



APPM: Introduction to HPC

CURC Alpine: New User Seminar

Instructor: Trevor Hall

- Website: www.rc.colorado.edu
- Helpdesk: rc-help@colorado.edu
- Slides: https://github.com/ResearchComputing/APPM_HPC
- Survey: <http://tinyurl.com/curc-survey18>

Learning Goals

- **Part 1: Overview**
 - Overview of CU Research Computing (CURC) and our resources
- **Part 2: Using Blanca**
 - Using Blanca
 - Logging in
 - Basic Linux Commands
 - File editing
 - Linux filesystem
 - Environment variables
 - Software modules on Blanca
 - Bash scripts and job scheduling

Part 1 - Overview

What is Research Computing?

- Provide services for researchers that include:
 - High performance computing (HPC)
 - Data visualization
 - Data storage
 - High speed data transfer
 - Data management support
 - Consulting
 - Training
- We are likely best known for:
 - Alpine Supercomputer (~22,000 cores)
 - Blanca "condo" cluster (~4,000 cores)
 - PetaLibrary storage

Primarily known for: High Performance Computing (HPC)



High Performance Computing (HPC) vs. Traditional Computing

- Traditional computing *generally* has access to a single processor (perhaps multiple cores)

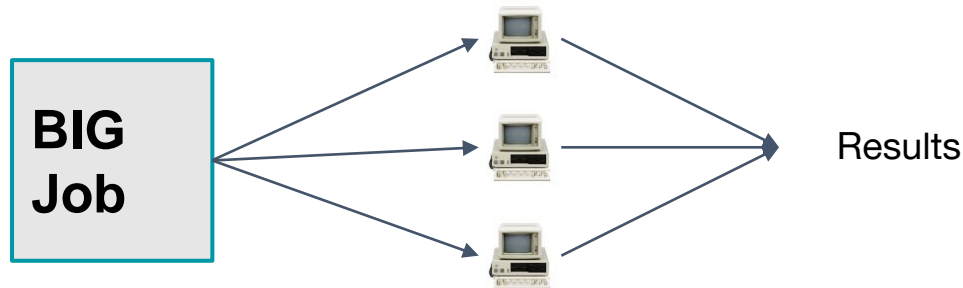


What can / use HPC for?

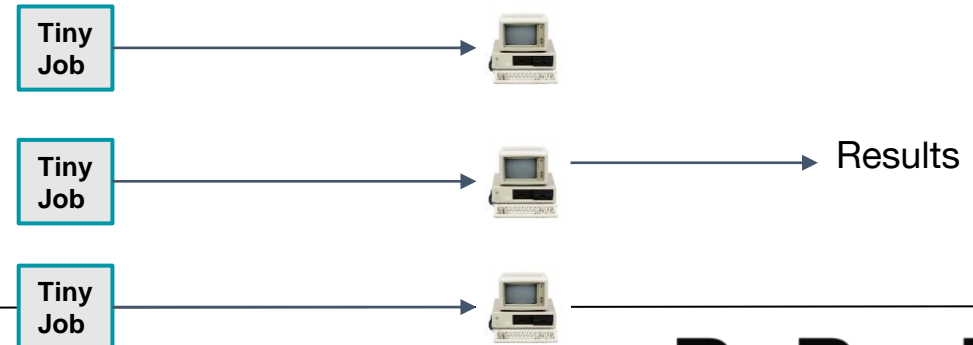
- Solving large problems that require more:
 - Memory than you have on your PC
 - cores/nodes/power than you have on your PC
- Jobs that require hardware you may not have:
 - High Performance GPU computing
 - Specific Operating System
- Visualization rendering

What can / use HPC for?

- Jobs that would take a long time on local machines can instead be distributed over hardware:
 - Parallelized to split up then joined (if software enabled)



