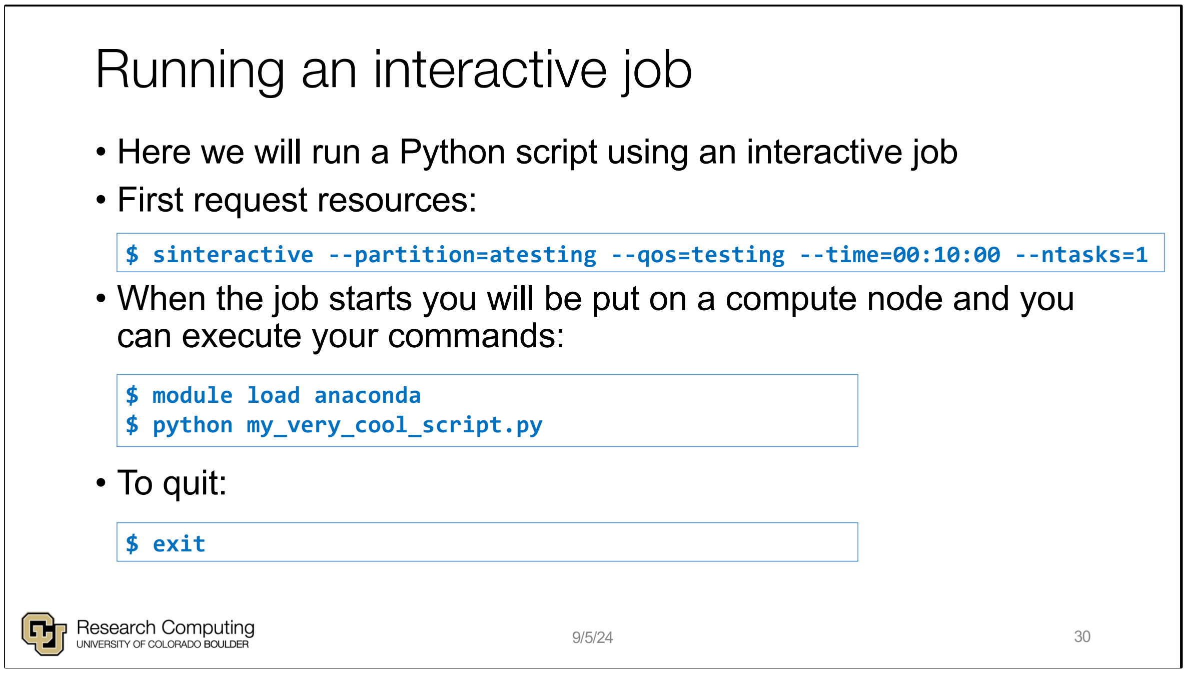
Interactive jobs

acompile

- Quick access to resources
- Limit of 4 CPUs for up to 12 hours
- Focused on compiling/building software and small workflows

`sinteractive`

- Request any partition, more resources, and longer walltime
- Subject to standard wait times (not immediate access)
- Focused on GUI-based software



Running an interactive job

- Here we will run a Python script using an interactive job
- First request resources:

```
$ sinteractive --partition=atesting --qos=testing --time=00:10:00 --ntasks=1
```

- When the job starts you will be put on a compute node and you can execute your commands:

```
$ module load anaconda
$ python my_very_cool_script.py
```

- To quit:

```
$ exit
```

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Batch Jobs

- **Batch Jobs** are jobs you submit to the scheduler that are run later without supervision
- A job script is simply a script that includes **SLURM directives** (resource specifics) ahead of any commands.

Anatomy of a job script

```
#!/bin/bash

## Directives
#SBATCH --<option>=<value>

## Software
module load <software>

## User scripting
<command>
```

