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 at:
https://github.com/ResearchComputing/Supercomputing_Spinup

Survey at: 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
  - Cluster resources

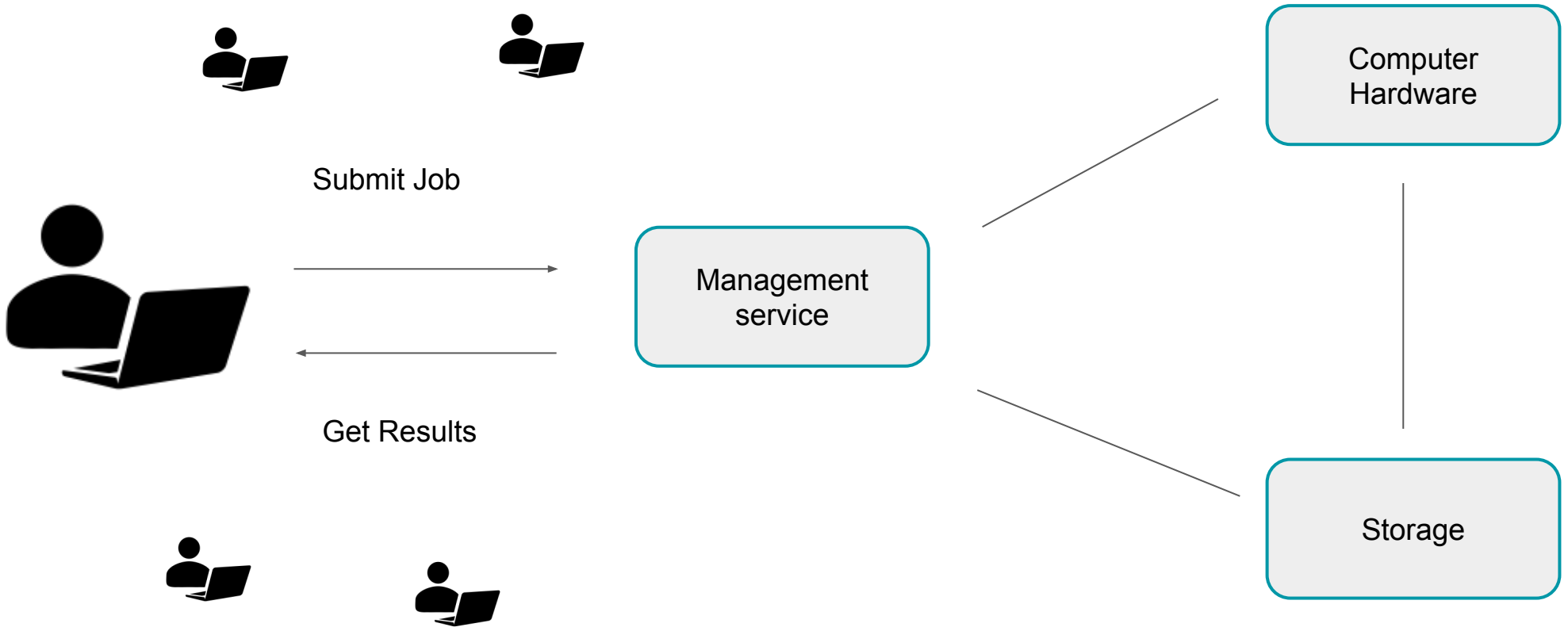
- Examples of submitting jobs to the supercomputer!
  - Traditional job submission (terminal)
    - Simple batch jobs: hello world, running programs
    - Advanced batch jobs: mpi, serial-parallel
    - Interactive jobs
  - Non traditional (gateways)
    - Interactive applications
    - Check jobs

