Introduction to Running Computations on the High Performance Clusters at the Center for Computational Research

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CENTER FOR COMPUTATIONAL RESEARCH
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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.

CCR Cluster

- Users run programs on the cluster as **jobs** submitted to queues.
  - A **job** is a request for computers, cores, memory, networking, queue, and time.
- The CCR cluster is a high performance.
  - Large parallel jobs run on the cluster.
- The CCR cluster is high through-put.
  - A large number of jobs run on the cluster at one time.

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.

CCR Cluster

- The CCR cluster provides over 8,000 cores.
- There is a mix of 8-core, 12-core , 16-core and 32-core compute nodes.
  - A **compute node** is a linux machine with memory, disks, and cores (cpus), as well as both ethernet and Infiniband network connections.
- The GPFS (IBM General Parallel File System) is used for storage.
- There is a login front-end server.
- SLURM (Simple Linux Utility Resource Manager) is the job scheduler.

CCR Cluster

- **IMPORTANT!**
- Recent and planned changes to the CCR cluster.
  - All users should look at the 2015 What's New guide.

Where are my files?

- GPFS provides storage space of user home directories, projects directories and global scratch space.
- All compute node access GPFS.
- A home directory has a 2GB quota by default. The path 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.

CCR Cluster Compute Nodes

- There are over 700 compute nodes providing ~8000 cores.
- 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.
- The maximum number of compute nodes that users can request in a job is the total for that group of nodes.

Number of Compute Nodes

- **12-core** compute nodes — **372**
- **8-core** compute nodes — **256**
- **16-core** compute nodes — **32**
- **32-core** compute nodes — **18**
- **12-core** nodes with GPUs — **32**

- [more on compute nodes]

How to choose a compute node

- Most users choose compute nodes based on number of nodes, number of cores, and memory per node required for the job.
- 8-core compute node 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**

How to choose a partition

- **viz** - partition for jobs running on the remote visualization nodes.
  - Users do not submit directly to the viz partition.
  - **per user limit of 32** running or pending jobs at a time.
  - maximum time limit of 24 hours
  - how to use the Remote Visualization compute nodes

How to choose a partition

- **supporters** - higher priority partition for users belonging to research groups that have contributed funds to CCR.
  - almost all compute nodes
  - **per user limit of 1000** running or pending jobs at a time
  - maximum time limit of 72 hours
- more on CCR SLURM partitions

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**.
- Only secure protocols, such as **ssh** and **sftp**, are permitted to access the front-end.
- Small test computations can run on the front-end machine.
    - CPU time limit of 15 minutes on the front-end. Processes that exceed the time limit are automatically terminated.

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.
- Windows users must install X-Win32 or PuTTY for the 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.
- **UBVPN** must be used to access the rush login machine from off campus.
- Users should setup UB-Secure on their laptops for connecting through wireless.
- more on how to transfer files
- Get the software from the UBit webpage.
  - UBit software

Command Line Environment

- The compute nodes and front-end machine run Linux. It is a command line **UNIX environment**.
- Users should have know basic UNIX commands, such as ls, cd and mkdir.
- There are several editors available: emacs, nano and vi.
- Use the dos2unix command to remove any hidden characters in text files transferred from Windows machines.
- more on basic UNIX commands
- CCR UNIX Reference Card

Using Software and Compilers

- Compilers, JAVA, Python, MPI and application software are available to use on cluster.
- Lmod is used to set paths and variables for the software.
- "**module avail**" shows all installed software packages.
- "**module load <package-name>**" puts the software in the user's path.
- more on using Lmod and modules

Compilers, MPI and more

- The Intel, PGI and GNU compilers are available on the cluster. GNU compilers are already in the user's default path.
- MPI (Message Passing Interface) implementations are installed on the cluster.
- More recent versions of JAVA are available.
- Anaconda Python is available.
  - more on using Anaconda Python

SLURM Commands

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

How to submit an interactive job

- Submit an interactive job using the **fisbatch** wrapper.
- Useful for debugging.
- Specify partition, nodes, cores or tasks, and time.
- Once the job starts the user is logged into the compute node.
- more on submitting an interactive job

SLURM script example

```
#!/bin/sh
#SBATCH --partition=general-compute
#SBATCH --time=00:15:00
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=8
#SBATCH --mem=24000
# Memory per node specification is in
MB. It is optional.
# The default limit is 3000MB per core.
```

SLURM script example

```
#SBATCH --job-name="hello_test"
#SBATCH --output=test-srun.out
#SBATCH --mail-
user=username@buffalo.edu
#SBATCH —mail-type=ALL
echo "SLURM_JOBID="$SLURM_JOBID
echo "SLURM_JOB_NODELIST"=
$SLURM_JOB_NODELIST
```

SLURM script example

```
echo "SLURM_NNODES"=$SLURM_NNODES
echo “SLURMTMPDIR="$SLURMTMPDIR

echo  "working directory =
"$SLURM_SUBMIT_DIR

module load intel/13.1
module load intel-mpi/4.1.3
module list
ulimit -s unlimited
```

SLURM script example

```
NPROCS=`srun --nodes=${SLURM_NNODES}
bash -c 'hostname' |wc -l`
echo NPROCS=$NPROCS
echo "Launch helloworld with srun"
#The PMI library is necessary for srun
export I_MPI_PMI_LIBRARY=/usr/lib64/
libpmi.so
srun ./helloworld
#
echo "All Done!"
```

Commonly used SLURM variables

- **$SLURM_JOBID**
- **$SLURM_JOB_NODELIST**
  - Node list in SLURM format; for example f16n[04,06].
- **$SLURM_NNODES**
  - Number of nodes
- **$SLURMTMPDIR**
  - /scratch/jobid
  - local to the compute node
- **$SLURM_SUBMIT_DIR**
  - Directory from which the job was submitted
- **NOTE!** Jobs start in the $SLURM_SUBMIT_DIR.