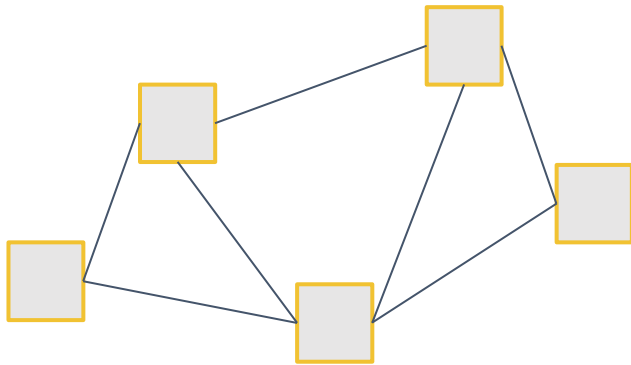
- Broken up into many serial jobs



Research Computing Resources

HPC Cluster: Alpine

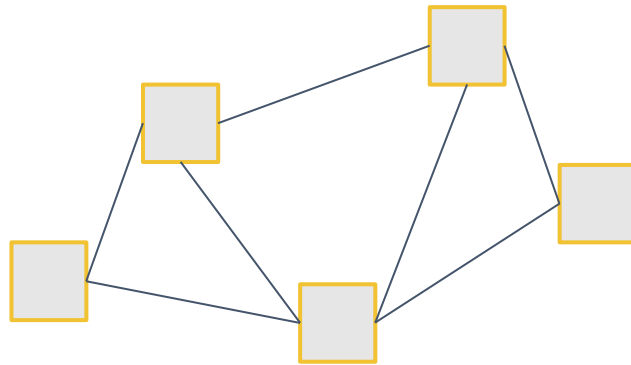
Alpine



- Alpine is the 3rd-generation HPC cluster at CURC, following:
 - Janus
 - RMACC Summit
- Alpine is a heterogeneous cluster with hardware currently provided by CU Boulder, CSU, and Anschutz
- Access available to CU Boulder, CSU, AMC and RMACC users

HPC Cluster: Alpine

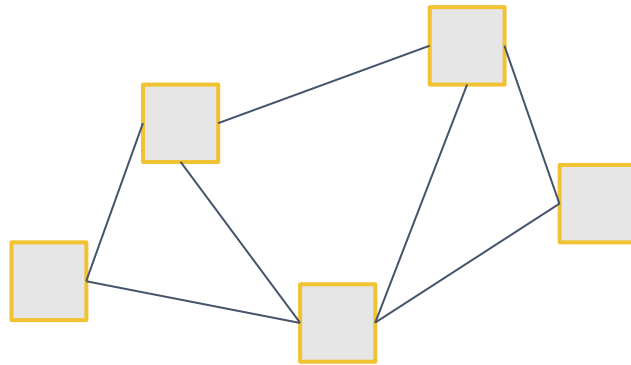
Alpine



- Hardware on Alpine will continue to be purchased and released in stages:
- Alpine (stage 4):
 - 256 General CPU Nodes
 - *AMD Milan, 64 Core, 3.74G RAM/Core*
 - 12 NVIDIA GPU Nodes
 - *3x NVIDIA A100 (atop General CPU node)*
 - 8 AMD GPU Nodes
 - *3x AMD MI100 (atop General CPU node)*
 - 22 AMD High-Memory Nodes
 - *AMD Milan, 48 Core, 21.5G RAM/Core*
 - Additional Hardware contributed by CSU, AMC
 - *Nodes which boost priority for CSU/AMC users*

HPC Cluster: Alpine

Alpine



- Interconnect

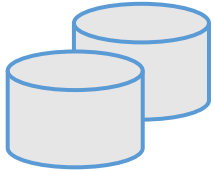
- **CPU nodes:** HDR-100 InfiniBand (200Gb inter-node fabric)
- **GPU nodes:** 2x25 Gb Ethernet +RoCE
- **Scratch Storage:** 25Gb Ethernet +RoCE

- Operating System

- RedHat Enterprise Linux version 8 operating system

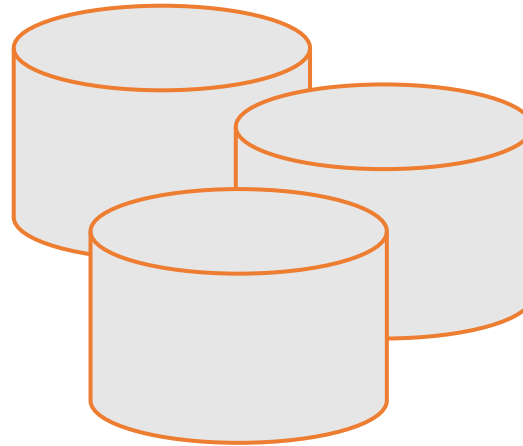
Storage at CURC

Core



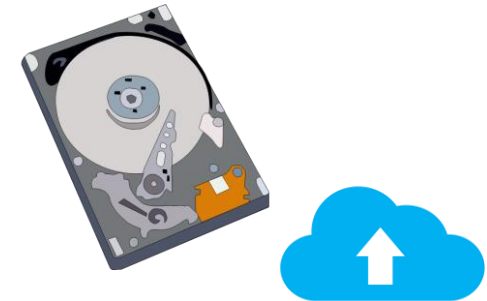
- Included with RC account
 - /home
 - /projects
 - scratch space

