Introduction to SLURM & SLURM batch scripts

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Overview of Talk

- What is SLURM
- Basic SLURM commands
- Accounts and Partitions
- SLURM batch directives
- SLURM Environment Variables
- SLURM Batch scripts
- 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

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

Basic SLURM commands

- **sinfo** - shows partition/node state
- **squeue** - shows all jobs in the queue
  - **squeue -u <username>** - shows only your jobs
- **sbatch <scriptname> -** launch a batch script
- **scancel <jobid>** - cancel a job
- **salloc** – start an interactive job

Notes:

For **sinfo, squeue** – can add **–M all** to see all clusters using given slurm installation (notchpeak, kingspeak, lonepeak, ash)

Can also add **–M cluster** OR use full path /uufs/<cluster>.peaks/sys/pkg/slurm/std/bin/<command> to look at the queue, or submit or cancel jobs for a different cluster

Redwood 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\""
```

- 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"‘
```

Can add **–M** to **si** and **sq** also

You can find these on the CHPC Slurm page
https://www.chpc.utah.edu/documentation/software/slurm.php#aliases

Accounts & Partitions

- **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.
- **Accounts**: to limit and track resource utilization at user/group level. Each user/group can have multiple Slurm accounts.
- To run a job, specify a pair of Slurm Account and a Slurm Partition
- What Partitions are there?
  - sinfo (or si, si2)
  - <CluserName>: *notchpeak, kingspeak* → general nodes
  - <CluserName>-freecycle: *notchpeak-freecycle* → general nodes - preemptable
  - <PILastName>-<ClusterCode>: baggins-np (-kp; -lp) → owner nodes (PI-specific)
  - <ClusterName>-guest: *notchpeak-guest* → owner nodes (from all PIs) -preemptable

  (variants: -gpu; -shared: …)

Accounts & Partitions

- What Accounts do I use for a Partition?
  - <PILastName>: *bargins* paired with → general nodes partitions *(see below)
  - <PILastName>-<ClusterCode>: *bargins-np* paired with → owner nodes partition (PI-specific) in owner mode
  - owner-guest paired with → owner nodes partition (from all PIs) in guest mode

- *General Nodes Partition V.S. Awarded Allocation
  - On Notchpeak (allocated cluster)
    - Have an awarded allocation --- use partition “notchpeak”
    - Without an awarded allocation --- use partition “notchpeak-freecycle” (not recommended)
  - On other clusters (unallocated cluster)
    - use partition <ClusterName>: eg kingspeak

More on Accounts & Partitions

Awarded allocations and node ownership status	**What resource(s) are available** (recommendation high to low)
No awarded general allocation, 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

Query your allocation

~]$ myallocation

You have a general allocation on kingspeak. Account: chpc, Partition: kingspeak
You have a general allocation on kingspeak. Account: chpc, Partition: kingspeak-shared
You can use preemptable mode on kingspeak. Account: owner-guest, Partition: kingspeak-guest
You can use preemptable GPU mode on kingspeak. Account: owner-gpu-guest, Partition: kingspeak-gpu-guest
You have a GPU allocation on kingspeak. Account: kingspeak-gpu, Partition: kingspeak-gpu
You have a general allocation on notchpeak. Account: chpc, Partition: notchpeak
You have a general allocation on notchpeak. Account: chpc, Partition: notchpeak-shared
You can use preemptable GPU mode on notchpeak. Account: owner-gpu-guest, Partition: notchpeak-gpu-guest
You can use preemptable mode on notchpeak. Account: owner-guest, Partition: notchpeak-guest
You have a GPU allocation on notchpeak. Account: notchpeak-gpu, Partition: notchpeak-gpu
You have a general allocation on lonepeak. Account: chpc, Partition: lonepeak
You have a general allocation on lonepeak. Account: chpc, Partition: lonepeak-shared
You can use preemptable mode on lonepeak. Account: owner-guest, Partition: lonepeak-guest
You can use preemptable mode on ash. Account: smithp-guest, Partition: ash-guest

