Introduction to HPC on Blanca

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- Andrew Monaghan
- *Email: Andrew.Monaghan@Colorado.edu*
- *RC Homepage: https://www.colorado.edu/rc*

- Slides available for download at: https://github.com/ResearchComputing/APPM_HPC_Spring_2021

Outline for this presentation

- Overview of RC, Blanca
- Logging in
- Basic Linux commands
- File editing
- Linux filesystem
- Environment variables
- Software modules on Blanca
- Bash scripts and Job Submission

What is Research Computing?

- Provide services for researchers that include:
  - Large scale computing
  - Data storage
  - High speed data transfer
  - Data management support
  - Consulting
  - Training

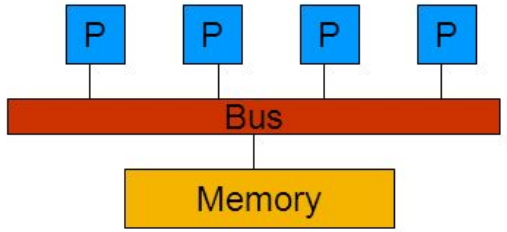
- We are likely best known for:
  - Summit Supercomputer (~12,000 cores)
  - Blanca ”condo” cluster (~4,000 cores)
  - PetaLibrary storage

What Would I Use Blanca For?

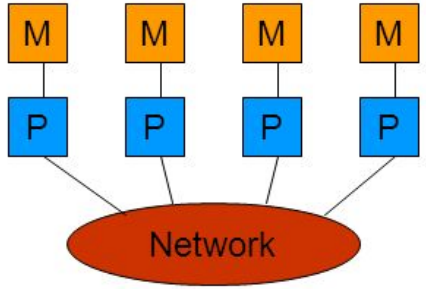
Solving large problems that require more:

- Memory than you have on your personal computer
- Cores/nodes/power than you have on your personal computer

- Blanca is set up for both shared memory (single node) and distributed memory (multi-node) parallelization.
  - Can also use Summit for"big" distributed memory parallelization



- **Shared memory**



- **Distributed memory**

Source: https://images.slideplayer.com/25/7599921/slides/slide_4.jpg

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)

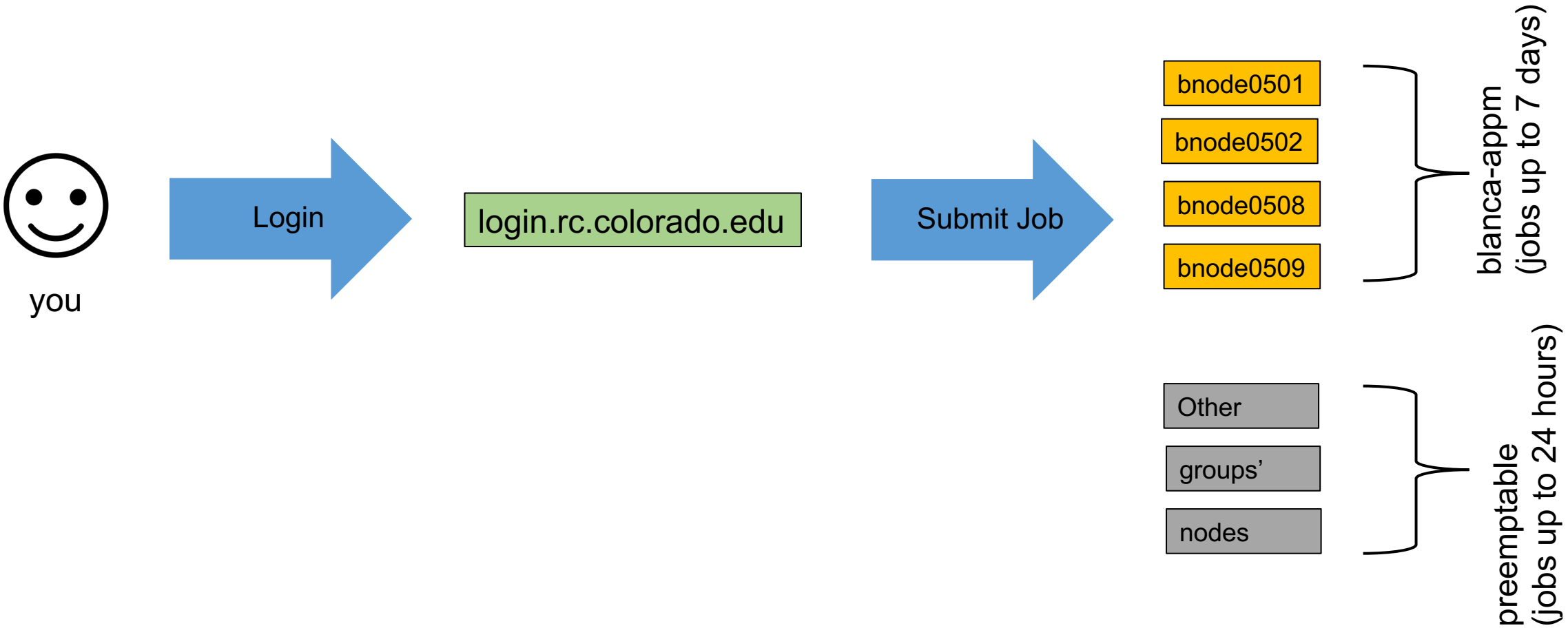
- More documentation on Blanca: https://curc.readthedocs.io/en/latest/access/blanca.html

