Introduction to SLURM & SLURM batch scripts

Zhiyu (Drew) Li & Anita Orendt
Research Consulting & Faculty Engagement
Center for High Performance Computing
{zhiyu.li; anita.orendt}@utah.edu

Overview of Talk

- What is SLURM
- Accounts and Partitions
- Basic SLURM Commands
- Node Sharing
- SLURM batch directives
- SLURM Environment Variables
- Running an Interactive Batch job
- Monitoring Jobs
- Where to get more Information

What is SLURM

- Formerly known as ***S***imple ***L***inux ***U***tility for ***R***esource ***M***anagement
- Open-source workload manager for supercomputers/clusters
  - Manage resources (nodes/cores/memory/interconnect/gpus)
  - Schedule jobs (queueing/prioritization)
- Used by 60% of the TOP500 supercomputers[1]
- Fun fact: development team based in Lehi, UT

slurm
workload manager

[1] https://en.wikipedia.org/wiki/Slurm_Workload_Manager (2023 Jun)

Partitions & Accounts

- **Partition**: a group of nodes that a job can be scheduled on. A node can belong to more than one partition, and each partition can be configured to enforce different resource limits and policies.

- **Account**: to limit and track resource utilization at user/group level. A user/group can have multiple Slurm accounts – each represents different privileges.

- To run a job on CHPC, you need to specify a pair of a **Partition** and an **Account.** (How to find out? -- There are 3 commands! More on this later)

Basic SLURM commands

- **sinfo** - shows all partitions/nodes state
  - **mysinfo*** **-** info on partitions/nodes and associated accounts you have access to on the cluster (***Method 1***)
- **squeue** - shows all jobs in queue
  - **squeue -u <username>** - shows only your jobs
  - **mysqueue*** **-** shows job queue per partition and associated accounts you have access to on the cluster (***Method 2***)
- **sbatch <scriptname.sbatch> -** launch a batch job
- **scancel <jobid>** - cancel a job
- **salloc** – start an interactive job

*CHPC developed programs. See CHPC Newsletter 2023 Summer

For **sinfo, mysinfo, squeue, mysqueue** – can use **–M <ClusterName>** (notchpeak, kingspeak, lonepeak, ash)

Redwood (PE) has own slurm setup, separate from others

Some Useful Aliases

- **Bash** to add to **.aliases** file:

alias **si**="sinfo -o \"%20P %5D %14F %8z %10m %10d %11l %16f %N\""

alias **si2**="sinfo -o \"%20P %5D %6t %8z %10m %10d %11l %16f %N\""

alias **sq**="squeue -o \"%8i %12j %4t %10u %20q %20a %10g %20P %10Q %5D %11l %11L %R\""

- **Csh/Tcsh** to add to **.aliases** file:

alias **si** 'sinfo -o "%20P %5D %14F %8z %10m %11l %16f %N"'

alias **si2** 'sinfo -o "%20P %5D %6t %8z %10m %10d %11l %N"'

alias **sq** 'squeue -o "%8i %12j %4t %10u %20q %20a %10g %20P %10Q %5D %11l %11L %R"‘

See: https://www.chpc.utah.edu/documentation/software/slurm.php#aliases

- si/si2 – check node specifications (CPU, Memory, GPU, PI)
- sq – check job priority, assigned nodes, reason/error…

Partitions & Accounts

- To run a job on CHPC, you need to specify a pair of a **Partition** and an **Account.**
  - Commands to check valid pairs:

    myinfo, mysqueue,

    myallocation (Method 3, gives info on all clusters)

- CHPC Cluster Partition Naming Convention
  - <CluserName>: *notchpeak, kingspeak, lonepeak* → general nodes (allocation required on notchpeak)
  - <CluserName>-freecycle: *notchpeak-freecycle* → general nodes - preemptable
  - <PILastName>-<ClusterCode>: baggins-np (-kp; -lp) → owner nodes (PI/Dept-specific)
  - <ClusterName>-guest: *notchpeak-guest* → owner nodes (from all PIs) -preemptable

  Variants: -gpu; -shared;

  notchpeak-shared: general nodes on notchpeak run in Shared mode (more on this later)

  baggins-gpu-kp: owner GPU nodes on kingspeak

More on Accounts & Partitions

Awarded allocations and node ownership status	**What resource(s) are available** (recommendation high to low)
No awarded general allocation (notchpeak), no owner nodes	Unallocated general nodes (eg kingspeak, lonepeak) Guest access on owner nodes Allocated general nodes in freecycle mode (notchpeak) - not recommended
Awarded general allocation, no owner nodes	Allocated general nodes (notchpeak) Unallocated general nodes (eg kingspeak, lonepeak) Guest access on owner nodes
Group owner nodes, no awarded general allocation	Group owned nodes Unallocated general nodes (eg kingspeak, lonepeak) Guest access on owner nodes of other groups Allocated general nodes in freecycle mode (notchpeak) - not recommended
Group owner node, awarded general allocation	Group owned nodes Allocated general nodes (notchpeak) Unallocated general nodes (eg kingspeak, lonepeak) Guest access on owner nodes of other groups