RC account check

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

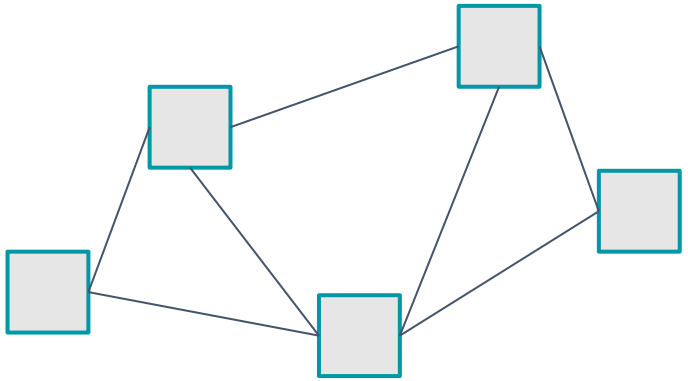
**only available during seminar*

HPC - High Performance Computing



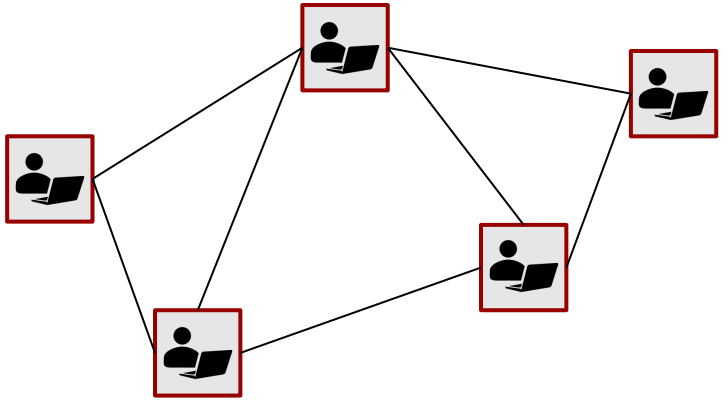
HPC Clusters at RC

Summit



- NSF-Funded
- Shared
- 450+ Nodes

Blanca



- Buy-in Cluster
- High priority use

RMACC Summit Supercomputer

- 450 General Compute nodes (Intel Xeon Haswell)
  - 24 cores per node
- GPU, High Memory, Phi Nodes
- **11,400 total cores**
  - Omni-Path network
  - 1.2 PB scratch storage

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

Additional Node Types on Summit

- 10 GPU Nodes
  - NVIDIA Tesla K80 (2 accelerators/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

Blanca Supercomputer

- **223 Compute nodes** (heterogeneous)
- **10 GPU nodes** (heterogeneous)
- Hardware owned by individual contributors
  - Preemptable access to all other nodes. i.e., you can use then when the node owners are not

- When you log in, the Summit queue is loaded in *by default*

```
$ module load slurm/blanca
# to load in Blanca queue
```

Submitting Jobs via Terminal

RC Access: Logging in

- If you have an RC 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 RC 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 a working directory (I’m using scratch here) and download the material for this workshop:

```
[user@shas0137 ~]$ git clone
https://github.com/ResearchComputing/Supercomputing_Spinup_Spring_2022.git
[user@shas0137 ~]$ cd Supercomputing_Spinup
[user@shas0137 ~]$ export SPINUP_ROOT=$(pwd)
```

