Research Computing New User Seminar

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- Slides: https://github.com/ResearchComputing/New_User_Seminar

Before We Begin

- **The focus of most of the seminar is UCB Summit users**
  - CSU and XSEDE Summit users please understand things are somewhat different for you.
  - Email rc-help@colorado.edu for exact discrepancies
- **Things to take particular note of:**
  - Confusing, ambiguous, highly nuanced concepts
  - Common mistakes or frustrations
  - Best Practices
- **Good questions to ask:**
  - Why? Questions
  - If a question is said to be covered later feel free to re-ask if it's not answered to your satisfaction.

- Slides: https://github.com/ResearchComputing/New_User_Seminar

Outline

- **What is RC?**
- **Steps to get access to our systems**
  - Accounts
  - Two-factor authentication
  - Allocations
  - Logging in
- **Navigating our systems**
  - Storage spaces
  - Data transfer - Globus
  - Software
- **Running jobs**

- Slides: https://github.com/ResearchComputing/New_User_Seminar

What is Research Computing?

- **Provide services for researchers that include:**
  - Large scale computing
  - Data storage
  - High speed data transfer
  - Data management support
  - Consulting
  - Training
- **We are likely best known for:**
  - Summit Supercomputer
  - PetaLibrary storage

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What Would I Use Summit For?

- **Research Computing is more than just Summit...**
  ...But it is what we are most known for
- **So what would you use Summit for?**
  - Solving large problems that require more:
    - Memory than you have on your personal computer
    - Cores/nodes/power than you have on your personal computer
  - High performance GPU computing
  - High memory jobs
  - Visualization rendering
- **Not a place for:**
  - Large data storage

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Hardware - Summit Supercomputer

- 450+ compute nodes
- 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 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
- **Phi Nodes**
  - 20 nodes
  - Intel Xeon Phi

How To Access RC Resources?

1. Get an account
2. Set up two factor authentication
3. Set up an allocation (Unnecessary for Blanca or PetaLibrary)
4. Log in
5. Create greatness

After you login, you will need to do many additional things that we will discuss today

Getting an RC Account

- **CU Boulder users and affiliates:**
  - Request an account through the RC Account request portal
    - https://rcamp.rc.colorado.edu/accounts/account-request/create/verify/ucb
- **CSU Users:**
  - Request an CSU eID if you don't have one
  - Fill out account application form
  - Duo authentication
  - Then get an RC user account
  - https://www.acns.colostate.edu/hpc/summit-get-started/
- **RMACC Users:**
  - Contact your local representative. They will help you get an XSEDE account
    - Need XSEDE account and Duo access through XSEDE
  - Contact us with your XSEDE username to start our local process if approved by your local contact and your XSEDE account is in place
  - If you don't have a local representative then contact rc-help@colorado.edu

Setting up Two-Factor Authentication

- **Require this to provide an extra level of authentication, we are outside the firewall!**
- Duo
  - Access through a smart phone app
  - Access through text
  - Access through phone call

Duo Authentication

- Once you get an account, contact rc-help@colorado.edu to request a Duo invitation
- Once you get the invitation, you'll get a series of steps to complete Duo enrollment
- RC supports Duo "push" and "phone call" for authentication
- Greatly prefer "push"
- Once in place UCB users can manage their Duo setup at duo.colorado.edu

Allocations

- You will need a compute allocation to use any of our resources
- Automatically added to UCB General when applying for your account
  - If you do not request access to Summit when signing up, then you won't have access to UCB General
  - Contact rc-help@colorado.edu if you are not part of UCB General
- Once you have some benchmarks, you will want to request an allocation

Why Do I Need An Allocation?

- **I have an account – why do I need an allocation?**
  - An account validates you are eligible to use RC compute resources
  - An allocation allows us to keep track of your use of the system
  - This is important because:
    - We need to make sure we have enough resources to accommodate all of our users
    - Helps for reporting to NSF and the CU Research & Innovation Office
  - Applying for an allocation beyond UCB General:
    - Gives you higher priority in the system and access to more compute time
- **CSU and RMACC users already have one set up.**
- **Not all UCB users need or want to use Summit**

What is Fair Share?

