Slurm Job Management

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Slurm

https://slurm.schedmd.com/

- **S**imple **L**inux **U**tility for **R**esource **M**anagement
- Development started in 2002 at Lawrence Livermore National Laboratory
- **Overview -** open source, fault-tolerant, and highly scalable cluster management and job scheduling system
- **Main functions**
  - allocates exclusive and/or non-exclusive access to resources (compute nodes) to users for some duration of time so they can perform work
  - provides a framework for starting, executing, and monitoring work (normally a parallel job) on the set of allocated nodes
  - arbitrates contention for resources by managing a queue of pending work
- Configuration specific to an HPC center; **CARC** has its own setup

Some terms

- **Head Node** – The system that controls the cluster
- **Worker (Compute) Node** – Systems that perform the computations in a cluster
- **Login Node** – System that users log into to use a cluster
- **Scheduler** – Software that controls when jobs are run and the node they are run on
- **Shell** – A program that users employ to type commands
- **Script** – A file that contains a series of commands that are executed
- **Job** – A chunk of work that has been submitted to the cluster

How does it work?

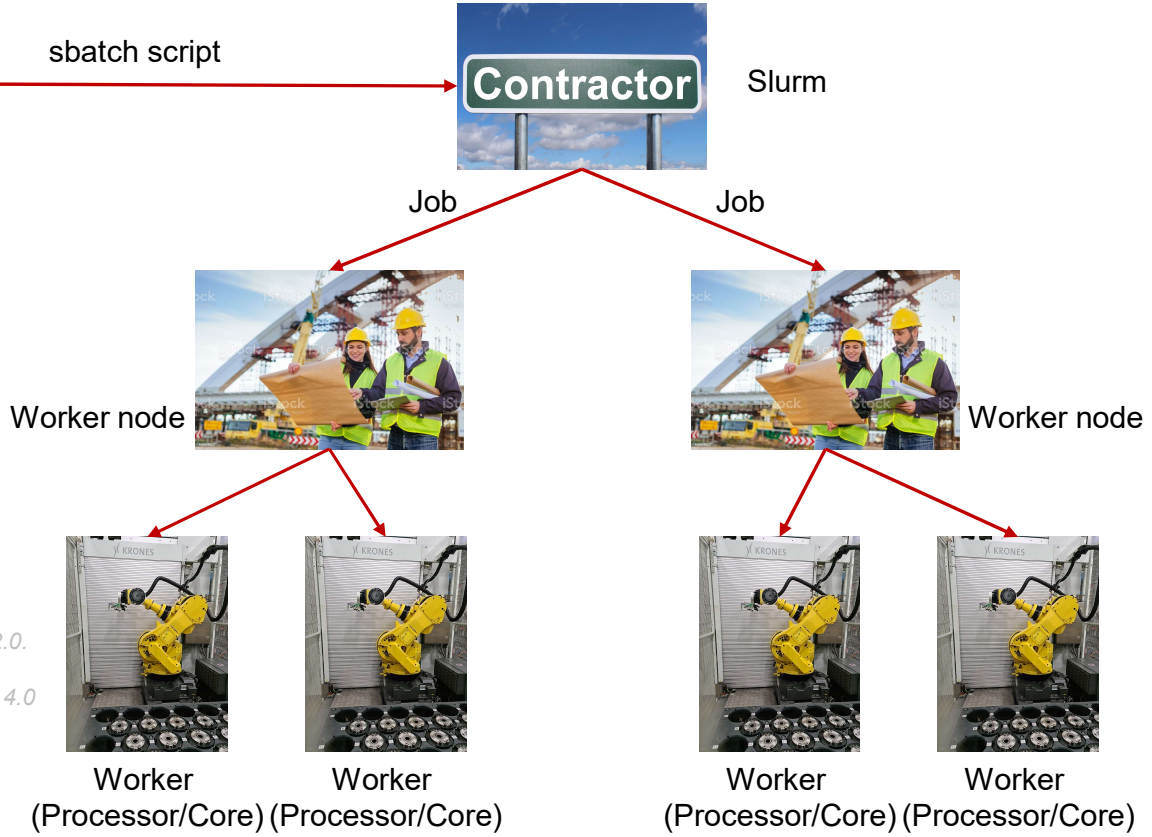

Image: "Love is Art Science 95" by Kollage Kid, licensed CC BY-NC 2.0.
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Image: "Industrial robot Fanuc M-710iC" by Biser Todorov CC BY-SA 4.0