Anatomy of a job script

```
#!/bin/bash

## Directives
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module load <software>

## User scripting
<command>
```
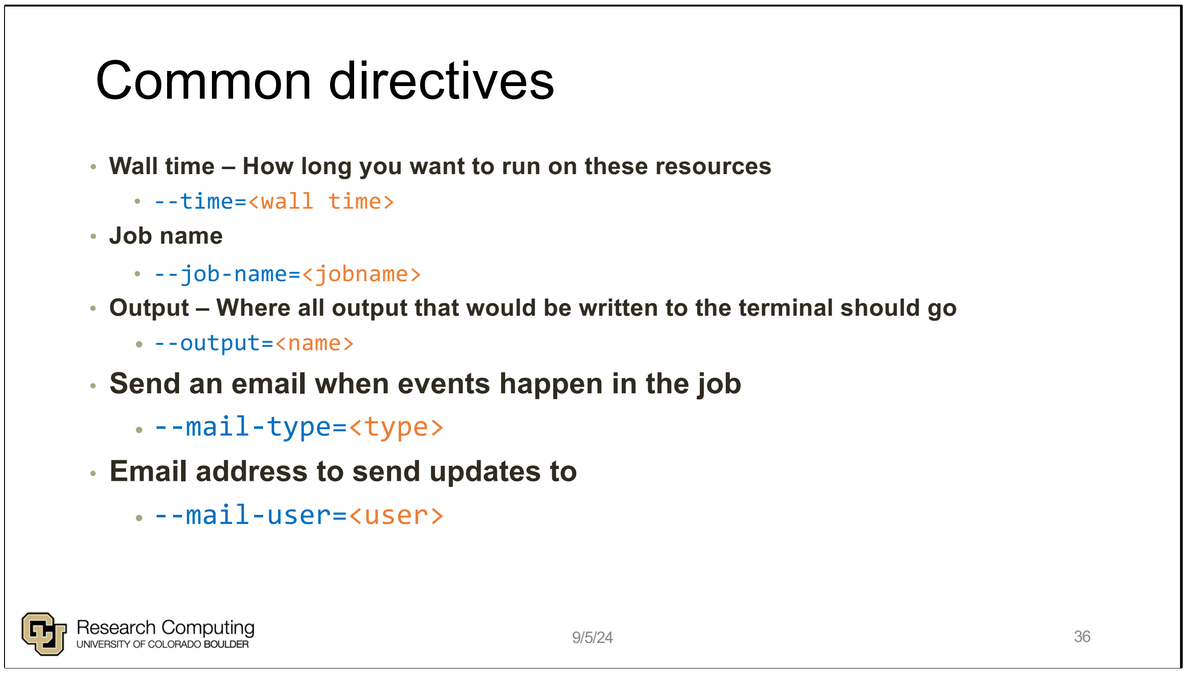

Directives in a job script

```
#SBATCH --<option>=<value>
```

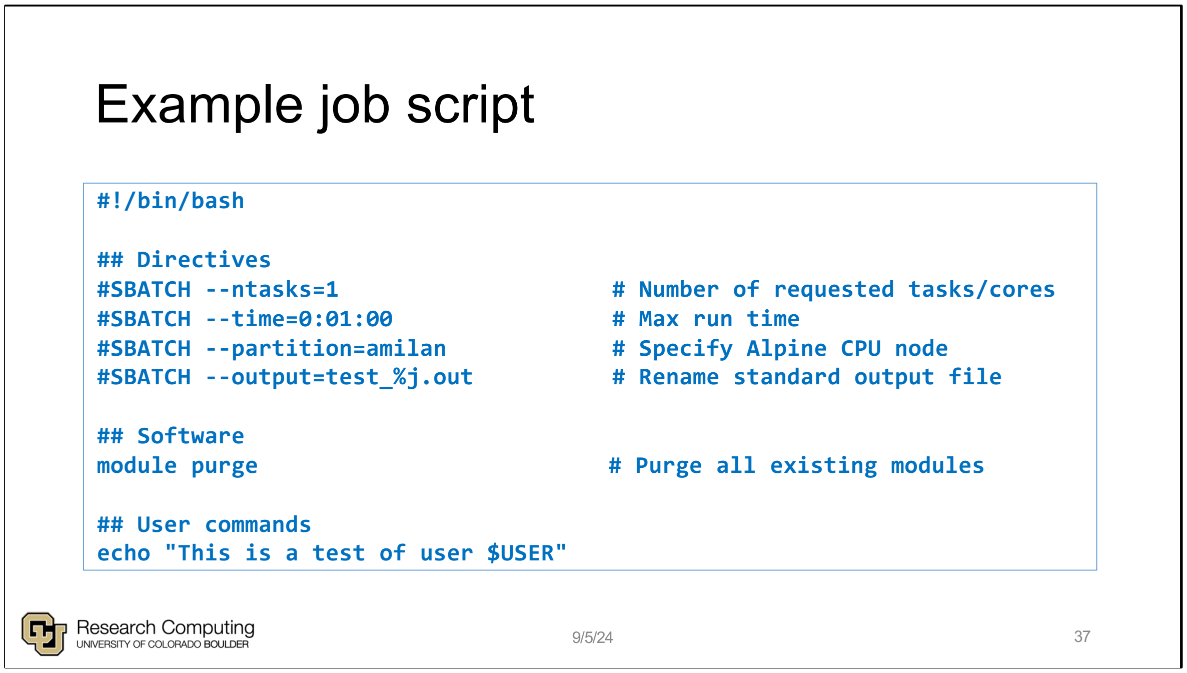
Common directives

- **Partition – A collection of compute nodes**
  - `--partition=<partition_name>`
- **Quality of service (QoS) – System defined constraints for a job (more on this later!)**
  - `--qos=<qos>`
- **Allocation – Account to “charge to”**
  - `--account=<account_name>`
- **Number of nodes to run on**
  - `--nodes=<nodes>`
- **Number of cores to run on**
  - `--ntasks=<number-of-tasks>`



