HPC Job Submission

Research Computing
UNIVERSITY OF COLORADO **BOULDER**

Be Boulder.

HPC Job Submission

Gerardo Hidalgo-Cuellar
gehi0941@colorado.edu
www.rc.colorado.edu
rc-help@colorado.edu

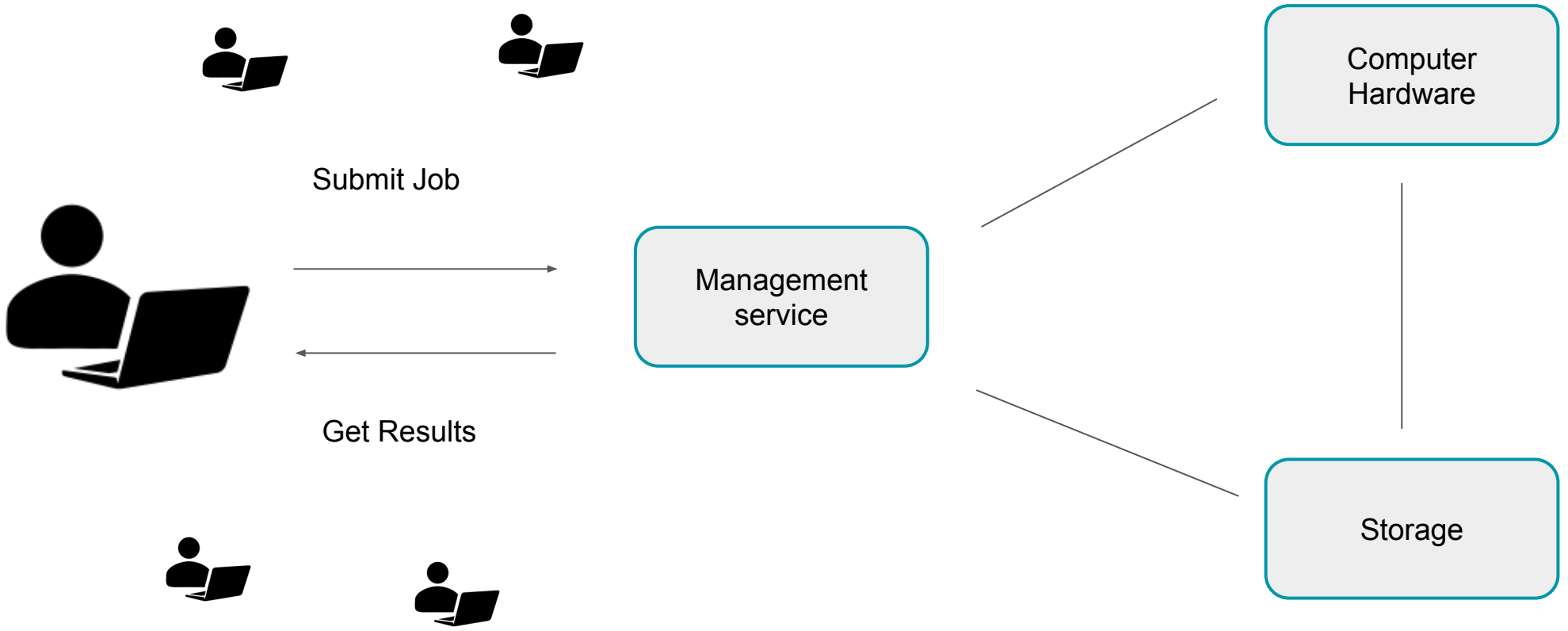
Slides available for download at:
https://github.com/ResearchComputing/Supercomputing_Spin_Up_Fall_2021