Working Directory

- Navigate to the “job_submission” directory

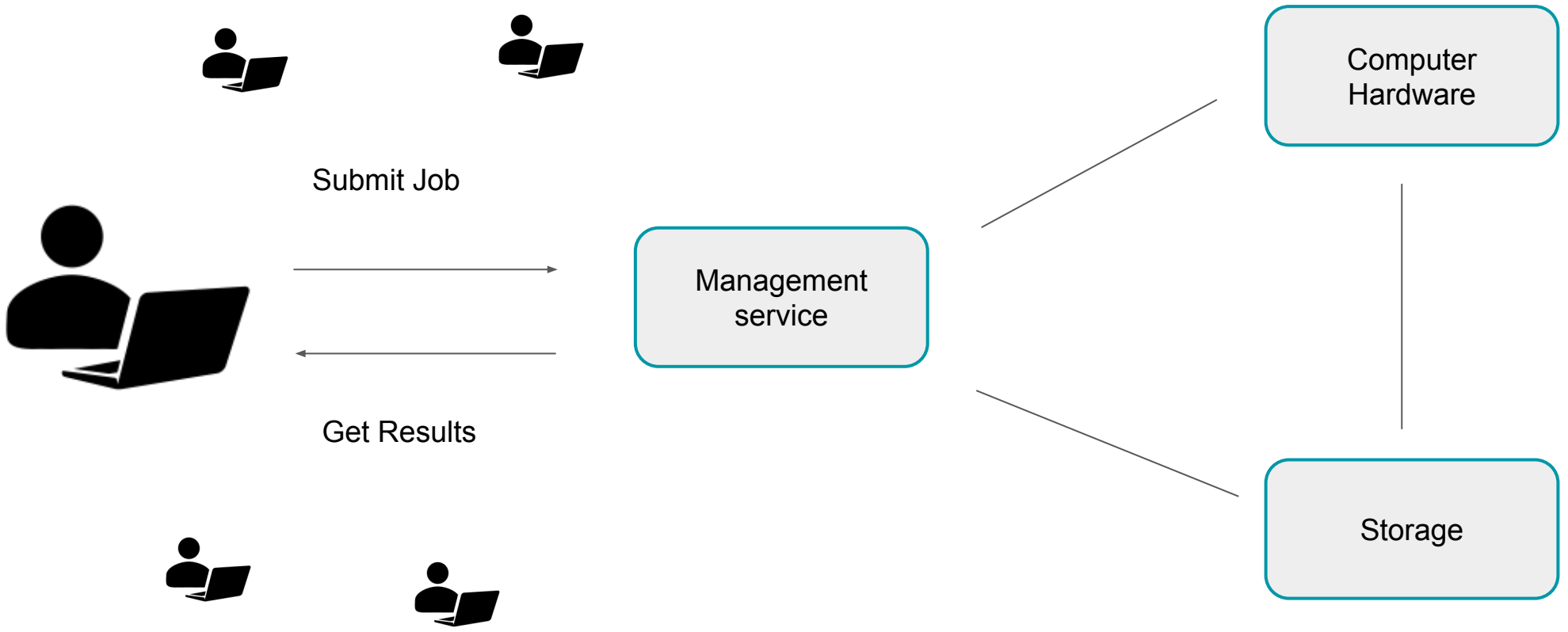
```
[user@loginNN ~]$ cd $SPINUP_ROOT/job_submission
```

