

Overview of RMACC Summit

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University of Colorado **Boulder**

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CMU - RMACC Summit overview

Overview of RMACC Summit

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www.colorado.edu/rc

- Slides: https://github.com/ResearchComputing/CMU_HPC_2019

Outline

- What is RC?
 - Resources and services/support
 - Summit overview
- Steps to get access to our systems
 - Accounts
 - Two-factor authentication
 - Logging in
- Navigating our systems
 - Job Scheduling
 - Allocations and Fair Share
 - Storage spaces
 - Data transfer - Globus
 - Software

Feel free to ask questions anytime
during this presentation!



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 best known for:
 - Summit Supercomputer (what you'll be using)
- Other resources (not covered today)
 - Blanca condo cluster (buy-in for dedicated nodes)
 - PetaLibrary storage (large-scale data storage system)

What Would I Use Summit For?

- Research Computing is more than just Summit
- 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



Hardware: RMACC Summit Supercomputer

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



Getting an RC Account for CMU Users

- Details: <https://curc.readthedocs.io/en/latest/access/rmacc.html>
 - Step 1: Create an XSEDE account on <https://portal.xsede.org>
 - Step 2: Configure Duo phone app for 2-factor authentication
 - Step 3: Email us at rc-help@colorado.edu to request access to RMACC Summit



Logging In

- Details: <https://curc.readthedocs.io/en/latest/access/rmacc.html>
- Login to XSEDE SSO:

`ssh <your-xsede-username>@login.xsede.org`

- Enter your XSEDE portal password
- Select an option for Duo

Enter a passcode or select one of the following options:

1. Duo Push to XXX-XXX-XXXX
2. Phone call to XXX-XXX-XXXX

- your Duo app or Phone Call will alert you to confirm the login

- SSH to RC:

`gsissh rmacc-summit`



Notes: Duo Authentication

- For RMACC users, this is handled by the XSEDE SSO (Single Sign On)
- Most users will use the "Push" smartphone app
 - Make sure you have a good broadband or wifi data network connection
- Duo accounts usually expire if left unused for 6-12 months
- Purged Duo accounts will need to be restored by XSEDE

Notes: 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 (namely Summit for RMACC/XSEDE users)



Navigating our Systems

- Now that you've logged in, now what?
 - How do I schedule a job?
 - 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? ...



Job scheduling

- Users submit “**jobs**” to do work (e.g. run python or R code, run a matlab script, run a model, etc.)
- Jobs are submitted to the compute nodes via a job management system called “**Slurm**
 - Slurm schedules the job and places it in a queue with all of the other jobs submitted by users
 - Users must have **allocations** (think “computing currency”) to submit jobs (covered in next slide)
 - Users are placed in the queue according to their “**Fair Share**” priority

Allocations

- All users need a compute time allocation to use any of our compute resources.
- New RMACC users are automatically added to the “rmacc-general” allocation when you sign up
- If this does not seem to be the case, to request access please email rc-help@colorado.edu and ask for access to the “rmacc-general” allocation
- If you plan heavy usage we can discuss an allocation to get access to a larger “share” of Summit (email us at rc-help)

What is Fair Share?

- Fair share scheduling uses a complex formula to determine priority in queue
- Looks at load for each user 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 for a given allocation
- If no other pending jobs and enough resources are available then your job will run regardless of your previous usage. You never get “cut off”

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
 - Great for script or code editing
 - Also Job submission, checking on jobs, looking at output
- Compile nodes
 - Where you compile code, install packages, etc.
 - 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/<username>**
 - Very small: 2GB. Not for computation.
 - Backed up daily.
 - Good for ‘can’t lose’ files
- **/projects/<username>**
 - 250 GB
 - Backed up regularly
 - Good for storing scripts, self-installed software, some data
- **/scratch/summit/<username>**
 - Large: 10 TB partition
 - Fast filesystem -- Good for jobs with lots of I/O – run your jobs on here!
 - Not backed up
 - Temporary: data deleted 90 days from creation.

What Belongs Where?

- **/home**
 - Scripts
 - Code
 - Small, important files/directories
 - Inappropriate for sharing files with others
 - Inappropriate for job output
- **/projects**
 - Code/files/libraries
 - Software you are installing
 - Mid-level size input files
 - Appropriate for sharing files with others
 - Inappropriate for job output
- **/scratch/summit**
 - Output from running jobs
 - Large files/datasets
 - Appropriate for sharing files with others
 - **THIS IS NOT AN APPROPRIATE SPACE FOR LONG TERM STORAGE (90-day purge policy)**

Transferring Data

- **Globus** is Research Computing's preferred method of data transfer for larger files or datasets
 - 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**, **scp** and **sftp** aren't viable options for RMACC users due to the need to use the XSEDE SSO (can't transfer data directly from local machine to RMACC Summit)

Setting Up Globus

- See: <https://curc.readthedocs.io/en/latest/compute/data-transfer.html>
 - Step 1: Create an account at Globus.org
 - Step 2: Make your personal computer an endpoint by installing ‘Globus Connect Personal’
 - Step 3: Login at www.globus.org
 - Step 4: Find your **personal endpoint** on one side of the screen
 - Step 5: Find ‘**CU Boulder Research Computing XSEDE**’ endpoint
 - Step 6: Transfer data to/from CU Research Computing

Software

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

Important Things to Know About Modules

- You need to be on an **scompile** node to browse the 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, you can type `module avail`
- To set up your environment to use a software package, type `module load <package>/<version>`



Questions?

Presenter: Andrew Monaghan
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Link to course evaluation:
<http://tinyurl.com/curc-survey18>

Documentation:
<https://curc.readthedocs.io>

Slides:
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