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

Outline

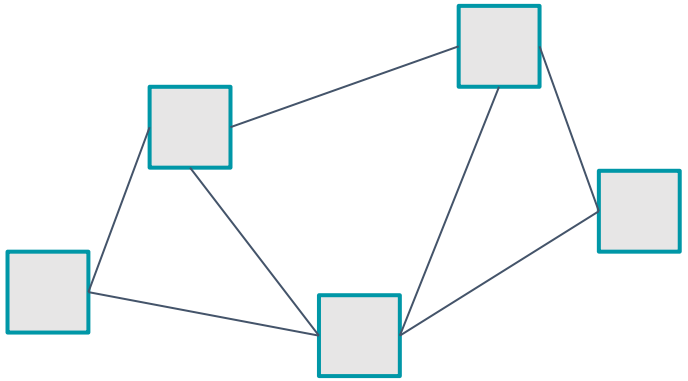
- General Information
  - Summit resources
- Examples of submitting jobs to the supercomputer!
  - Simple batch jobs
  - Advanced batch jobs: running programs, mpi
  - Interactive jobs

HPC - High Performance Computing



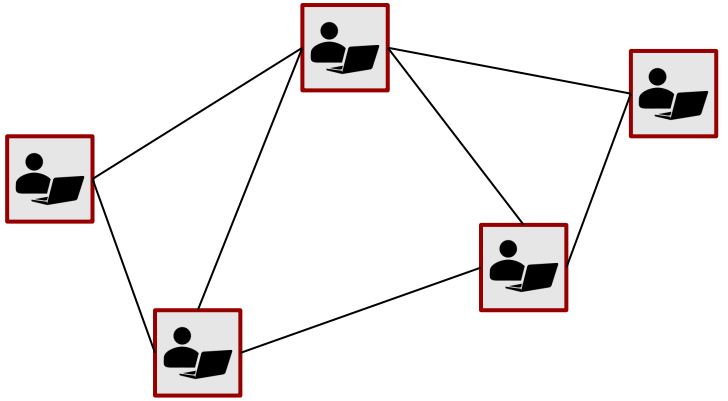
HPC Clusters at RC

Summit



- NSF-Funded
- Shared
- 450+ Nodes

Blanca



- Buy-in Cluster
- High priority use

RMACC Summit Supercomputer

- 450 compute nodes (Intel Xeon Haswell)
- 24 cores per node
- 11,400 total cores
- Omni-Path network
- 1.2 PB scratch storage
- GPFS File system

- 67% CU, 23% CSU, 10% RMACC

Additional Types of RMACC Summit Compute Nodes

- 10 Graphics Processing Unit (GPU) Nodes
  - NVIDIA Tesla K80 (2/node)
- 5 High Memory Nodes
  - 2 TB of memory/node, 48 cores/node
- 20 Phi Nodes
  - Intel Xeon Phi
  - 68 cores/node, 4x threads/core

RC Access: Logging in

- If you have an RMACC account already, login as follows from a terminal:

```
$ ssh <username>@login.rc.colorado.edu
# Where username is your identikey
```

- If you do not have an RMACC account use one of our temporary accounts:

```
$ ssh user<XXXX>@tlogin1.rc.colorado.edu
# Where user<XXXX> is your temporary username
```

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 Summit we will go to a compile node.

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

- Now go to your working directory and download the material for this workshop:

```
[user@shas0137 ~]$ cd /scratch/summit/$USER
[user@shas0137 ~]$ git clone
https://github.com/ResearchComputing/Supercomputing_Spin_Up_Fall_2021
```