PetaLibrary



- Paid Service for:
 - Storage
 - Archive
 - Sharing of research data

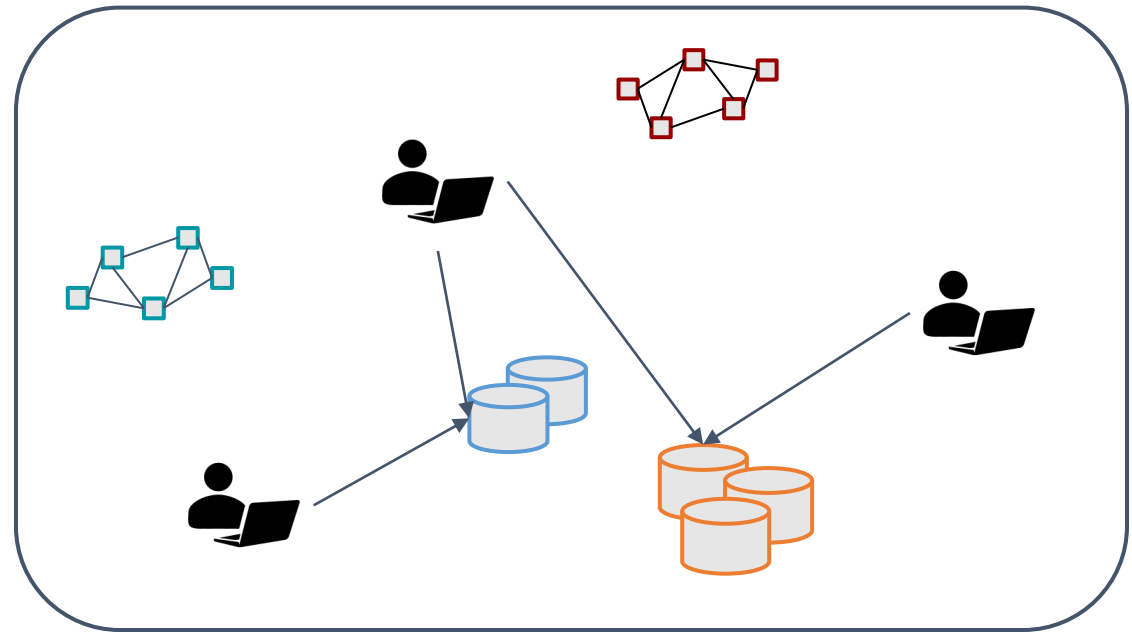
Local or Cloud



- You can download your data locally or to a variety of other cloud resources
- Cloud Foundations at Research Computing

Data Sharing: Within RC

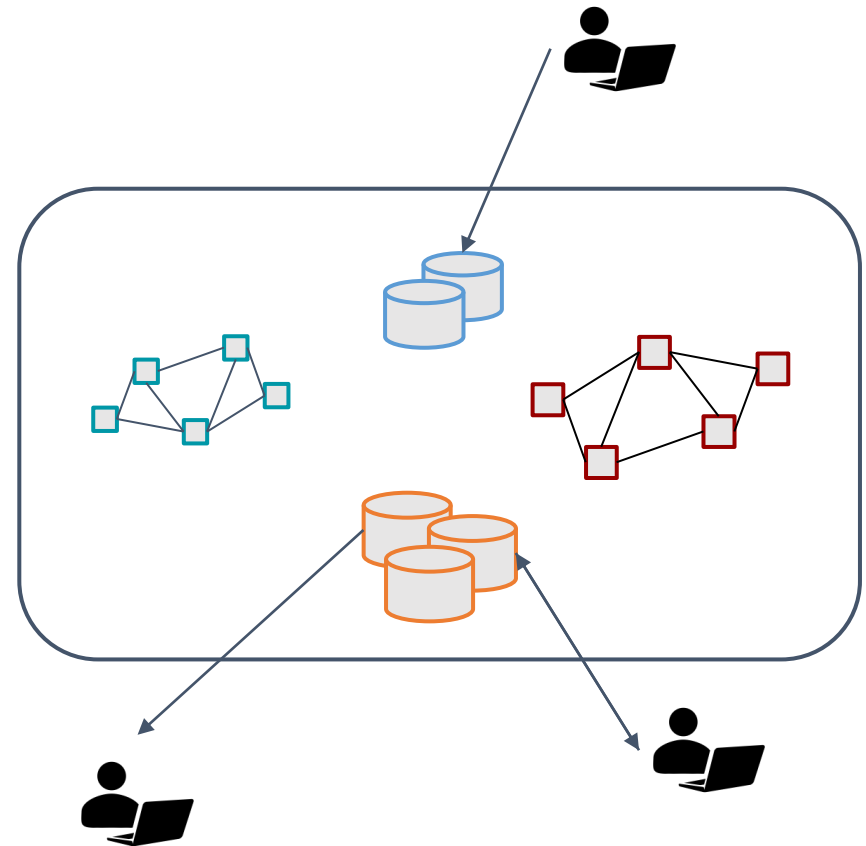
- Sharing workspaces
 - Project space
 - Scratch Space
 - PetaLibrary Space*