See https://www.chpc.utah.edu/documentation/guides/index.php#parts

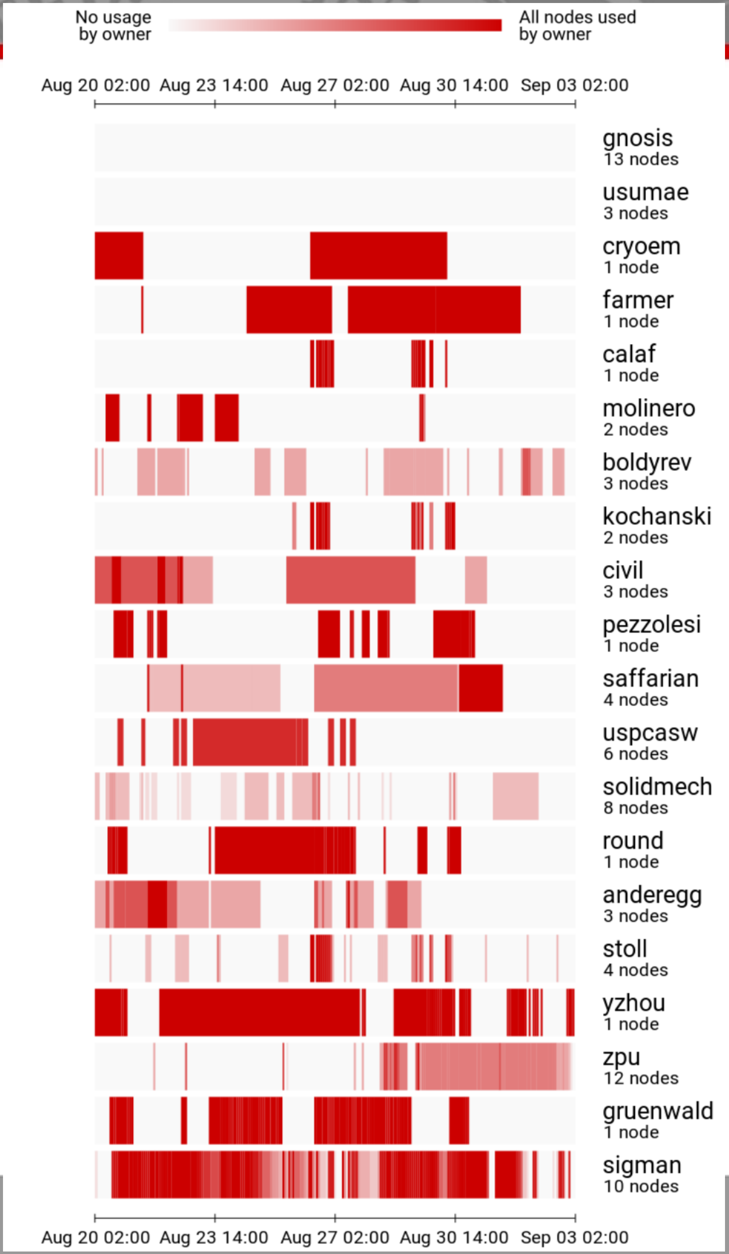
Node Sharing

- A partition can be configured to run jobs in 2 modes: **Exclusive** V.S. **Shared**
- **Exclusive partition**: Slurm gives whole node(s) (all CPU cores) to your job (and you will be charged on whole nodes);
- **Shared partition**: Slurm gives a portion of node (CPU core & Memory) as requested; The remain resources can be used by other jobs; (you will be charged on the portion of the node)
- **How to tell on CHPC clusters** -- Identifiable by partition names
  - **Exclusive**: notchpeak, kingspeak, baggins-np, baggins-kp
  - **Shared**: notchpeak-shared, kingpeak-shared-guest, baggins-shared-kp
  - Exception: GPU partitions are all in Shared mode (even no '–shared" in names) on CHPC: notchpeak-gpu
- Use **Shared Partition** wherever possible
  - Save your group allocations/credits
  - Shorten queueing time for You and Others: allow multiple jobs on same node
  - Help increase utilization and save energy/environment
  - CHPC may reach out to you to promote resources sharing

https://www.chpc.utah.edu/documentation/software/node-sharing.php

Owner/Owner-guest

- CHPC provides heat maps of usage of owner nodes by the owner over last two weeks
- https://www.chpc.utah.edu/usage/constraints/
- Use information provided to target specific owner partitions with use of constraints (more later) and node feature list