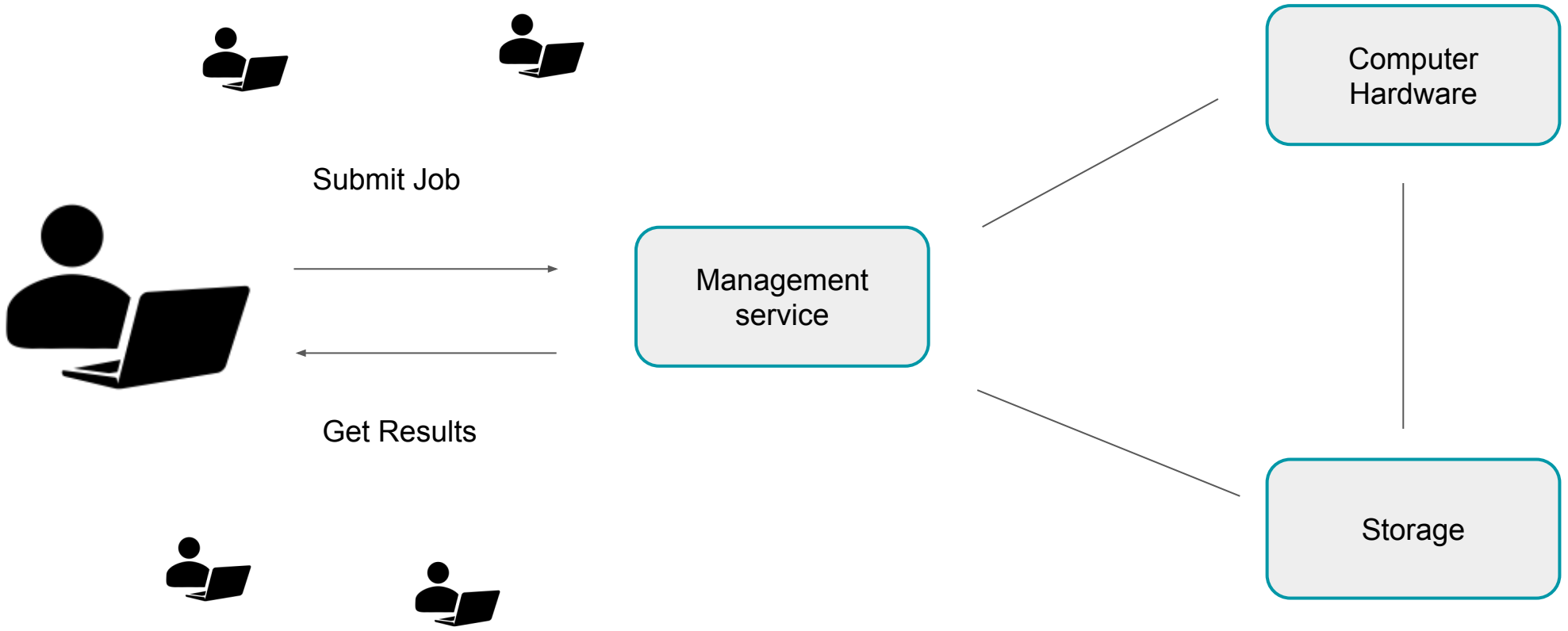
Jobs

- Because Summit is a shared resource with many users trying to utilize available compute with their applications, we need a system to divide compute in a simple and fair system.

