Introduction to Running Computations on the High Performance Cluster at the Center for Computational Research
CCR Seminar: MATLAB Example

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CCR Resources

The Center for Computational Research provides high performance computing resources to the University at Buffalo.

- Supporting faculty research and classroom education, as well as local business and University collaborations.
- High performance and high through-put cluster.
- High performance remote visualization.

What is a cluster?

- A cluster is a collection of individual computers connected by a network that can act as a single more powerful machine.
  - Each individual computer has its own CPUs, memory and disks. It runs an operating system and it connected to a network that is usually private to the cluster. An individual computer is referred to as a compute node.

What is a cluster?

- A High Performance Cluster is a cluster that can run computations that require large number of compute nodes each. There are software packages and a high speed network that make this possible.
- A High Throughput Cluster is a cluster that can run a great many computations that require a single compute node or a single CPU on a compute node.

CCR Cluster

- The CCR cluster is collection of linux computers, private networks, a shared file system, a login computer, and job scheduler.
- Resources must be requested from the **job scheduler**.
- The user must decide what resources are required for the job.
- The user must control and optimize the job.

CCR Cluster

- The CCR cluster is **NOT a cloud**.
- Resources are NOT on demand.
- There is NO rapid elasticity.
- There is NO measured service to optimize the use of resources.

Access to the CCR Cluster

- The front-end machine is **rush.ccr.buffalo.edu**
- 32-core node with 256GB of memory.
- Accessible from **UB network only**.
- On campus your machine must be on the LAN or connected to UBsecure wireless.
- Off campus use the UB provided VPN client.

How to login

- Login from Linux or Mac
- ssh -X rush.ccr.buffalo.edu
- **ssh -X UBITusername@rush.ccr.buffalo.edu**
  - The -X flag enables a graphical display. This is optional.
  - Note: MAC users should in the XQuartz package.
- Windows users must install X-Win32, PuTTY, or OpenSSH for a secure login.
- The **X-Win32** program allows for a graphical display.
  - more on how to login

How to transfer files

- **Filezilla** is graphical file transfer program, which is available for Windows, Linux and MAC computers.
- **WinSCP** is available on Windows.
- **Cyberduck** is available on MACs.
- more on how to transfer files
- Get the software from the UBit webpage.
  - UBit software

Basic UNIX Commands

- The cluster compute nodes and front-end machine run Linux (CentOS).
- It is a command line **UNIX environment**.
- Here are two references for learning the basic commands:
  - more on basic UNIX commands
  - CCR UNIX Reference Card

Basic UNIX Commands

- Users should start with the basic UNIX commands, such as **ls** (list), **cd** (change directory), **cp** (copy), and **mkdir** (make directory).
- There are several editors available: emacs, nano and vi.
- Users can edit file on their laptops and transfer the files to the CCR cluster.
- The dos2unix command will remove any hidden characters in text files transferred from Windows machines

Where are my files?

- GPFS (IBM General Parallel File System) provides storage space of user home directories, projects directories and global scratch space.
- All compute node access GPFS.
- The path for a home directory is **/user/<username>**.
- Faculty can request projects space for the research group. The path is **/projects/<faculty-username>**
- Home and project directories are backed up daily.

Where are my files?

- **/gpfs/scratch** is global scratch space.
  - This space is for temporary use.
  - Use scratch space for running jobs only.
  - Files older than 3 weeks are automatically removed.
  - There is no backup of files in /gpfs/scratch.
- Every compute node has a **/scratch** directory on the local disk. Jobs can use this local scratch directory.

Class Exercise

- When you login are will be in your home directory.
- Login to **rush.ccr.buffalo.edu**
- List the contents of you home directory:
  - **TYPE:** ls
  - **TYPE:** ls -latr
    - (long, all, time, reverse)
- Show the path of the directory:
  - **TYPE:** pwd

Class Exercise

- Show my group membership:
  - **TYPE:** id username
- Show the quota on my home directory:
  - **TYPE:** gquota
    - the default quota is 2GB
- Show the quota on the group's projects space:
  - **TYPE:** gquota -g group
    - hint: use the gid name from the id command.
- What is the quota for your projects space?

Class Exercise

- Many application are already installed on the CCR cluster.
- LMOD module files are used to set environment variables and paths of application software.
- Show what modules you have loaded.
  - **TYPE:** module list
- List all available modules.
  - **TYPE:** module avail
- List all matlab modules.
  - **TYPE:** module avail matlab

Class Exercise

- Show the module for matlab/R2014b.
  - **TYPE:** module show matlab/R2014b
  - hint: this shows what the module files does when you load it.
- Load the matlab/R2014b module.
  - **TYPE:** module load matlab/R2014b
  - hint: now you can run matlab
- Unload the matlab module.
  - **TYPE:** module unload matlab/R2014b

Class Exercise

- Create a directory in your home directory.
  - **TYPE:** mkdir class
- List the current directory.
  - **TYPE:** ls -l
- Note the permissions on the class directory.
  - drwxr-xr-x
  - from left to right: d for directory, rwx (read, write, execute) for the user, r-x (read and execute) for members of the group, r-x for world.