*If you have purchased PetaLibrary space

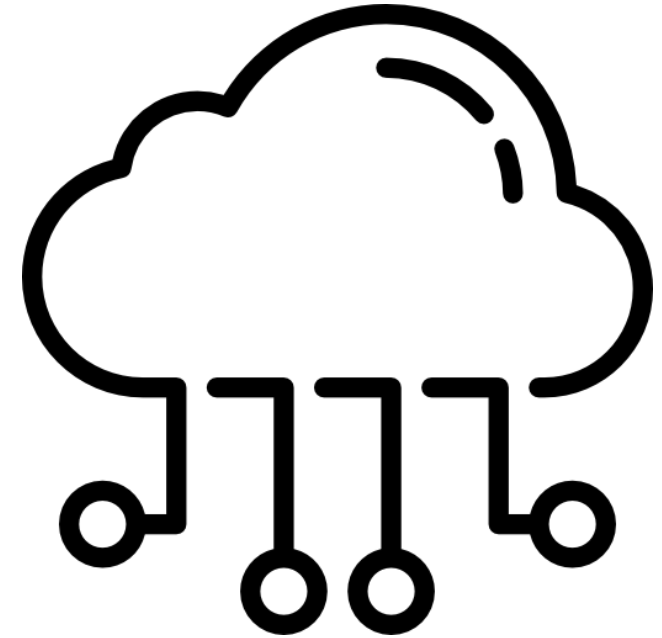
Data Sharing: Outside RC

- Globus (recommended):
 - GUI Web Application
 - Automates large transfers
 - Resumes failed transfers
 - Distributes large transfers across DTNs
 - Endpoints that can shared
- Data Transfer Nodes (DTN)
 - Internal CU network needed (VPN)
- Command line tools
 - scp, sftp, rsync, rclone



Cloud Computing

- CURC supports both AWS and on-premise cloud via CUMulus
 - For use cases not well-supported by HPC
- Can be used as an alternative to HPC
- Can be used to enhance HPC
 - Automatic job submission, high availability, etc.



Request a CUMulus application by contacting the RC helpdesk at rc-help@colorado.edu