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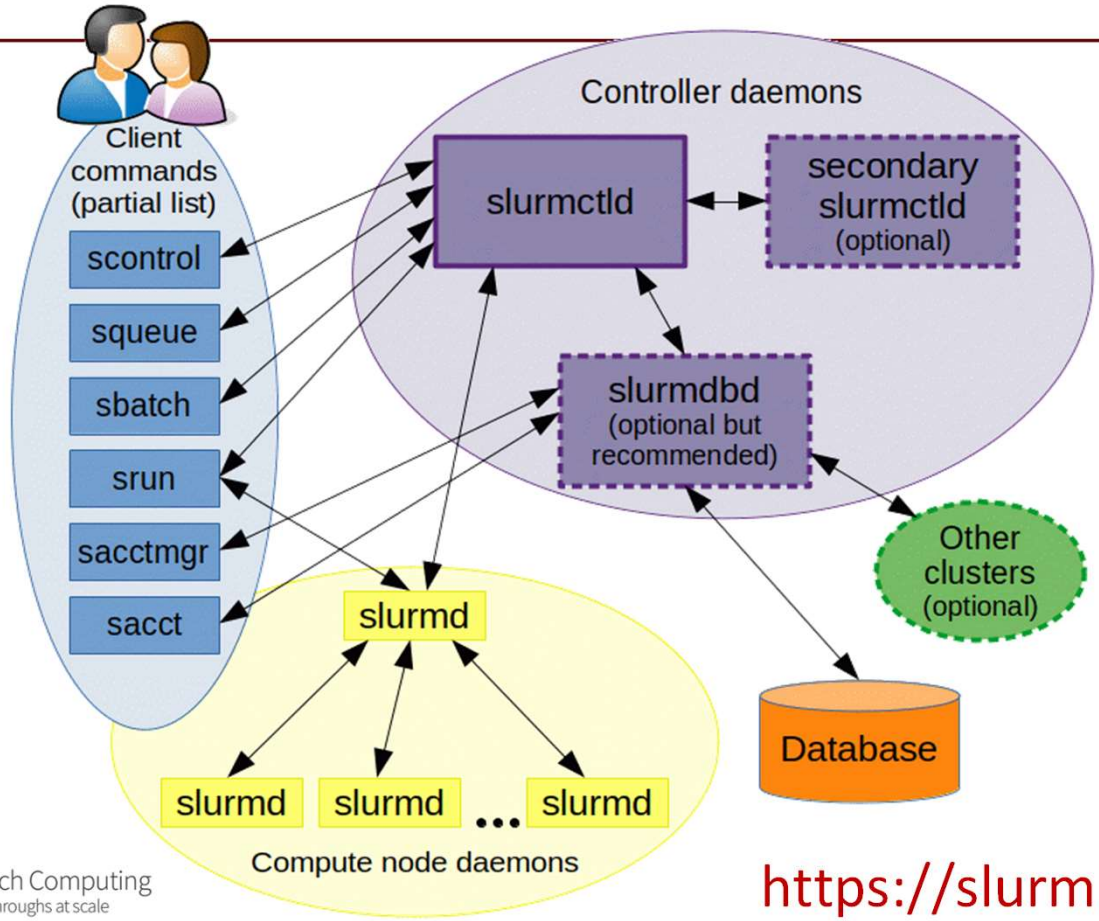
How does it work? – the details



https://slurm.schedmd.com/

Commands

https://slurm.schedmd.com/quickstart.html

- **sinfo** – reports state of the partitions and nodes
- **squeue** – reports state of jobs or job steps
- **salloc** – allocates resources for a job in real time
- **sbatch** – submits a job script to queue for a later execution
- **srun** – submits a job for execution or initiate job steps in real time
- **scancel** – is used to cancel a job or job step
- **sprio** – displays a detailed view of the components affecting job's priority
- **sstat** – is sed to get information about the resources utilized by a job or job step
- **sacct** – is used to report job accounting information about active or completed jobs
- **seff** – is used to display job efficiency for past jobs
- **scontrol** – is used to display or modify slurm configuration and state

Lets get going

- Detailed policies and directions
  - https://carc.usc.edu/user-information/getting-started
- Do not install software yourself, contact us
  - https://carc.usc.edu/education-and-outreach/office-hours:
    - Virtual (Tue, 2:30-5:00)
    - In-person: Leavey Library, room 3L (Tue, 2:30-5:00)
  - Submit a ticket! (https://carc.usc.edu/user-support/)
  - When we install software, it is available to everyone
- Program running slow? *Submit a ticket!*
- Don't know what resources to use? *Submit a ticket!*
- Any other questions? *Submit a ticket* or *visit our forum*