Common directives

- Wall time – How long you want to run on these resources
  - `--time=<wall time>`
- Job name
  - `--job-name=<jobname>`
- Output – Where all output that would be written to the terminal should go
  - `--output=<name>`
- Send an email when events happen in the job
  - `--mail-type=<type>`
- Email address to send updates to
  - `--mail-user=<user>`



Example job script

```
#!/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"
```

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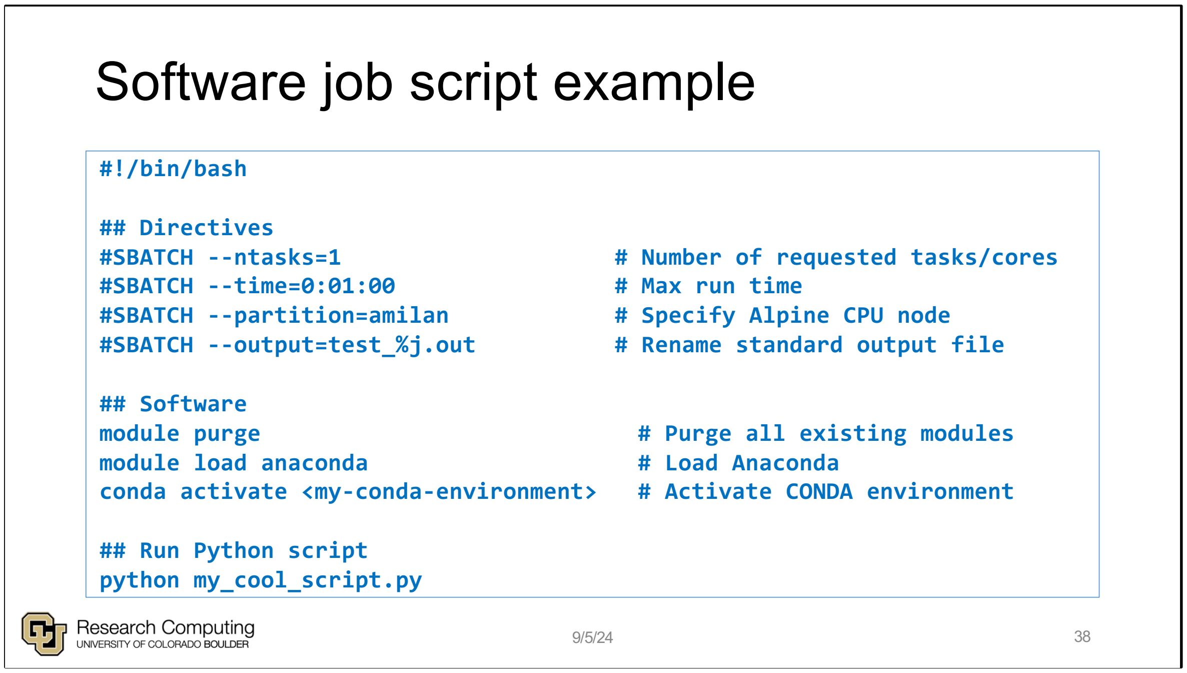
Output files are important for debugging and verifying a job has completed successfully. Always include a --output directive!

The output 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).



Software job script example

```
#!/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
module load anaconda                    # Load Anaconda
conda activate <my-conda-environment>   # Activate CONDA environment

## Run Python script
python my_cool_script.py
```

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Software can be loaded using the software module system or by accessing user installed software in their /projects directory.

https://curc.readthedocs.io/en/latest/compute/modules.html

Be careful not to run GUI or other software that requires user interaction!