Blanca APPM nodes

- 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)

Blanca Workflow



Logging In

- `ssh <identikey>@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

Linux

- Part of the Unix-like family of operating systems.
- Started in early ‘90s
- Several distributions are available – from enterprise-grade, like RedHat Linux (RHEL), to more consumer-focused, like Ubuntu.
  - Blanca nodes presently run RHEL7
- Runs on everything from embedded systems to supercomputers.
- Linux is simple, flexible, fast, many potent tools

Anatomy of a Linux command

- command [flags] [flag arguments] [target(s)]
  - ls -l myworkdir/
- Case is important!
- Help on commands is available through the ”man” command (short for manual). E.g.,
  - 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
- **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)
- **chmod/chown** – change permissions or ownership
- **df** – displays filesystems and their sizes
- **du** – shows disk usage (`du -sh` more useful)

Process and Program related commands

- **ps** – lists processes
- **top** – shows processes currently using the CPUs
- **kill** – sends a signal to a process (use “kill -9” for best results)
- **time** – shows how much time a process has used
- **free** – memory usage

File-viewing commands

- **more** – 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
- **diff** – shows differences between two files
- **grep** – prints lines containing a string or other regular expression (ps –ef | 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

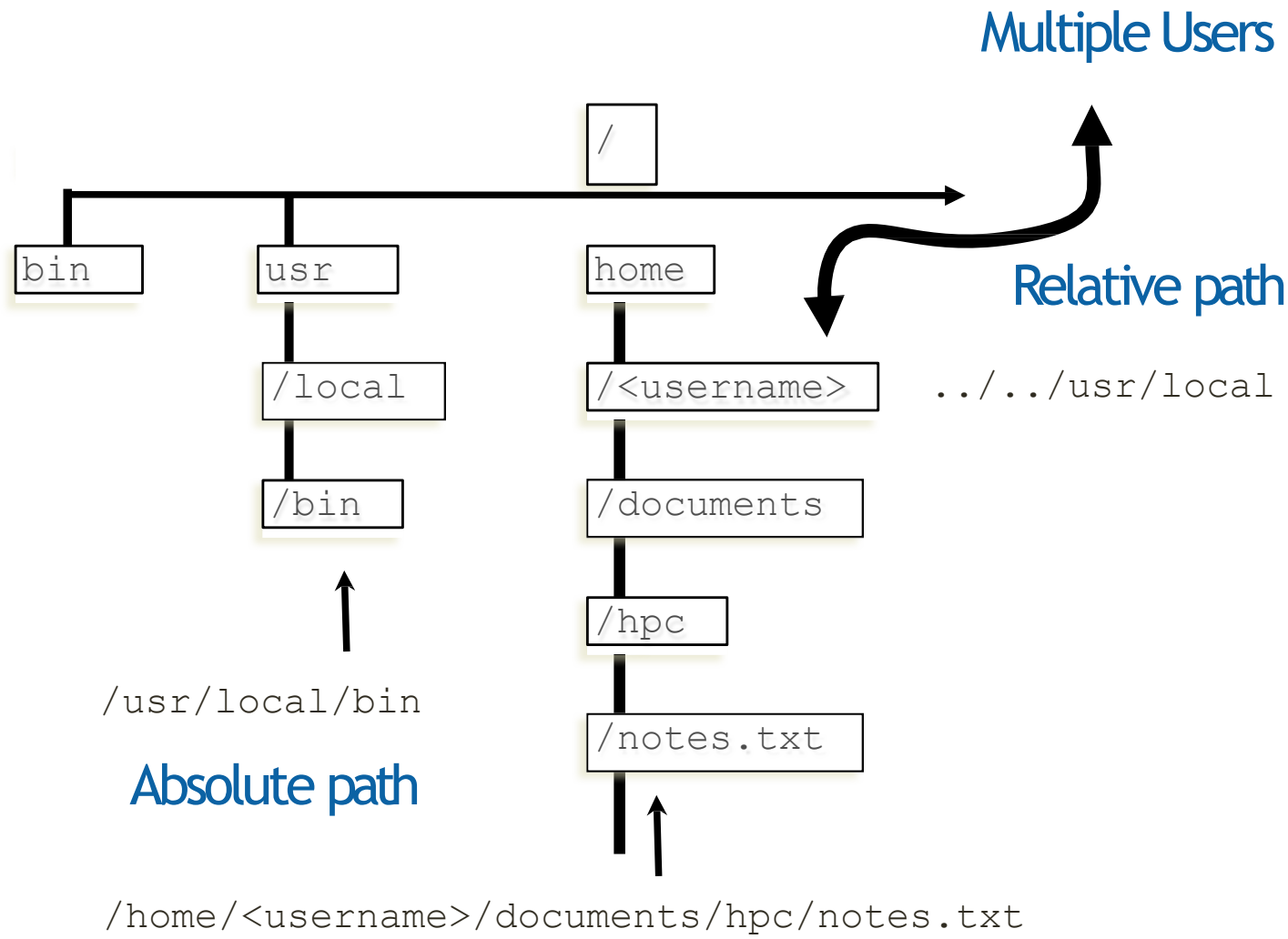
File editing with nano

- To edit a file:
  - nano myfile.txt
- From within Nano:
  - Ctrl+o save (need to confirm filename)
  - Ctrl+x exit
  - Ctrl+k cut
  - Ctrl+u paste
- Other population Linux editors: vi, emacs

The Linux Filesystem

- System of arranging files on disk
- Consists of directories (folders) that can contain files or other 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)

Filesystem


Multiple Users
/
bin
usr
home
Relative path
/local
/<username>
../../usr/local
/bin
/documents
/hpc
/usr/local/bin
/notes.txt
Absolute path
/home/<username>/documents/hpc/notes.txt

Your personal directories on Blanca

- /home/<username>
  - Very small: 2GB.
  - 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
- /rc_scratch/<username>
  - Group-shared 100 TB partition.
  - Good for jobs with lots of I/O
  - Not backed up
  - Temporary: data deleted 90 days from creation.

Environment variables

- Environment variables store important information needed by Linux users, programs, etc.