Class Exercise

- Note: the write permission means write, modify, and delete.
  - **Exception:** projects spaces do not allow one user to modify or delete another user's files.
- Use the chmod command to remove access to work for the class directory.
  - **TYPE:** chmod o-rwx class
  - hint: the syntax is chmod ugo+-rwx name
- View the manual page for chmod.
  - **TYPE:** man chmod

Class Exercise

- Change directory to the class directory.
  - **TYPE:** cd class
- Copy the following files from /gpfs/scratch/cdc/matlab-examples directory.
  - **TYPE:** cp /gpfs/scratch/cdc/ccr-class/slurmMATLAB slurmMATLAB
  - **TYPE:** cp /gpfs/scratch/cdc/ccr-class/test.m test.m
- List the contents of the class directory.
  - **TYPE:** ls -l

CCR Cluster Resources

- You must select resources for each job.
  - partition (job queue)
    - default is general-compute
  - compute nodes
    - default is 1 node
  - number of cores (CPUs) per node
    - default is 1 core
  - memory (per compute node)
    - default is 2800MB per core

CCR Cluster Resources

- time limit
  - default for the general-compute partition is 72 hours
  - default for debug partition is 1 hour
- type of compute node (constraint)
  - default is to run on any node that fulfills the core and memory requirements of the job
- Note: compute nodes are shared by default

CCR Cluster Compute Nodes

- There are over **700 compute nodes** providing ~8000 cores.
  - Hint: think of a core as a CPU.
- Compute nodes are grouped according to number of cores.
- A job will always be assigned nodes with the same number of cores.
  - No job would ever have a mix of 8-core and 12-core compute nodes.

Number of Compute Nodes

- 372 **12-core** compute nodes
- 256 **8-core** compute nodes
- 32 **16-core** compute nodes
- 18 **32-core** compute nodes
- 32 **12-core** compute nodes with 2 GPUs each
- more on compute nodes

How to choose a compute node

- Most users choose compute nodes based on **number of nodes**, **number of cores per node**, and **memory per node** required for the job.
- 8-core compute nodes have 24GB of memory.
- 12-core compute nodes have 48GB of memory.
- 16-core compute nodes have 128GB of memory.
- 16 of the 32-core compute nodes have 256GB, while 2 have 512GB of memory.
- GPU Compute nodes have 48GB of memory and 2 Nvidia Fermi GPUs.

How to choose a partition

- SLURM **job queues** are referred to as partitions. Here are the **partitions** for the CCR cluster.
- **general-compute** - default partition if no partition is specified for a job.
  - almost all compute nodes
  - **per user limit of 1000** running and pending jobs at a time
  - maximum time limit of 72 hours

How to choose a partition

- **gpu** - higher priority for only the compute nodes with GPUs.
  - **per user limit of 32** running or pending jobs at a time.
  - maximum time limit of 72 hours
- **largemem** - higher priority for only the 32-core compute nodes.
  - **per user limit of 32** running or pending jobs at a time.
  - maximum time limit of 72 hours

How to choose a partition

- **debug** - small partition for quick debugging.
  - 8 dedicated compute nodes
    - 4 8-core compute nodes,
    - 2 12-core compute nodes
    - 1 16-core node with 2 GPUs
    - 1 16-core node with a XEON PHI coprocessor
  - **per user limit of 4** running or pending jobs at a time.
  - maximum time limit of **1 hour**

SLURM Commands

- **squeue** — shows the status of jobs.
- **sbatch** —submits a script job.
- **scancel** —cancels a running or pending job.
- **snodes** — shows details of the compute nodes.
- **slurmjobvis** – graphical job monitoring tool.
- more on SLURM commands

Class Exercise

- List the jobs in the queues.
  - **TYPE:** squeue
- List the jobs in the debug partition.
  - **TYPE:** squeue -p debug
- List the compute nodes in the queues
  - **TYPE:** snodes
- List the compute nodes in the debug partition.
  - **TYPE:** snodes all debug

SLURM Script Example

- The #SBATCH lines are directives to the scheduler. The directives are the resource requests, job output file, and email preferences.

```
#!/bin/sh
#SBATCH --partition=debug
#SBATCH --time=00:15:00
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=8
#SBATCH --mem=23000
#SBATCH --constraint=CPU-L5630|CPU-L5520
#SBATCH --job-name="test"
#SBATCH --output=test.out
##SBATCH --mail-user=username@buffalo.edu
##SBATCH --mail-type=END
```

SLURM Script Example

- The following lines print information to the job output file.

```
echo "SLURM_JOB_ID="$SLURM_JOB_ID
echo "SLURM_JOB_NODELIST"=$SLURM_JOB_NODELIST
echo "SLURMTMPDIR="$SLURMTMPDIR

echo "working directory = "$SLURM_SUBMIT_DIR
```

- The job starts in the directory from which you submitted it. This is the working directory.

SLURM Script Example

- Load the module file for MATLAB.
- List the loaded modules.

```
module load matlab/R2014b
module list
ulimit -s unlimited
#
```

- The ulimit command removes the size limit on the instruction stack. This helps large programs to run.