Submitting a Job script

```
sbatch <job_file> <other-directives>
```

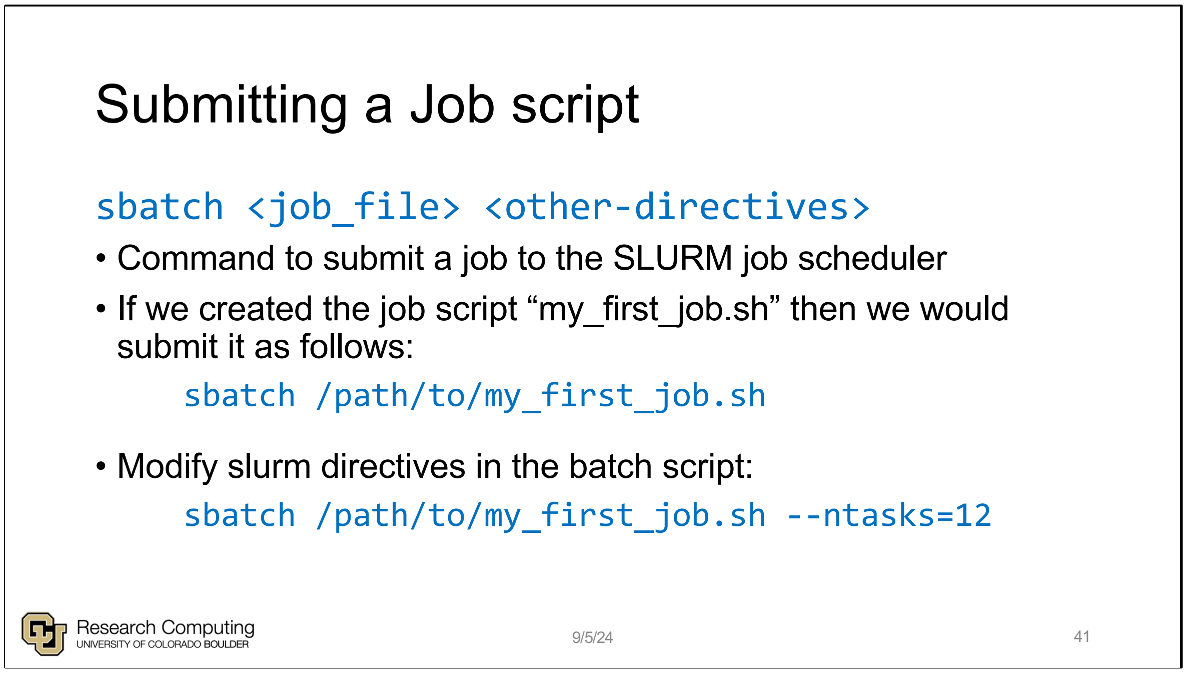
- Command to submit a job to the SLURM job scheduler

Submitting a Job script

```
sbatch <job_file> <other-directives>
```

- Command to submit a job to the SLURM job scheduler
- If we created the job script “my_first_job.sh” then we would submit it as follows:

```
    sbatch /path/to/my_first_job.sh
```



Submitting a Job script

```
sbatch <job_file> <other-directives>
```

- Command to submit a job to the SLURM job scheduler
- If we created the job script “my_first_job.sh” then we would submit it as follows:

```
sbatch /path/to/my_first_job.sh
```

- Modify slurm directives in the batch script:

```
sbatch /path/to/my_first_job.sh --ntasks=12
```