- Type ‘env’ to see your currently set environment variables

- Useful Environment variables:
  - `PATH`: directories to search for commands
  - `HOME`: home directory
  - `PWD`: current working directory
  - `USER`: username
  - `LD_LIBRARY_PATH`: directories to search for shared objects (dynamically-loaded libs)

Shell Wildcards and Special Characters

- `*` - matches zero or more characters
- `?` - matches a single character
- `#` - comment; rest of the line is ignored
- `\` - escape; don't interpret the next character

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 also install your own software
  - It is best if you are responsible for support
  - We are happy to assist

Using Modules

- Must be on a compute node to browse the modules (e.g, bnode0501)
- To set up your environment to use a software package, type `module load <package>/<version>`
- 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`

Using Anaconda for Python, R

- Many users prefer to use conda to manage python (and R, etc) packages and environments.

- We have Anaconda python installed on our system!
  - (but it isn't a module…)

- Documentation on use: https://curc.readthedocs.io/en/latest/software/python.html

Next Topics:
Bash Scripting and Job submission

- Bash scripts (needed to submit jobs)
- Examples of submitting jobs to the supercomputer
  - Batch jobs
  - Interactive jobs

Bash

- A shell is the environment in which commands are interpreted in Linux

- GNU/Linux provides various shells; **bash is the most popular**
  - sh Bourne-again Shell (Bash)
  - csh C-Shell
  - tcsh Tc-Shell
  - ksh Korn-shell

- Shell scripts are files containing collections of commands for Linux systems that can be executed as programs…

Bash Script

- To create a bash shell script file, the first line must be:

```
#!/bin/bash
```

- Program loader recognizes the `#!` as an interpreter directive. This is followed by `/bin/bash` which tells the OS which shell should be used.
- Example:

```
#!/bin/bash

cd /home/$USER

hostname
echo “Hello!” > file.out
```

Why I am learning this?

Bash shell scripts are used to create job scripts that -- when submitted to the Slurm job manager -- request resources and execute commands and software on RMACC Summit.

Let’s get started!...

Jobs and Job Scripting

- **Job** – a system allotment of resources that run a particular application.
- **Slurm** -- resource manager
- Because Summit and Blanca are shared resources among a variety of groups on campus, users must run their applications through jobs.
  - Ensures everyone can utilize the system
  - No one person taking up too much of the system!
- Blanca is a bit different - APPM owns a portion of the system that is solely shared between APPM researchers.
  - Substantially shorter wait times!

Job Types

- **Batch Jobs**
  - Non-interactive allotment of resources that run applications in the background
  - Think “baking a batch of cookies”
  - Useful for:
    - Applications that take a substantial amount of time
    - Non-interactive Applications
- **Interactive Jobs**
  - Interactive allotments or resources where user run their applications manually
  - Useful for:
    - Debugging Applications
    - Running GUI Applications

Submitting Batch Jobs

- `sbatch` command: submit a batch job to Slurm
- The sbatch command usually takes in 1 parameter: A job script.
  - Job scripts provide all information on what is needed for the job.
  - Parameters can be overwritten or added externally by specifying the parameter as a flag.
- Example:

```
sbatch test.sh
```

or

```
sbatch test.sh --time=02:00:00
```

Anatomy of a job script

Job parameters

Your job commands

```
#!/bin/bash

#SBATCH --ntasks=1                      # Number of requested tasks
#SBATCH --time=0:01:00                  # Max wall time
#SBATCH --partition=blanca-appm         # Specify APPM nodes
#SBATCH --qos=blanca-appm-student       # Specify you are student
#SBATCH --output=test_%j.out            # Rename standard output file

# Now run job (commands below here)

# Purge and load needed modules
module purge
module load R

# Run commands
Rscript myscript.R
```