- Fair share scheduling uses a complex formula to determine priority in queue
- Looks at load for each user and each QOS and balances utilization to fairly share resources
  - Involves historical use by user plus how long job has been in the queue
- System will first look at weighted average utilization of user mostly over the last 4 weeks
- Then compare it to the fair share target percentage of a user

Fair Share Target Percentage

- The target percentage depends on your priority based on your project proposal
- Everyone not associated with a project shares a target percentage of 13% (20% of the CU fraction)
  - No guaranteed level per user
- If you are under (over) your target percentage (based on a 4 week average) your priority is increased (decreased)
- Reminder this all only impacts pending jobs
- If no other pending jobs and enough resources are available then your job will run regardless of your previous usage

Logging In

- It’s important to note that you are NOT logging into any specific resource
  - Summit, etc.
- When you log in, you land on our login nodes
- From there, you can access our other resources

RC Resource Access

- To login to an RC login node:

```
ssh username@login.rc.colorado.edu
```

- Enter your password as:

```
duo:identikey_password
```

Navigating our Systems

- Now that you've logged in, now what?
  - What are the different node types we have?
  - What are the different storage spaces?
    - What should I be putting in these storage spaces?
  - How do I transfer data around?
  - How do I deal with software?

Different Node Types

- **Login nodes**
  - Four virtual machines
  - This is where you are when you log in
  - No heavy computation, interactive jobs, or long running processes
  - Script or code editing
  - Job submission
- **Compile nodes**
  - Where you compile code
  - Explore the Summit software environment
- **Compute/batch nodes**
  - This is where jobs that are submitted through the scheduler run
  - Intended for heavy computation

Storage Spaces

- **Home Directories**
  - /home/$USER
  - Not for direct computation
  - Small quota (2 GB)
  - Backed up
- **$PROJECT Space**
  - /projects/$USER
  - Mid level quota (250 GB)
  - Large file storage
  - Backed up

- **Scratch Directory**
  - /scratch/summit/$USER
  - 10 TB
    - Can ask for more if needed
  - Files purged around 90 days

What Belongs Where?

- /home
  - Code and Scripts
  - Very small files
  - Inappropriate for sharing files with others
  - Inappropriate for job output
- /projects
  - Code/files/libraries relevant for any software you are installing (if you want to share files with others)
  - Mid-level size input files
  - Appropriate for sharing files with others
  - Inappropriate for job output
- /scratch/summit
  - Output from running jobs
  - Large files
  - Appropriate for sharing files with others
  - THIS IS NOT APPROPRIATE FOR LONG TERM STORAGE

Transferring Data

- Globus is Research Computing's preferred method of data transfer
- Designed with researchers in mind
- End points between computers make for efficient data transfer with an easy to use interface
  - Endpoints are different locations that data can be moved to/from
  - Personal or multi-user
- Rsync and sftp through the login nodes is good for small transfers

Setting Up Globus

- **Log into your account through Globus.org with your identikey and identikey password**
- **Make your personal computer an endpoint**
  - Not needed if you are transferring between two other endpoints, like a repository and RC
- **Transfer data**
  - www.globus.org

Software

- **Common software is available to everyone on the systems**
- **You can install your own software**
  - But you are responsible for support
  - We are happy to assist
- **Research Computing uses modules to manage software**
  - You can load modules to prepare your environment for using software
    - Set any environment variables
    - Set environment so application can find appropriate libraries, etc.

Important Things to Know About Modules

- Some modules might require a specific hierarchy to load
  - For some modules, you may need to specify a specific version
    - For example: `module load R/3.3.0`
  - For other modules, you may be able to be more generic
    - For example: `module load matlab`
- Some modules may require you to first load other modules that they depend on
- To find dependencies for a module, type: `module spider <package>`
- To find out what software is available, type: `module avail`
- To set up your environment to use a software package, type: `module load <package>/<version>`

Job Submission

Running Jobs

- **What is a "job"?**
- **Batch jobs**
  - Submit job that will be executed when resources are available
  - Create a text file containing information about the job
  - Submit the job file to a queue
- **Interactive jobs**
  - Work interactively at the command line of a compute node

Job Scheduling

- On a supercomputer, jobs are scheduled rather than just run instantly at the command line
  - Shared system
  - Jobs are put in a queue until resources are available
- Need software that will distribute the jobs appropriately and manage the resources
  - Simple Linux Utility for Resource Management (Slurm)
    - Keeps track of what nodes are busy/available, and what jobs are queued or running
    - Tells the resource manager when to run which job on the available resources