Checking your jobs

- squeue: Monitor your jobs status **in queue and while running**:
  - By default, shows all jobs in queue can specify using:

```
$ 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 can specify using:

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

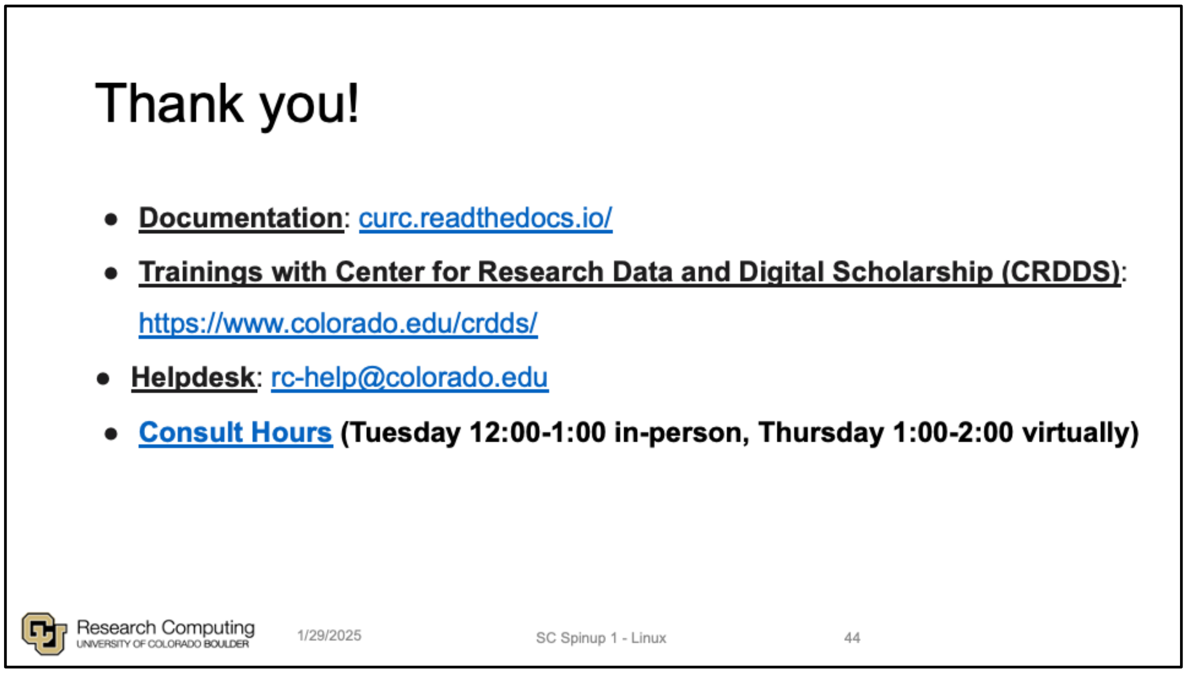
Checking your jobs

- To check the percentage of CPU and memory usage of a job **after it completes,** use seff

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

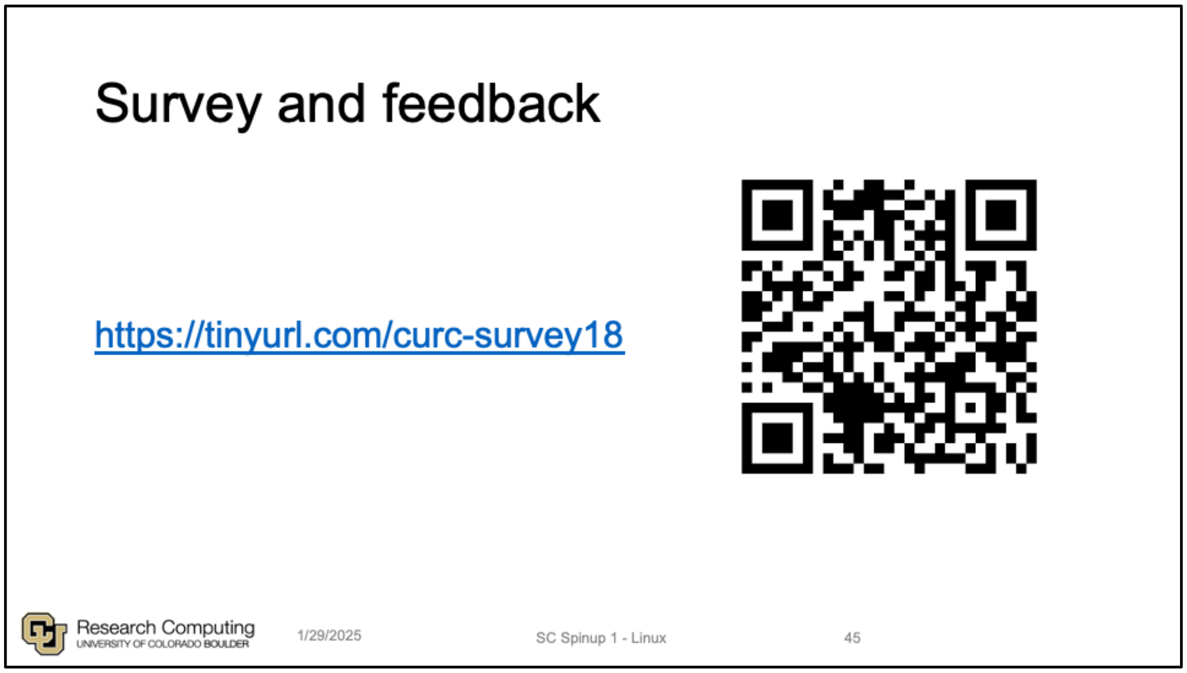
- To see general statistics for your submitted jobs, use jobstats

```
$ module load slurmtools
$ jobstats <username> <# of days>
```



Thank you!

- **Documentation**: curc.readthedocs.io/
- **Trainings with Center for Research Data and Digital Scholarship (CRDDS)**: https://www.colorado.edu/crdds/
- **Helpdesk**: rc-help@colorado.edu
- **Consult Hours (Tuesday 12:00-1:00 in-person, Thursday 1:00-2:00 virtually)**



Survey and feedback

https://tinyurl.com/curc-survey18

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