Job Parameters

- Allocation: `--account=<account-name>`
- Partition: `--partition=<partition-name>`
- Number of nodes: `--nodes=<nodes>`
- Number of Tasks: `--ntasks=<number-of-tasks>`
- Quality of service: `--qos=<qos>`
- Reservation: `--reservation=<name>`
- Wall time: `--time=<wall-time>`
- Job Name: `--job-name=<jobname>`
- Output File: `--output=<outputname>`

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

APPM QoS, Account, and Partition

- When using the APPM Blanca nodes, job scripts should specify the following information:

```
--account=blanca-appm
--partition=blanca-appm
--qos=blanca-appm-student #for some in APPM qos may just be blanca-appm
```

- Users of Blanca also have access to a low-priority preemptible QoS that will attempt to run your job on any available node on Blanca
  - Preemptable jobs will be booted off the node and restarted at a later time if a high priority user runs a job on the node.

```
--qos=preemptable
```

Submitting Your First Job!

Submit a slurm job with the following instructions:

1. The job should run the Linux “hostname” command
2. The job script will be named: `submit_hostname.sh`
3. The job will run on 1 core of 1 node
4. We will request a 1 minute wall time
5. Run from the blanca-appm-student QOS
6. Run on the blanca-appm partition and account
7. Use the ‘appm’ reservation
   - *This is only for this workshop*

submit_hostname.sh

```
#!/bin/bash
#SBATCH --nodes=1                       # Number of requested nodes
#SBATCH --ntasks=1                      # Number of requested cores
#SBATCH --time=00:01:00                 # Max wall time
#SBATCH --qos=blanca-appm-student       # Specify QOS; may be just “blanca-appm” for some
#SBATCH --partition=blanca-appm         # Specify APPM nodes
#SBATCH --account=blanca-appm           # Specify account
#SBATCH --output=hostname_%j.out        # Rename standard output file
#SBATCH --job-name=hostname             # Job submission name

# purge all existing modules
module purge

hostname
```

Running the job script

Submit the job:

```
$ sbatch --reservation=appm submit_hostname.sh
```

(note “–reservation=appm” for this class only)

Check the status of the job:

```
$ squeue / $ squeue –u <user> /
$ squeue –q <qos>
```

…or

```
$ sacct / $ sacct --format=<options>
```

…or

```
$ scontrol show job <job number>
```

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

Look at the job output:

```
$ cat hostname_<job-id>.out
```

*(*note that <job-id> is your job number)*

Interactive jobs

- Sometimes we want to work with a program in real time
    - Great for testing, debugging
- For example, let's run an interactive job and use "R"…

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 --reservation=appm --time=00:10:00
```

*note “--reservation=appm” is only for this workshop

- Once we receive a prompt, then:

```
module load R
R
```

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

Topics we didn't cover today

- Job arrays (when you need to run lots of similar tasks)
- Running preemptable jobs
- CURC JupyterHub (for running Jupyter Notebooks on Blanca)
- 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

Thanks!

- Please fill out the survey: http://tinyurl.com/curc-survey18
- Contact: rc-help@Colorado.edu, *Andrew.Monaghan@Colorado.edu*
- Course materials for today:
  - https://github.com/ResearchComputing/APPM_HPC_Spring_2021
- Blanca (and other) documentation: https://curc.readthedocs.io/en/latest/access/blanca.html
- Slurm Commands: https://slurm.schedmd.com/quickstart.html
- More detailed tutorials from our “HPC Fundamentals” course:
  - https://github.com/ResearchComputing/Fundamentals_HPC_Fall_2019

Supplemental Slides

Modes (aka permissions)

- Three classes of users:
  - User (u) aka “owner”
  - Group (g)
  - Other (o)
- Three types of permissions
  - Read (r)
  - Write (w)
  - Execute (x)

.. own grp oth

-|---|---|---

```
drwxr-xr--
```

Modes (continued)

- `chmod` changes modes:
- To add write and execute permission for your group:

```
chmod g+wx filename
```

- To remove execute permission for others:

```
chmod o-x filename
```

- To set only read and execute for your group and others:

```
chmod go=rx filename
```