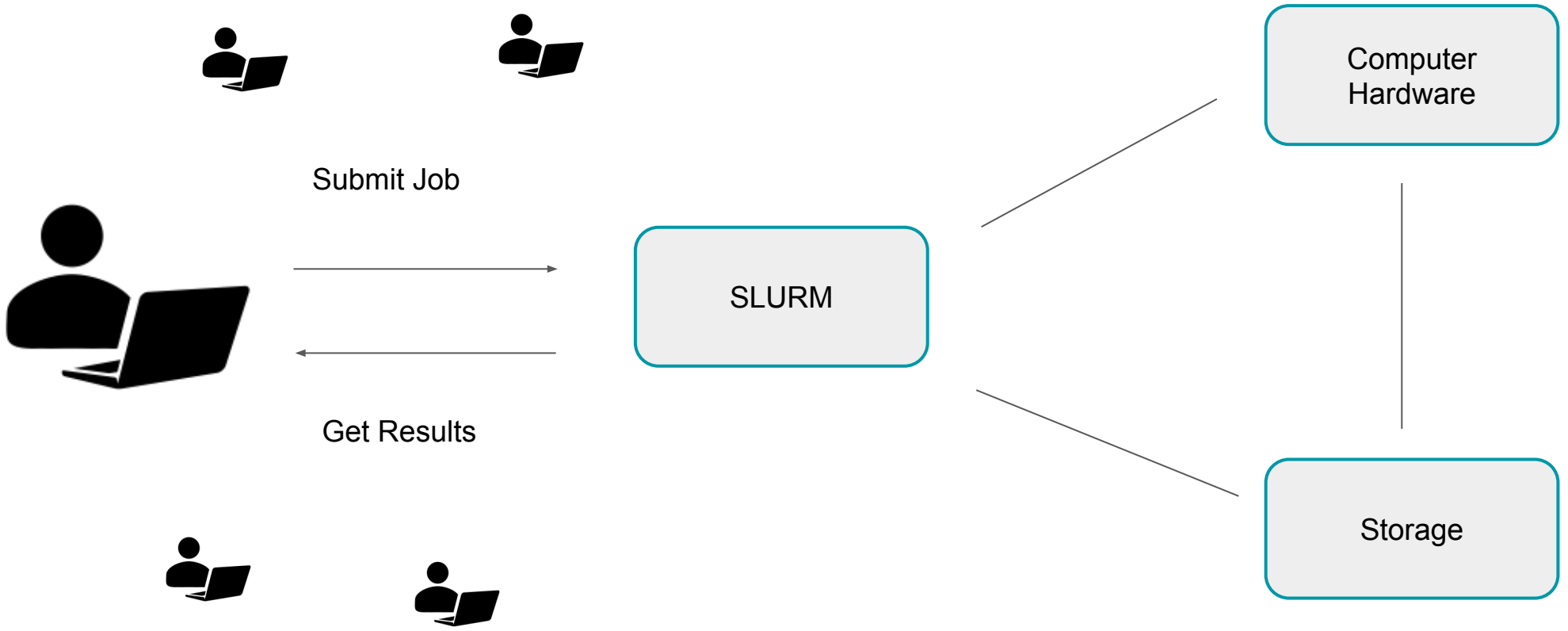
- SLURM
  - **S**imple **L**inux **U**tility for **R**esource **M**anagement

- 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 your submit to the scheduler where they are run later without supervision.
  - By far the most common job on Summit
  - "batch of cookies"
  - Requires a job script

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

Submit your first batch job

- `sbatch`: submit a batch job
- Submit your first job! :

```
$ cd Supercomputing_Spin_Up_Fall_2021/job_submission
$ sbatch submit_test.sh
```

- Script contains most of the parameters needed to define a job
- Additional flags can be used to temporarily replace any set parameters.

```
$ sbatch --reservation=scs submit_test.sh
```

http://slurm.schedmd.com/sbatch.html

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 (submit_test.sh)

```
#!/bin/bash

## Directives
#SBATCH --ntasks=1                          # Number of requested tasks
#SBATCH --time=0:01:00                      # Max wall time
#SBATCH --partition=shas-testing            # Specify Summit Haswell nodes
#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

Partitions

- Partitions specify the type of compute node that you wish to use
  - Specify with the `--partition` flag

```
#SBATCH --partition=shas
```

Partition	Description	# of nodes	RAM/core (GB)	cores/node	GPUs/node
shas	General Compute (Haswell)	~450	4.84	24	0
sgpu	GPU-enabled nodes	10	4.84	24	effectively 4
smem	High-memory nodes	5	42.7	48	0
sknl	Phi (Knights Landing) nodes	20	5.25	68	0

Sub-Partitions

- In addition to normal compute partitions, Summit Users also have access to several testing and interactive partitions
  - Quick access to get your applications functional!

Partition	Description	Max wall time	Max jobs/user	Max nodes/user
shas-testing sgpu-testing sknl-testing	For quick turnaround when testing	30 M	1	2 12 cores/node
shas-interactive	For interactive jobs (command or GUI)	4 H	1	1 core

Quality of Service (--qos)

- Quality of Service specifies additional constraints Job
  - On Summit, 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	Derived from partition	n/a	256
long	For jobs needing longer wall times	7 D	n/a	20

Writing your first job script

Your turn!

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

1. Navigate to the 'job_submission' directory
2. Create file 'submit_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 submit_sleep.sh

1. The job will run on 1 core of 1 node
2. We will request a 1 minute wall time
3. Run on the shas-testing partition
4. Set the output file to be named “sleep.%j.out”
5. Name your job “sleep”
6. Bonus: Email yourself when the job ends
7. Contains the following commands ->

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