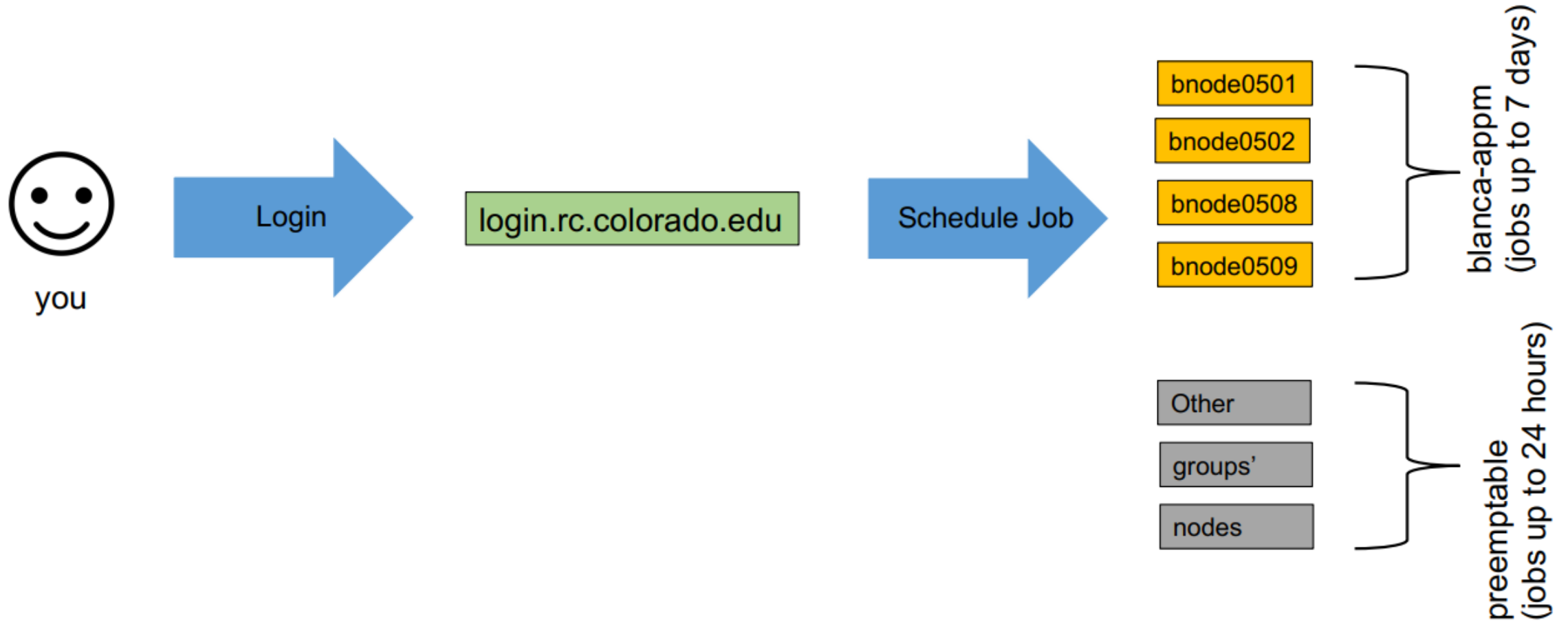
Blanca

- A “condo” cluster whereby individual research groups own nodes
- List of nodes and groups can be found [here](#)
- Users have dedicated access to their group’s nodes (e.g., blanca-appm)
 - Jobs up to 7 days long
 - Can also run ‘preemptable’ jobs on other groups nodes (jobs up to 24 hours long)
- More documentation on Blanca:
<https://curc.readthedocs.io/en/latest/access/blanca.html>

blanca-appm

- bnode0501, bnode0502 (2 nodes)
 - 32 (effectively 64) cores, avx2, Cascade, 2.3 GB RAM/core)
- bnode0508, bnode0509 (2 nodes)
 - 40 (effectively 80) cores, avx2, Cascade, 2.3 GB RAM/core)

Accessing Research Computing



How to Access RC Resources?

1. Get an RC account
2. Set up two-factor authentication with Duo
3. (Inform us of any specific needs)
4. Log in
5. Create greatness! (responsibly)

Getting an RC Account

- **University of Colorado, Boulder users and affiliates:**
 - Request an account through the RC Account request portal
 - <https://rcamp.rc.colorado.edu/accounts/account-request/create/organization>

Your RC Account

Access to:

1. Alpine Cluster
2. Core Storage
3. PetaLibrary Storage*
4. Open OnDemand
5. Approximately 2,000 Service Units (SUs) per month

*If purchased

Your RC Account

How can I use more computational time?:

- Trailhead Allocation (Default)
 - ~2,000 SUs / Month
- Ascent Allocation
 - 350,000 SUs
- Peak Allocation
 - >350,000 SUs

Request an allocation at

<https://curc.readthedocs.io/en/latest/clusters/alpine/allocations.html?highlight=alpine%20allocation#comparing-trailhead-auto-allocation-ascent-allocation-and-peak-allocation-tiers>

Your RC Account

How much storage do I have available?:

- /home directory
 - 2GB
- /projects directory
 - 250GB
- /scratch and /rc_scratch
 - 10TB*

More documentation at: <https://curc.readthedocs.io/en/latest/compute/filesystems.html>

Logging In

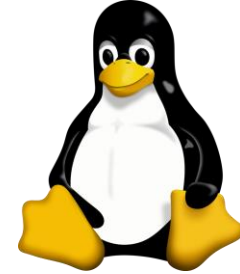
- It's important to note that you are ***NOT*** logging into any specific resource, Alpine, Blanca, etc.
- When you log in, you land on our ***login nodes***
- From ***there***, you can access our other resources:
 - Alpine
 - Blanca
 - Petalibrary