SLURM Batch Directives

#SBATCH --time 1:00:00 ← wall time of a job (or -t) in hour:minute:second

#SBATCH --partition=name ← partition to use (or -p)

#SBATCH --account=name ← account to use (or -A)

#SBATCH --nodes=1 ← number of nodes (or -N)

#SBATCH --ntasks=32 ← total number of tasks (cpu cores) (or -n)

#SBATCH --mem=128GB ← memory per node

#SBATCH --mail-type=FAIL,BEGIN,END ← events on which to send email

#SBATCH --mail-user=name@example.com ← email address to use

#SBATCH -o slurm-%j.out-%N ← name for stdout; %j is job#, %N node

#SBATCH -e slurm-%j.err-%N ← name for stderr; %j is job#, %N node

Guest Job --Target on Owner nodes

```
#SBATCH --time 10:00:00
#SBATCH --partition=notchpeak-shared-guest
#SBATCH --account=owner-guest
#SBATCH --nodes=1
#SBATCH --ntasks=32
#SBATCH --mem=128GB

#SBATCH --mail-type=FAIL,BEGIN,END
#SBATCH --mail-user=name@example.com
#SBATCH -o slurm-%j.out-%N
#SBATCH -e slurm-%j.err-%N
#SBATCH --constraint  “<Owner-Nodes-Label-Found-On-Chart>”
```

Basic SLURM script flow

1. Set up the #SBATCH directives for the scheduler to request resources for job
2. Set up the working environment by loading appropriate modules
3. If necessary, add any additional libraries or programs to $PATH and $LD_LIBRARY_PATH, or set other environment needs
4. Set up temporary/scratch directories if needed
5. Switch to the working directory (often group/scratch)
6. Run the program
7. Copy over any results files needed
8. Clean up any temporary files or directories

Basic SLURM script - bash

```
#!/bin/bash
#SBATCH --time=02:00:00
#SBATCH --nodes=1
#SBATCH --ntasks=8
#SBATCH --mem=32G
#SBATCH -o slurmjob-%j.out-%N
#SBATCH -e slurmjob-%j.err-%N
#SBATCH --account=owner-guest
#SBATCH --partition=kingspeak-shared-guest
#Set up whatever package we need to run with
module load <some-modules>
#set up the temporary directory
SCRDIR=/scratch/general/vast/$USER/$SLURM_JOB_ID
mkdir -p $SCRDIR
#copy over input files
cp file.input $SCRDIR/.
cd $SCRDIR
#Run the program with our input
myprogram < file.input > file.output
#Move files out of working directory and clean up
cp file.output $HOME/.
cd $HOME
rm -rf $SCRDIR
```

```
# Save the script as XXXXX.sbatch
# submit it
sbatch XXXXX.sbatch
# slurm returns a <jobid>
squeue –u <jobid>
```

Basic SLURM script - tcsh

```
#!/bin/tcsh
#SBATCH --time=02:00:00
#SBATCH --nodes=1
#SBATCH --ntasks=8
#SBATCH --mem=32G
#SBATCH -o slurmjob-%j.out-%N
#SBATCH -e slurmjob-%j.err-%N
#SBATCH --account=owner-guest
#SBATCH --partition=kingspeak-shared-guest
#Set up whatever package we need to run with
module load somemodule
#set up the scratch directory
set SCRDIR /scratch/local/$USER/$SLURM_JOB_ID
mkdir -p $SCRDIR
#move input files into scratch directory
cp file.input $SCRDIR/.
cd $SCRDIR
#Run the program with our input
myprogram < file.input > file.output
#Move files out of working directory and clean up
cp file.output $HOME/.
cd $HOME
```

SLURM Environment Variables

- Depends on SLURM Batch Directives used
- Can get them for a given set of directives by using the "env" command inside a script (or in a srun session).
- Some useful environment variables:
  - $SLURM_JOB_ID
  - $SLURM_SUBMIT_DIR
  - $SLURM_NNODES
  - $SLURM_NTASKS

