

Overview of RMACC Summit

Be Boulder.



University of Colorado **Boulder**

Overview of RMACC Summit

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 - www.rc.colorado.edu
- Slides: https://github.com/ResearchComputing/CU_DENVER_HPC_2019

Before We Begin

- Goals
 - Inform people about RC resources, expectations, etc.
 - Reduce user frustrations, questions
 - Avoid misunderstandings, lost time, lost work
 - Inform users about best practices
- Things to take note
 - 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.

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
 - Blanca
 - Petalibrary
- Summit (and other RC cluster) New user
 - Allocations
 - Storage spaces
 - Data transfer - Globus
 - Software

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

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
- Not a place for:
 - Large data storage

Hardware - Summit Supercomputer

- 500+ compute nodes (450 Intel Xeon Haswell general compute nodes)
- 24 cores per “shas” (general compute) node, different core counts for other node types
- 12,000+ total cores
- Omni-Path interconnect
- 1.2 PB scratch storage
- GPFS Scratch File system
- Allocation: 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

Getting an RC Account

- UCD / Anschutz Users:
 - Email rc-help@colorado.edu and we'll guide you through the process
 - CC your local RMACC representative, NICHOLAS.RAFAELS@CUANSCHUTZ.EDU (or we'll add him to the cc list after we get your email)
 - There is a form for grant supported projects using the system Nicholas will link you to
 - Light usage for learning/exploration of the system is a reasonable use case.

Two-Factor Authentication

- Provides an extra level of authentication
 - We are outside the firewall!
 - Valuable resources
 - Inviting, high-profile target
 - Lost time investigating/fixing and damage to our reputation if compromised
- Duo
 - Most users use the Duo smartphone app
 - “Phone Call” or Passcode are alternatives

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 data network connection if you are having trouble authenticating.
 - Make sure your WiFi is working or use 4G
- Duo accounts usually expire if left unused for 6-12 months
- Purged accounts will need to be restored by XSEDE

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
 - RC users have used the same hostname to log in and accessed the same non-scratch storage for over 9 years and 5 clusters
- From there, you can access our other resources

Accessing RC Resources

- <https://curc.readthedocs.io/en/latest/access/rmacc.html>
- `ssh -l <your-xsede-username> login.xsede.org`
- `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`

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?

Blanca

- If you are a new Blanca user you need an RC account, and we need to know what resources to connect you to.
- 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

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

Using Summit (and other RC clusters)

Allocations

- You will need a compute time allocation to use any of our compute resources.
- Blanca allocations are part of the buy-in
- New RMACC users should be added to the Summit 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 General allocation
- If you plan heavy usage we can discuss an allocation to get access to a larger “share” of 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

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 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
 - 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 APPROPRIATE FOR LONG TERM STORAGE**

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 and sftp through the login nodes is good for small transfers – transfers that take a few minutes.
 - This may require an SSH tunnel from your host or a firewall exception.

Setting Up Globus

- Create an account at Globus.org
- Make your personal computer an endpoint if you want
 - 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
- Can install your own software
 - It is best if you are responsible for support
 - We are happy to assist
- 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.

Important Things to Know About Modules

- You need to be on a compile 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: Joel Frahm
- Email rc-help@colorado.edu
- Twitter: @CUBoulderRC
- Link to survey on this topic:
<http://tinyurl.com/curc-survey18>

Slides:

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