```
$ sbatch --reservation=scs submit_sleep.sh
```

Solution are prefixed with 'answer'

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 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>
```

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

Checking your jobs (2)

- Another method of checking details of your job 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>
```

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

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!
```

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

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, but *installs are best effort*
  - For more assistance contact rc-help@colorado.edu

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

Example 1: Serial R Code

Running an external program

- Let's run R on an R script
- This script calls and runs the script *R_program.R*
  - Let's take a look at the R script

- Let's examine the batch script submit_R.sh
  - Note how R is loaded
- Go ahead and submit the batch script submit_R.sh

Example 2: Serial Matlab Code

Launch Matlab!

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

1. Name it 'submit_matlab.sh'
2. Load the 'matlab' module
3. The job should contain the following commands:

```
cd progs
matlab -nodisplay -nodesktop -r "matlab_tic;"
```

Details on job script parameters are in the next slide

Job details of submit_matlab.sh

1. The job will run on 1 core of 1 node
2. We will request a 2 minute wall time
3. Run on the shas-testing partition
4. Set the output file to be named “matlab.%j.out”
5. Name your job “matlab”

   Bonus: Email yourself when the job ends
6. Contains the following commands

```
cd progs
matlab -nodisplay -nodesktop -r "matlab_tic;"
```

```
$ sbatch --reservation=scs submit_matlab.sh
```

Solution are prefixed with 'answer'

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 --reservation=scs submit_python_mpi.sh
```

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

- 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 Summit
- When the resources become available the job starts
- Commands to run:

```
$ sinteractive –-time=00:10:00 --reservation=scs
```

- Once we receive a prompt, then:

```
$ module load R
$ cd ./progs
$ Rscript R_program.R
```

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

```
$ exit
```

Tools for submitting many small jobs at once

- CURC Load Balancer
  - https://curc.readthedocs.io/en/latest/software/loadbalancer.html
- Slurm job arrays
  - https://slurm.schedmd.com/job_array.html

Thank you!

- Please fill out the survey: http://tinyurl.com/curc-survey18
- Contact information: rc-help@Colorado.edu

- Slides and Examples from this course:
  https://github.com/ResearchComputing/Supercomputing_Spin_Up_Fall_2021

- Slurm Commands: https://slurm.schedmd.com/quickstart.html

Minimal Batch Script

What is the *minimum* required by a batch script?

```
#!/bin/bash

## Directives (HPC Resources)


## Software


## User Scripting
```

Minimal Batch Script

```
sacct -j 9151881 --format=account,elapsed,ncpus,qos,reqmem

Account     | Elapsed   | NCPUS   | QOS      | ReqMem |
ucb-general | 00:00:03 | 1       |  normal | 4848Mc |
ucb-general | 00:00:03 | 1       |          | 4848Mc |
ucb-general | 00:00:03 | 1       |          | 4848Mc |
```

Running from Different Directory

- What happens if we try to run a script from a different directory?
  - either by giving full or relative address?

- Where does the output go?
- Potential benefits?

Running from Different Directory

```
#!/bin/bash

## Directives (HPC Resources)

## Software

## User Scripting
pwd
touch test.txt
```

Running to Different Directory

- What happens if we try to run a script and change into a different directory?

- Where does the output go?
- Potential benefits?

Running to Different Directory

```
#!/bin/bash

## Directives (HPC Resources)

## Software

## User Scripting
echo "starting dir: $(pwd)"
touch start.txt
cd ../test
touch end.txt
echo "ending dir: $(pwd)"
```