See: https://slurm.schedmd.com/sbatch.html#SECTION_OUTPUT-ENVIRONMENT-VARIABLES

Slurm for use of GPU Nodes

- GPU nodes are on lonepeak, kingspeak, notchpeak (and redwood in the PE)
- Info on GPU nodes found at https://chpc.utah.edu/documentation/guides/gpus-accelerators.php
- There are both general (open to all users) and owner GPU nodes (available via owner-gpu-guest, with preemption, to all uses)
- At this time, general GPU nodes are run without allocation (no charge)
  - Must get added to the gpu accounts – Request via helpdesk@chpc.utah.edu
- GPU partitions set up in a shared mode only as most codes do not yet make efficient use of multiple GPUs so we have enabled node sharing
- **Use only if you are making use of the GPU for the calculation**

Node Sharing on GPU nodes

- In Addition to submitting to a GPU partition, at least you need to specify flag "--gres=gpu", number of CPU cores, amount of memory

Option	Explanation
#SBATCH --gres=gpu:p100:1	request one p100 GPU (others types names are titanx, rtx3090, p100, v100, titanv, 1080ti, 2080ti, p40, t4, a40,a100)
#SBATCH --mem=4G	request 4 GB of RAM (default is 2GB/core if not specified)
#SBATCH --mem=0	request all memory of the node; use this if you do not want to share the node as this will give you all the memory
#SBATCH --ntasks=1	request 1 cpu core

GPU Job

```
#SBATCH --time 10:00:00
#SBATCH --partition=notchpeak-gpu-guest
#SBATCH --account=owner-gpu-guest
#SBATCH --nodes=1
#SBATCH --ntasks=4
#SBATCH --mem=16G
#SBATCH --gres=gpu:a100:1

#SBATCH --mail-type=FAIL,BEGIN,END
#SBATCH --mail-user=name@example.com
#SBATCH -o slurm-%j.out-%N
#SBATCH -e slurm-%j.err-%N
```

Running interactive batch jobs

- An interactive command is launched through the salloc command

```
salloc --time=8:00:00 --ntasks=4 --nodes=1 --mem=16G
--account=<account>  --partition=kingspeak-shared
```

```
 salloc --time=8:00:00 --ntasks=4 --nodes=1 --mem=16GB
--account=notchpeak-gpu --partition=notchpeak-gpu --gres=gpu
```

- Use of FastX connection is highly recommended
  - support GUI applications
  - keep your sessions alive

OpenOnDemand is another option to start interactive sessions

Strategies for Job Arrays

- https://www.chpc.utah.edu/documentation/software/slurm.php#jobarr
- Useful if you have many similar jobs when each use all cores on a node or multiple nodes to run where only difference is input file
- sbatch --array=1-30%n myscript.sh – where n is maximum number of jobs to run at same time
- In script: use $SLURM_ARRAY_TASK_ID to specify input file:
  - ./myprogram input$SLURM_ARRAY_TASK_ID.dat

Job Priorities

- https://www.chpc.utah.edu/documentation/software/slurm.php#priority
- **sprio** give job priority for all jobs
  - sprio –j JOBID for a given job
  - sprio –u UNID for all a given user's jobs
- Combination of three factors added to base priority
  - Time in queue
  - Fairshare
  - Job size
- Only 5 jobs per user per slurm account (qos) will accrue priority based on time on queue

Checking Job Performance

- With an active job
  - can ssh to node
    - Useful commands, top, ps, sar, atop
  - Also from interactive node can query job
    - /uufs/chpc.utah.edu/sys/installdir/pestat/pestat
  - Can query node status
    - scontrol show node notch024
- After job complete -- XDMoD Supremm
  - Job level data available day after job ends
  - XDMoD sites https://xdmod.chpc.utah.edu and https://pe-xdmod.chpc.utah.edu
  - usage info: https://www.chpc.utah.edu/documentation/software/xdmod.php

Slurm Documentation at CHPC

https://www.chpc.utah.edu/documentation/software/slurm.php

https://www.chpc.utah.edu/documentation/software/serial-jobs.php

https://www.chpc.utah.edu/documentation/software/node-sharing.php

https://www.chpc.utah.edu/usage/constraints/

https://www.chpc.utah.edu/documentation/guides/index.php#GenSlurm

Other good documentation sources

http://slurm.schedmd.com/documentation.html

http://slurm.schedmd.com/pdfs/summary.pdf

http://www.schedmd.com/slurmdocs/rosetta.pdf

Getting Help

- CHPC website
  - www.chpc.utah.edu
    - Getting started guide, cluster usage guides, software manual pages, CHPC policies
- Service Now Issue/Incident Tracking System
  - Email: helpdesk@chpc.utah.edu
- Help Desk: 405 INSCC
- We use chpc-hpc-users@lists.utah.edu for sending messages to users