Partitions and ‘Quality of Services’

- There are several ways to define where your job will run
- Partitions (basically a queue):
  - Resources/hardware
- QoS:
  - Tells what the limits or characteristics of a job should be
    - Maximum wall time
    - Number of nodes
- One partition might have multiple QoS
- A QoS might exist on multiple partitions

Available Partitions

Partition	Description	# of nodes	cores/node	GPUs/node
shas	General Compute (Haswell)	380	24	0
shas-testing	General Compute Testing (Haswell)		24	0
shas-interactive	General Compute Interactive (Haswell)		24	0
sgpu	GPU-enabled nodes	10	24	effectively 4
sgpu-testing	GPU-enabled testing nodes		24	effectively 4
smem	High-memory nodes	5	48	0
sknl	Phi (Knights Landing) nodes	20	68	0
sknl-testing	Phi (Knights Landing) testing nodes		68	0

Quality of Service

QoS	Description	Maxwall	Max jobs/user	Max nodes/user
normal	Default QoS	Derived from partition	n/a	256
testing	For quick turnaround when testing	0.5 H	1	24
interactive	For interactive jobs with few nodes	4 H	1	1
long	For jobs needing longer wall times	7 D	n/a	20
condo	For groups who have contributed to the Summit condo	7 D	n/a	n/a

Useful Slurm Commands - sbatch

- **sbatch**: submit a batch script to slurm
- You can use a bunch of flag options in a batch script or on the command line
- Useful to put in script so have for future use

- Example:

```
sbatch test.sh
```

OR

```
sbatch --partition=shas test.py
```

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

SBATCH Options

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

`#SBATCH <options>` `sbatch <options>`

- Allocation: `--account=<account_no>`
- Partition: `--partition=<partition_name>`
- Sending emails: `--mail-type=<type>`
- Email address: `--mail-user=<user>`
- 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>`

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

Working on Summit

- Make sure you load the appropriate slurm module – if on a Login Node:

```
$ module load slurm/summit
$ ml slurm/summit #shorthand
```

  - If on a scompile node, this is not needed and will return an error.
  - After you run this command you can run sbatch to submit jobs

Blanca

- If you are a Blanca user, you need an RC account
- To run jobs as a Blanca user, once you've logged into a login node, load the Blanca slurm module

```
module load slurm/blanca
```

Use `--qos=blanca-<group-identifier>` for high priority access

`--qos=blanca` for low-priority access

- Only certain users have access to Blanca – paid service
- If you are unsure, you can ask your advisor or RC
  - But likely if you are unsure you don't have access

PetaLibrary

- To access the PetaLibrary, you login in to one our RC's login nodes as normal
- Then you `cd` to either `/work/<groupname>` or `/archive/<groupname>`, depending on your PetaLibrary service
  - `<groupname>` is the name set for your group when you set up the PetaLibrary service
  - You do not include the `<>`
- Only certain users have access to PetaLibrary – paid service
- If you are unsure, you can ask your advisor or RC
  - But likely if you are unsure you don't have access

Practice Examples

Submit Your First Job!

Submit a slurm job with the following instructions:

1. The job should run the Unix “hostname” command
2. The job will be submitted from a bash script named hostname_summit.sh
3. The job will run on 1 node
4. We will request 1 minute wall time
5. Run from the testing QOS
6. Run on the shas-testing partition

Hostname_summit.sh

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

# purge all existing modules
module purge

hostname
```

Running the script

- Submit the job:
  ```
  sbatch hostname_summit.sh
  ```
- Check output

Another slurm command

- **squeue**
  - View information about jobs located in the slurm scheduling queue
- OPTIONS:
  - User: `-u <user list>`
  - Queues: `--qos=<qos_list>`

- EXAMPLE:

  squeue: `--qos=debug`

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

Your turn

Submit a slurm job with the following instructions:

1. The job should run first the whoami command, then the Unix "sleep" command for 30 seconds, then the hostname command
   - Syntax for these Unix commands are below:

```
whoami
sleep 30
hostname
```

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

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

Your turn

Submit a slurm job with the following instructions:

1. The job will be submitted from a bash script named sleep.sh
2. The job will run on 1 node
3. Request a 1 minute wall time
4. Run the job from the normal QOS
5. Run the job from the Summit haswell partition
6. Name your job sleep
7. Email yourself the results at the end of the job run
   Hint: This requires two SBATCH directives to do this – see link at top of this slide

Sleep.sh

```
#!/bin/bash
#SBATCH --nodes=1                       # Number of requested nodes
#SBATCH --time=0:01:00                  # Max walltime
#SBATCH --qos=testing                   # Specify testing QOS
#SBATCH --partition=shas-testing        # Specify Summit Haswell nodes
#SBATCH --output=sleep_%j.out           # Rename standard output file
#SBATCH --job-name=sleep                # Job submission name

# purge all existing modules
module purge

whoami
sleep 30
hostname
```

Running an external script

- Let's run a Matlab program
- We will run the bash script matlab.sh
- This script calls and runs matlab_tic.m

Running the script

- Submit the job:

```
sbatch matlab.sh
```

- Check output

Matlab.sh

```
#!/bin/bash
#SBATCH --nodes=1                       # Number of requested nodes
#SBATCH --time=0:02:00                  # Max walltime
#SBATCH --qos=testing                   # Specify debug QOS
#SBATCH --partition=shas-testing        # Specify Summit haswell nodes
#SBATCH --output=matlab_%j.out          # Output file name

# purge all existing modules
module purge

# Load Matlab module
module load matlab

# Run matlab without a GUI
matlab -nodisplay -nodesktop -r "clear; matlab_tic;"
```

Your turn

Submit a slurm job with the following instructions:

1. Create an R program called `R_program.R` that creates a vector called “planets” and then list the planets in the vector
   a. Syntax: `planets <- c("Mercury", "Venus", "Earth", "Mars", "Jupiter", "Saturn", "Uranus", "Neptune", "Pluto”)`
2. Print off the vector
   a. Syntax: `print(planets)`
3. Create a bash script called `R_code.sh` that runs the R script
   a. Syntax: `Rscript R_program.R`
4. The job will run on 1 node
5. We will request a 1 minute wall time
6. Specify the debug QOS
7. Specify the shas partition
8. The output will be put in a file called `R_code_%j.out`
9. Don’t forget to load the R module!

Solution – R_code.sh

```
#!/bin/bash
#SBATCH --nodes=1                          # Number of requested nodes
#SBATCH --time=0:01:00                     # Max walltime
#SBATCH --qos=testing                      # Specify debug QOS
#SBATCH --partition=shas-testing           # Specify Summit haswell nodes
#SBATCH --output=R_code_%j.out             # Output file name

# purge all existing modules
module purge

# Load the R module
module load R/3.3.0

# Run R Script
Rscript R_program.R
```

Solution – R_program.R

```
# Simple R code example by Shelley Knuth (shelley.knuth@colorado.edu)


# Create vector
planets <- c("Mercury", "Venus", "Earth", "Mars", "Jupiter", "Saturn", "Uranus",
"Neptune", "Pluto")


# Print off vector
print(planets)
```

Interactive jobs!

- Sometimes we want our job to run in the background
- Sometimes we want to work in program in real time
- For example, Matlab
- Let's run an interactive Matlab job

Interactive job

- In this example we'll use X windows to access the Matlab GUI
- To do this, we are going to log out and log back in
  - Only necessary for demo
  - Need to add something to the sign in process

- For Mac Users:

```
ssh -X username@login.rc.colorado.edu
```

- For Windows Users, must set up X-forwarding through your SSH client program
- Also must have an X-server package on your laptop
  - Xming for Windows or XQuartz for Mac

Interactive job

- To work with Matlab interactively, we're going to request some time from the supercomputer
- When the resources become available then we will start up Matlab
- Commands to run:

```
module load slurm/summit
sinteractive --qos=debug --time=00:05:00
```

  Once we receive a prompt, then:

```
module load matlab
matlab
```

- Once we finish we must exit!

Questions?

- Email rc-help@colorado.edu
- Twitter: @CUBoulderRC

- Link to survey on this topic:
  http://tinyurl.com/curc-survey16

- Slides: https://github.com/ResearchComputing/New_User_Seminar