Node Sharing

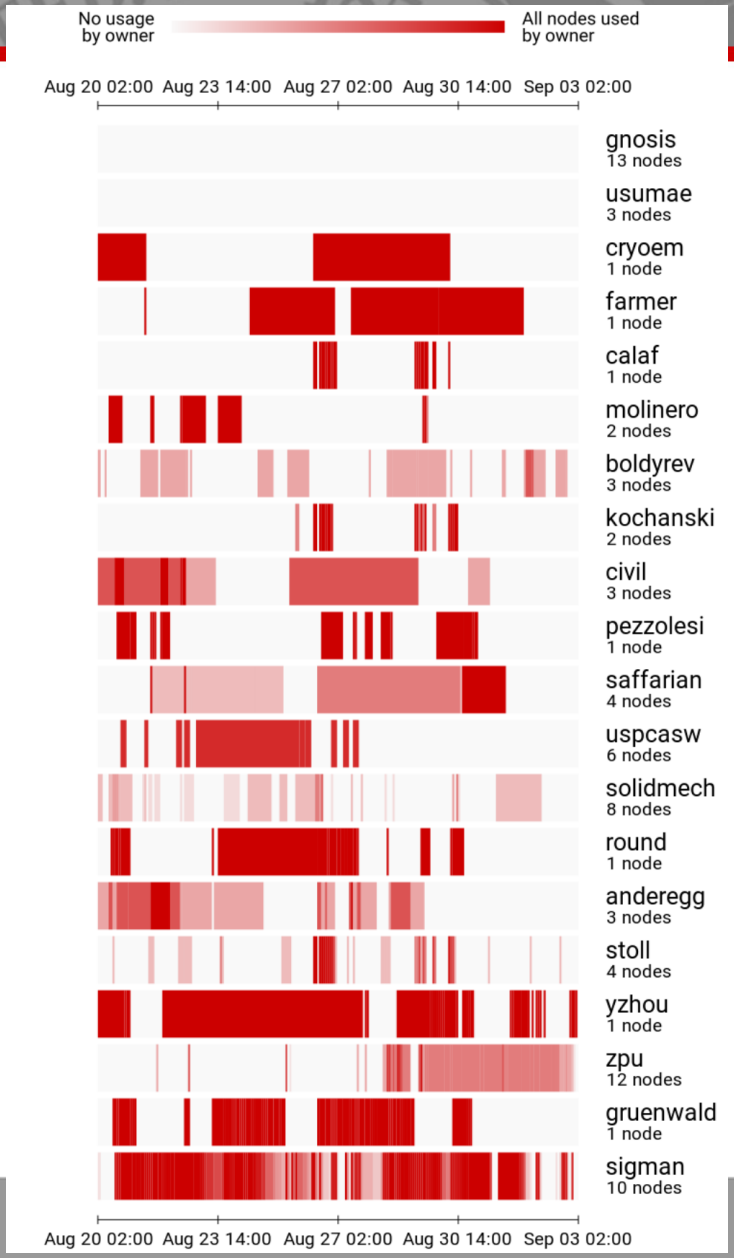
- Use the shared partition for a given set of nodes (using normal account for that partition)