Part 2 (Using Blanca)

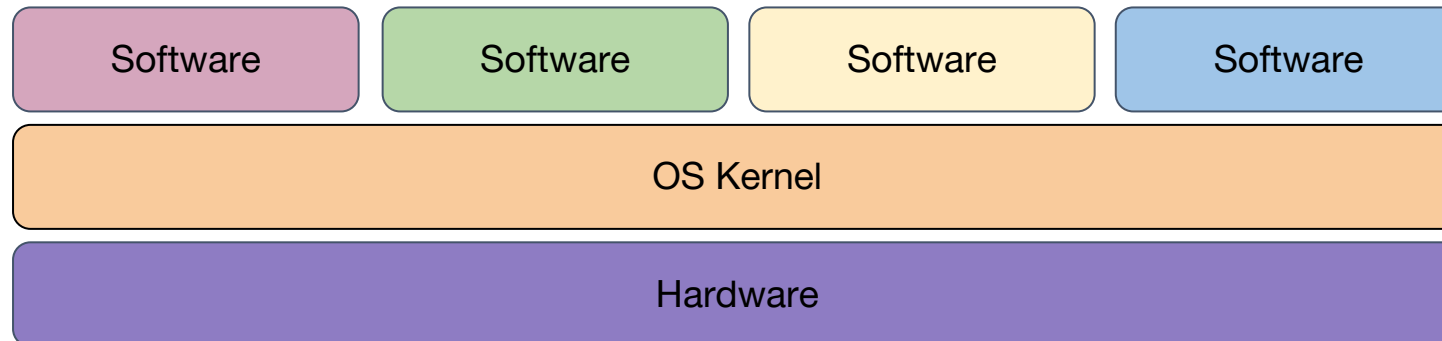
Logging into CURC

- `ssh <identkey>@login.rc.colorado.edu`
- Enter your identikey password
- Authenticate by accepting the Duo push to your smartphone
 - - Can also authenticate by text message, phone call, or token
- More info here: <https://curc.readthedocs.io/en/latest/access/logging-in.html>

What is Linux?



- Part of the Unix-like family of operating systems.
- Started in early '90s by Linus Torvalds.
- Typically refers only to the kernel with software from the GNU project and elsewhere layered on top to form a complete OS. Most is open source.



images courtesy of wikicommons

Why Use Linux?

- Default operating system on virtually all HPC systems and the foundation for many business services globally
- Extremely flexible
- Fast and powerful
- Many tools for software development
- You can get started with a few basic commands and build from there

Anatomy of a Linux command

- command [flags] [target(s)]

`ls -l myworkdir/`

- Case is important!
- Help on commands is available through the “man” command (short for manual)

`man ls`

File and Directory related commands

- **pwd**– prints full path to current directory
- **cd** – changes directory; can use full or relative path as target
- **mkdir** – creates a subdirectory in the current directory
- **rmdir** – removes an empty directory
- **rm** – removes a file (**rm -r** removes a directory and all of its contents)
- **cp** – copies a file
- **mv** – moves (or renames) a file or directory
- **ls** – lists the contents of a directory (**ls -l** gives detailed listing)