Task Launching

- The number of cores/processes can be computed.
  - Use srun to get the total number of cores.
  - NPROCS=`srun --nodes=${SLURM_NNODES} bash -c 'hostname' |wc -l`
- Intel-MPI mpirun and mpiexec are SLURM aware.
- srun will execute a command across nodes.
  - Typically, this is the best choice for launching a parallel computation.

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

Check the status of the job

```
squeue -u <username>
squeue -j <job_id>
```

```
 JOBID PARTITION NAME USER ST TIME NODES
NODELIST(REASON)
4832 general-c hello_te cdc R 0:20 2 f16n[10-11]
```

- Job status:
  - **R** – job is running.
  - **PD** – job is waiting for resource.
    - Reasons are usually (Resources) or (Priority).
  - Others commons reasons are CA (cancelled) and CD (completed).

Partition and node status

sinfo -p general-compute

```
PARTITION      AVAIL  TIMELIMIT  NODES  STATE
NODELIST
general-comput*    up 3-00:00:00    264   idle
d07n07s[01-02],d07n08s[01-02], …
```

- Node states:
  - **alloc** – all cores are in use.
  - **mix** – some cores are available.
  - **idle** – node is free. All cores are available.
  - **down**- node is down.
  - **drained** – node is offline.

Node status and details

```
[cdc@rush:~]$ snodes k14n16s01
HOSTNAMES  STATE    CPUS S:C:T    CPUS(A/I/O/T)   CPU_LOAD
MEMORY   GRES     PARTITION          FEATURES
k14n16s01  alloc    12   2:6:1    12/0/0/12      12.06    48000
(null)   general-compute*   IB,CPU-E5645

cdc@rush:~]$ snodes k05n22
HOSTNAMES  STATE    CPUS S:C:T    CPUS(A/I/O/T)   CPU_LOAD
MEMORY   GRES     PARTITION          FEATURES
k05n22     idle     16   2:8:1    0/16/0/16      0.04     128000   mic:1
debug            CPU-E5-2660,MIC
[cdc@rush:~]$
```

Node Sharing

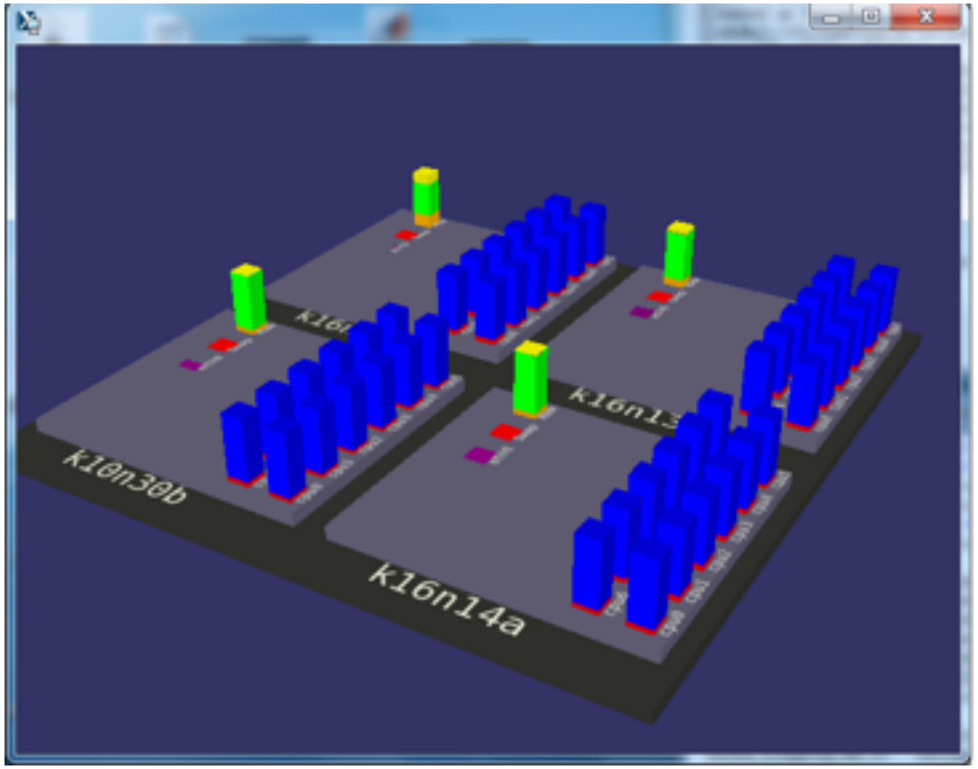
- Compute nodes are **shared** among different jobs and users.
- Tasks are limited to the number of cores and memory specified.
- The integration of CPUSETS and SLURM makes this possible.
  - **CPUSET** is a Linux kernel level mechanism that can be used to control access to individual cores.
- The default memory limit per core is 3000MB.

Node Sharing

- --mem=24000
  - Requests 24GB per node.
- --mem-per-core=16000
  - Requests 16GB on a core; use for serial job.
- Jobs exceeding the memory limit will be terminated by the resource manager.
- Check the General Compute Cluster webpage for node memory and core details.
- The --exclusive flag will request the nodes as dedicated. The nodes will not be shared.

Job monitoring

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



Putting it all together

- Login to the cluster login front-end machine.
- Transfer files to home directory.
- Locate necessary software with “module avail”
- Load modules and compile the code.
- Create a job script.
- Submit a script.
- Monitor job with squeue and slurmjobvis.

More Information and Help

- CCR SLURM web pages
- **/gpfs/courses/class-notes** for sample jobs.
- 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.