notchpeak*	2	2/0/0/2	2:16:2	768000	1700000	3-00:00:00	chpc,skl,c32,m768	notch[044-045]
notchpeak*	32	32/0/0/32	4:16:2	255000	700000	3-00:00:00	chpc,rom,c64,m256	notch[172-203]
notchpeak*	4	4/0/0/4	2:16:2	95000	1800000	3-00:00:00	chpc,skl,c32,m96	notch[005-008]
notchpeak*	19	19/0/0/19	2:16:2	191000	1800000	3-00:00:00	chpc,skl,c32,m192	notch[009-018,035-043]
notchpeak*	1	1/0/0/1	2:18:2	768000	7400000	3-00:00:00	chpc,skl,c36,m768	notch068
notchpeak*	7	7/0/0/7	2:20:2	191000	1800000	3-00:00:00	chpc,csl,c40,m192	notch[096-097,106-107,153-155]
notchpeak-shared	2	2/0/0/2	2:16:2	768000	1700000	3-00:00:00	chpc,skl,c32,m768	notch[044-045]
notchpeak-shared	32	32/0/0/32	4:16:2	255000	3700000	3-00:00:00	chpc,rom,c64,m256	notch[172-203]
notchpeak-shared	4	4/0/0/4	2:16:2	95000	1800000	3-00:00:00	chpc,skl,c32,m96	notch[005-008]
notchpeak-shared	19	19/0/0/19	2:16:2	191000	1800000	3-00:00:00	chpc,skl,c32,m192	notch[009-018,035-043]
notchpeak-shared	1	1/0/0/1	2:18:2	768000	7400000	3-00:00:00	chpc,skl,c36,m768	notch068
notchpeak-shared	7	7/0/0/7	2:20:2	191000	1800000	3-00:00:00	chpc,csl,c40,m192	notch[096-097,106-107,153-155]

- In script:
  - #SBATCH --partition=<ClusterName>-shared
  - #SBATCH --ntasks=2
  - #SBATCH --mem=32G
- If there is no memory directive used the default is that 2G/core will be allocated to the job.
- Allocation usage of a shared job is based on the percentage of the cores and the memory used, whichever is higher

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=2 ← number of nodes (or -N)
#SBATCH --ntasks 32 ← total number of tasks (or -n)
#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
#SBATCH --constraint “C20” ← can use features given for nodes (or -C)

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

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 -o slurmjob-%j.out-%N
#SBATCH -e slurmjob-%j.err-%N
#SBATCH --account=owner-guest
#SBATCH --partition=kingspeak-guest
#Set up whatever package we need to run with
module load somemodule
#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
```

Basic SLURM script - tcsh

```
#!/bin/tcsh
#SBATCH --time=02:00:00
#SBATCH --nodes=1
#SBATCH -o slurmjob-%j.out-%N
#SBATCH -e slurmjob-%j.err-%N
#SBATCH --account=owner-guest
#SBATCH --partition=kingspeak-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
rm -rf $SCRDIR
```

Running interactive batch jobs

- An interactive command is launched through the salloc command

```
salloc --time=1:00:00 -ntasks=2 --nodes=1 --
account=chpc  --partition=kingspeak
```

- Launching an interactive job automatically forwards environment information, including X11 forwarding allowing for the running of GUI based applications

OpenOnDemand is another option to start interactive sessions (presentation – Tuesday, June 20, 2023)

Parallel Execution

- MPI installations at CHPC are SLURM aware, so mpirun will usually work without a machinefile (unless you are manipulating the machinefile in your scripts)
- If machinefile or host list needed, create the node list:
  - `srun hostname | sort -u > nodefile.$SLURM_JOB_ID`
  - `srun hostname | sort > nodefile.$SLURM_JOB_ID`
- Alternatively, you can use the srun command instead, but you need to compile with a more recently compiled MPI
- Mileage may vary, and for different MPI distributions, srun or mpirun may be preferred (check our slurm page on the CHPC website for more info or email us)

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=rs
- At this time, general GPU nodes are run without allocation
- 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
- Must get added to the gpu accounts – request via helpdesk@chpc.utah.edu
- **Use only if you are making use of the GPU for the calculation**

Node Sharing on GPU nodes

- Need to specify number of CPU cores, amount of memory, and number of GPU
- Core hours used based on highest % requested among cores, memory and GPUs

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	requests 1 core

Strategies for Serial Applications

- https://www.chpc.utah.edu/documentation/software/serial-jobs.php
- When running serial applications (no MPI, no threads) unless memory constrained, you should look to options to bundle jobs together so using all cores on nodes
- There are multiple ways to do so, including
  - srun --multi-prog
  - submit script
- Also consider OpenScienceGrid (OSG) as an option (especially if you have a large number of single core, short jobs)

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 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, 581-6440 (9-6 M-F)
- We use chpc-hpc-users@lists.utah.edu for sending messages to users