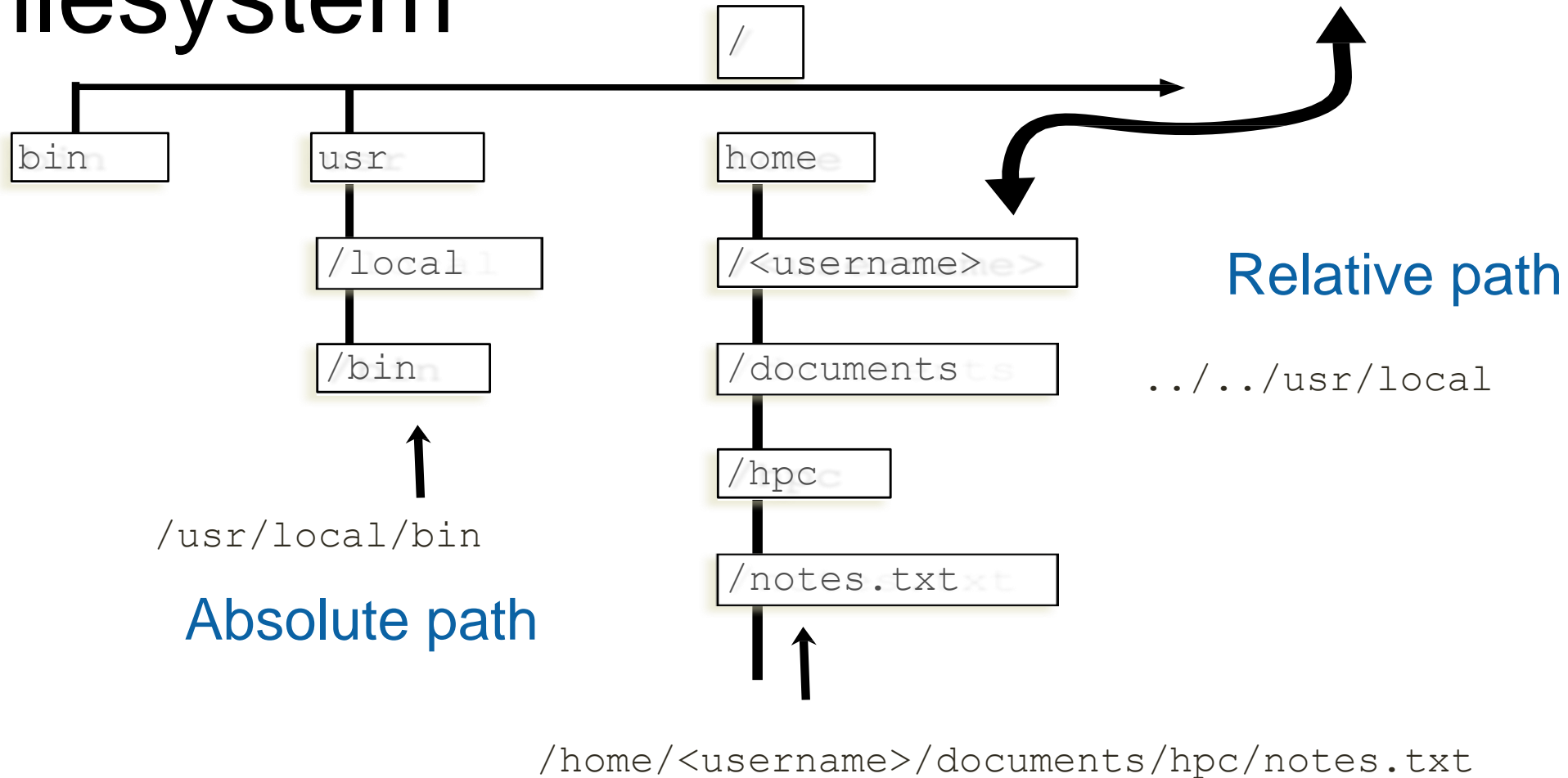
File-viewing commands

- **less**– displays a file one screen at a time
- **cat** – prints entire file to the screen
- **head** – prints the first few lines of a file
- **tail** – prints the last few lines of a file (with **-f** shows in realtime the end of a file that may be changing)
- **diff** – shows differences between two files
- **grep** – prints lines containing a string or other regular expression
`ps -df | grep xx`
- **sort** – sorts lines in a file
- **find** – searches for files that meet specified criteria
- **wc** – count words, lines, or characters in a file

The Linux Filesystem

- System of arranging files on disk
- Consists of directories (folders) that can contain files or directories
- Levels in full paths separated by forward slashes:
e.g. `/home/user/scripts/analyze_data.sh`
- Case-sensitive; spaces in names discouraged
- Some shorthand:
 - `.` (the current directory)
 - `..` (the directory one level above)
 - `~` (home directory)
 - `-` (previous directory, when used with `cd`)

Filesystem



Jobs

What is a “**job**”?