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

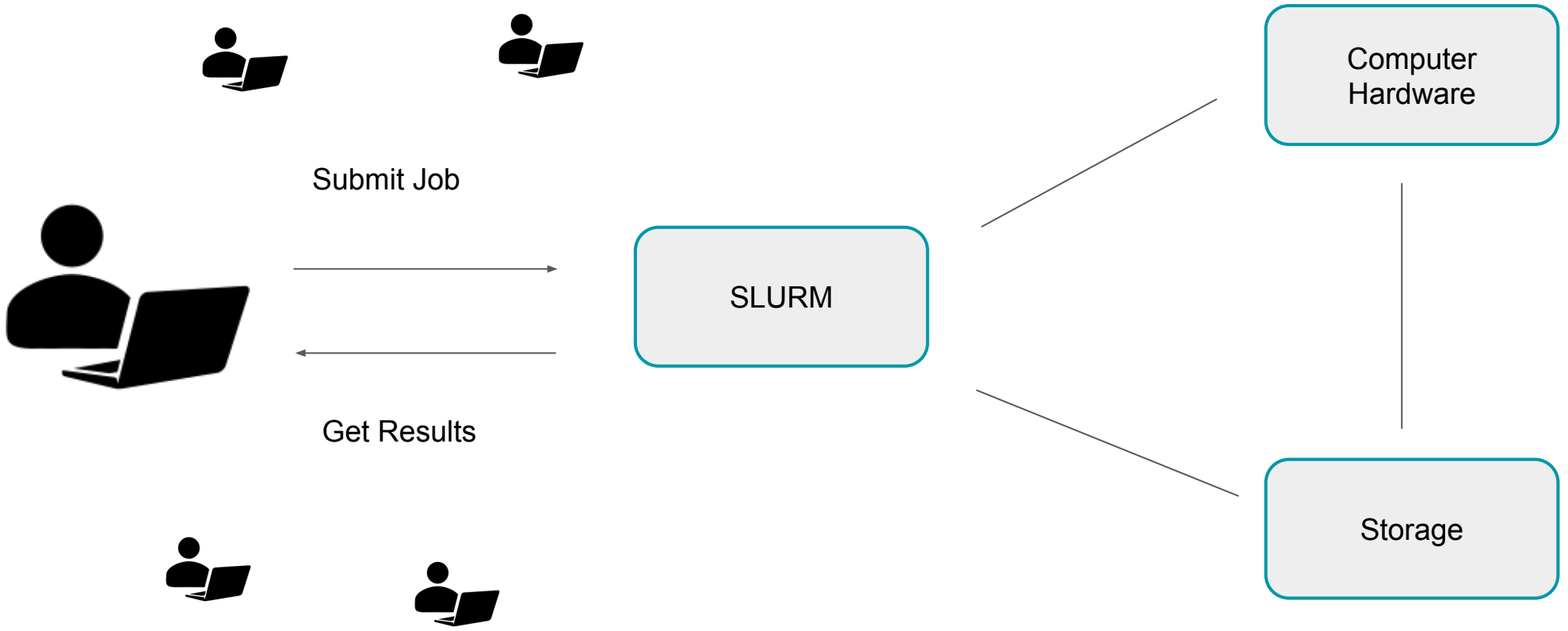
Jobs

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

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

Submit your first batch job

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

```
$ cd $SPINUP_ROOT/job_submission
$ sbatch summit_scripts/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

- open `summit_scripts/test.sh` (nano or vim)

```
#!/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"
```

Anatomy of a job script

```
#!/bin/bash

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

## Software
module load <software>

## User scripting
<command>
```

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	~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
    - only `shas` and `sknl`
  - 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 summit_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 submit_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 **shas-testing partition**
4. Set the output file to be named **"./output/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 summit_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>
```

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

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>
```

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, *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
- Batch script calls and runs *programs/R_program.R*
  - Let's take a look at the R program

- Let's examine the batch script summit_scripts/R.sh
  - Note how R is loaded
  - R program can be run with "Rscript <script>"

- Go ahead and submit the batch script:

```
$ sbatch summit_scripts/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 summit_scripts/matlab.sh'
2. Load the matlab module (module load matlab)
3. The job should contain the following commands:

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

Details on job script parameters are in the next slide

Job details of 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 **"./output/matlab.%j.out"**
5. Contains the following commands

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

*Bonus: Email yourself when the job ends

```
$ sbatch summit_scripts/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 python_mpi.sh

```
$ sbatch summit_scripts/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: `summit_scripts/python_loadbalance.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

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

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

- Once we receive a prompt, then:

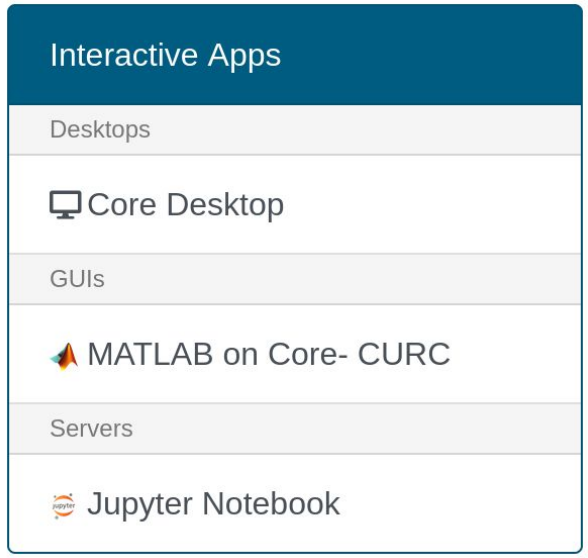
```
$ module load R
$ cd programs
$ Rscript R_program.R
```

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

```
$ exit
```

Open OnDemand (demo)

- If you are new to linux, submitting jobs to an HPC system can be overwhelming
- We have browser-based applications that give you the power to connect to a compute node straight away
- CURC Open OnDemand
  - JupyterHub
  - MATLAB
  - Virtual Desktop



Thank you!

- Survey: http://tinyurl.com/curc-survey18
- Contact information: rc-help@Colorado.edu

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