SLURM Script Example

- Run the MATLAB computation using the command line.

```
#
echo "run matlab computation"
matlab -nodisplay < test.m
date
echo "All Done!"
```

- Once all the lines of the SLURM have been executed, then the job completes and exits the compute node.

How to submit a SLURM script job

- Submit an interactive job using the **sbatch** <your_slurm_script>
- The job will be submitted to the SLURM scheduler.
- The job will wait in the queue until the scheduler assigns resources to it. This is a pending state.
- more on submitting a job script

Class Exercise

- View the slurmMATLAB script file.
  - **TYPE:** more slurmMATLAB
  - hint: press space bar to page
  - Note: a sleep was added so that you will see the job in the queue. The computation runs very quickly.
- What resources are requested by the SLURM job script?
- View the test.m file.
  - **TYPE:** more test.m

Class Exercise

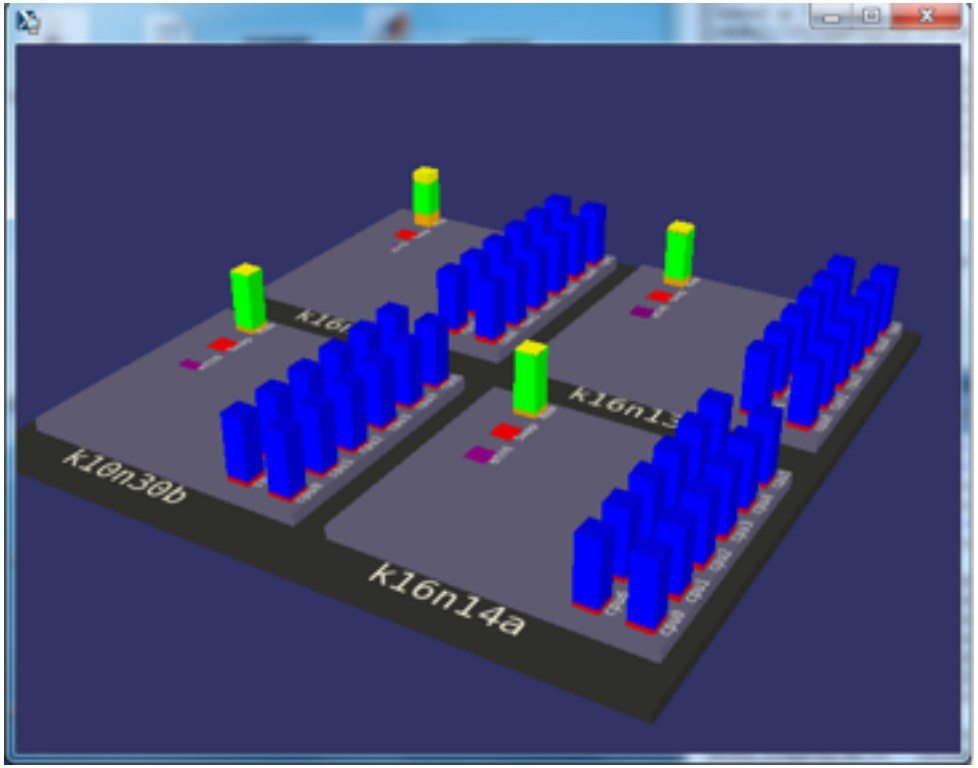
- Submit the job.
  - **TYPE:** sbatch slurmMATLAB
- Check the status of the job.
  - **TYPE:** squeue -u username
  - **TYPE:** squeue -j jobid
- Check the status of the debug partition.
  - **TYPE:** squeue -p debug
- Note: The PD state is pending. The job is waiting in the queue.

Class Exercise

- Monitor the job using slurmjobvis.
  - **TYPE:** slurmjobvis jobid
- Monitor the using ssh and top:
  - **TYPE:** ssh cpn-XXX-xx
  - hint: get the compute node running the job using the squeue command
  - **TYPE**: top
  - The top command show the CPU and memory utilization.
- Leave the compute node.
  - **TYPE:** exit

Job monitoring

- The **slurmjobvis** is a graphical display of the activity on the node.
- CPU, memory, network, as well as GPU utilization, are displayed.



How to submit an interactive job

- Submit an interactive job using the **fisbatch** wrapper.
- Although the job is interactive it still waits in the queue.
- Useful for debugging.
- Specify partition, nodes, cores or tasks, and time.
- Once the job starts the user is logged into the compute node.

How to submit an interactive job

- **TYPE:** fisbatch --partition=debug --nodes=1 --ntasks-per-node=8 —time=01:00:00
- When the job starts you will be logged into the compute node.
- Now load the matlab module and type matlab. The matlab GUI will launch.
  - This can be a bit slow.
- more on submitting an interactive job

More Information and Help

- CCR SLURM web pages
- More sample SLURM scripts can be found in the /util/academic/slurm-scripts directory on rush.
- Compute Cluster web page
- Remote Visualization web page
- Users can get assistance by sending an email to ccr-help@ccr.buffalo.edu.