- Work for the cluster to perform on
- Has a unique ID

1. Batch jobs

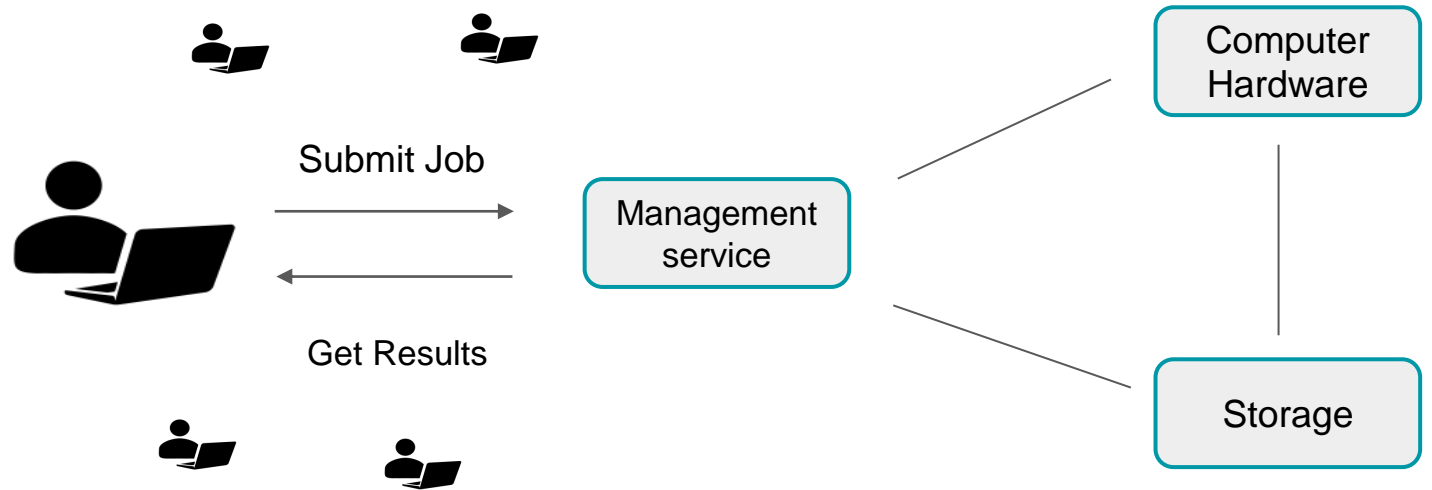
- Submit job script which will be executed when resources are available
 - Create script containing information about the job
 - Submit the job file to a queue

2. Interactive jobs

- Work interactively at the command line of a compute node

Job Scheduling

- CURC Clusters are shared resources, jobs are:
 - Submitted to a queue
 - When the required resources become available, the scheduler determines which set of nodes to use
 - Executes your job



Job Script: 3 main parts

1. Directives

- Specify resource requirements

1. Software

- Because jobs run on a different node than from where you submitted...
- ...software that is needed must be loaded via the job script

1. User scripting

- the actual user scripting that will execute when the job runs

```
#!/bin/bash

## Directives
#SBATCH --<resource>=<amount>

## Software
module purge

## User Scripting
hostname # example bash command
```

Slurm Options (directives)

#SBATCH <options>

sbatch <options>

- Allocation: --account=<account_no>
 - Partition: --partition=<partition_name>
 - Sending emails: --mail-type=<type>
 - Output file: --output=<file name> (%j gives you job id)
 - 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> ...etc...
- FYI: You do NOT actually type <> above – this designates something specific you as a user must enter about your job

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!
```

Software and Jobs

- More LMOD commands:

```
$ module purge           #Unloads all current modules  
$ module unload python   #Unloads python  
$ module spider python   #Searches for python 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

Topics we didn't cover today

- Job arrays (when you need to run lots of similar tasks)
- Running preemptable jobs
- CURC OnDemand (Interactive interface <https://ondemand.rc.colorado.edu>)
- Use of conda on CURC
- ..and lots of other cool stuff
- See: <https://curc.readthedocs.io> ; or email rc-help@colorado.edu to schedule a consultation

Help! I'm stuck, where do I go?

- **Documentation:** curc.readthedocs.io/
- **Trainings with Center for Research Data and Digital Scholarship (CRDDS):**
<https://www.colorado.edu/crdds/>
 - **Coming up:**
 - [RC Quick Byte – Getting an Account](#) (1/23)
 - [Alpine New User Seminar](#) (1/25)
 - [Supercomputing Spin Up Part 1 – Working with Linux](#) (1/30)
 - [Supercomputing Spin Up Part 2 – Job Submission](#) (2/1)
- **Helpdesk:** rc-help@colorado.edu
- **[Consult Hours](#)** (Tuesday 12:00-1:00, Thursday 1:00-2:00)

Questions?

CURC User Policies: <https://curc.readthedocs.io/en/latest/additional-resources/policies.html?highlight=policies#curc-user-policies>

Survey and feedback

<http://tinyurl.com/curc-survey18>