Log into CARC

- Open the terminal:
  - Mac: Applications>Utilities>Terminal or open Spotlight and start typing “terminal”
  - Windows: Start menu>cmd (or use PuTTY or Cygwin)
  - Linux: System tools>Terminal or Accessories>Terminal or search for Terminal
- Type `ssh ttrojan@discovery1.usc.edu`
- Enter your password
- Choose an option in Duo-2FA, and confirm your access
- (optional) Answer “No” when asked to save your password
- If successful, your prompt should look something like:
  `[ttrojan@discovery1 ~]`

sinfo

https://slurm.schedmd.com/sinfo.html

- reports state of the partitions and nodes

```
$ sinfo
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    1:00:00      7   idle a02-26,e05-[42,76,78,80],e09-18,e23-02
epyc-64      up 2-00:00:00     10    mix b22-[10,12-13,15,21-24,29-30]
epyc-64      up 2-00:00:00     22  alloc b22-[01-09,11,14,16-20,25-28,31-32]
main*        up 2-00:00:00    178    mix d05-[05-42],d06-[15-18,20,22-26,28],d18-[01,05,08,12-13,16,23-24,27-30,32-
38],d22-[51-52],e06-[01-04,09-10,12-13,16-19,22],e07-[02,05,08-09,14-16,18],e11-[26,29,45,47],e13-[11,28-29,32,38-47]
main*        up 2-00:00:00     59  alloc d06-[19,21,27],d17-[03-05,22],d18-[17,22,31],e06-[06-08,20-21,24],e07-[01,03]
main*        up 2-00:00:00     68   idle d11-[09-41],d17-[12,18,31-37],d18-[02-26],e06-[05,11,14-15
gpu          up 2-00:00:00     10   resv e17-[10-19]
gpu          up 2-00:00:00     21    mix d11-[02-04],d13-[02,04-07,09],d14-[03-04,07-10],d23-[10,13-14,16],e22-[01-02]
gpu          up 2-00:00:00     46   idle d13-[03,08,10-11],d14-[05-06,11-18],d23-15,e21-[01-16],e22-[03-16],e23-01
oneweek      up 7-00:00:00      2  alloc e02-[45,72]
oneweek      up 7-00:00:00     45   idle e01-[46,48,52,60,62,64,76],e02-[40-44,46,48-71,73-80]
largemem     up 7-00:00:00      2    mix a16-[02-03]
largemem     up 7-00:00:00      1   idle a16-04
```

sinfo (continued)

https://slurm.schedmd.com/sinfo.html

- Useful options `–Node`, `--partition`, and `--states`

```
$ sinfo --partition largemem
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
largemem     up 7-00:00:00      2    mix a16-[02-03]
largemem     up 7-00:00:00      1   idle a16-04
```

```
$ sinfo -lNp largemem
Thu Sep 16 08:12:37 2021
NODELIST   NODES PARTITION       STATE CPUS    S:C:T MEMORY TMP_DISK WEIGHT AVAIL_FE REASON
a16-02         1  largemem       mixed 40     4:10:1 103160        0      1 xeon-485 none
a16-03         1  largemem       mixed 40     4:10:1 103160        0      1 xeon-485 none
a16-04         1  largemem        idle 40     4:10:1 103160        0      1 xeon-485 none
```

- Formatting is manageable through `–format`
- `SINFO_FORMAT` environment variable can be used (`export SINFO_FORMAT="…"`)
- sinfo2 is an alias to `sinfo -o "%60N %10P %8t %8D %10X %10Y %10m %25G %b "`

Codes for common node states

https://slurm.schedmd.com/sinfo.html

- **ALLOCATED –** the node has been allocated to one or more jobs
- **DOWN –** the node is unavailable for use
- **DRAINING –** the node is currently executing a job, but will not be allocated additional jobs
- **IDLE –** the node is available for use
- **MAINT –** the node is currently in a reservation with a flag value of “maintenance”
- **MIXED –** the node has some of its CPUs ALLOCATED while others are IDLE
- **RESERVED –** the node is in advanced reservation and not generally available

sinfo (continued)

https://slurm.schedmd.com/sinfo.html

- Use `--states=idle` to help in choosing a partition for your job to run

```
$ sinfo --states=idle
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug        up    1:00:00      7   idle a02-26,e05-[42,76,78,80],e09-18,e23-02
epyc-64      up 2-00:00:00      0    n/a
main*        up 2-00:00:00     48   idle d11-[11,16,18,20,27,41],d17-[11-12,18,31-38],d18-[02-04,06-07,09-11,14-15],e07-
[06-07,10-12],e13-[30-31,33,35-37],e16-[08-12,16-17],e17-[02,04,06]
gpu          up 2-00:00:00     10   resv e17-[10-19]
gpu          up 2-00:00:00     46   idle d13-[03,08,10-11],d14-[05-06,11-18],d23-15,e21-[01-16],e22-[03-16],e23-01
oneweek      up 7-00:00:00     45   idle e01-[46,48,52,60,62,64,76],e02-[40-44,46,48-71,73-80]
largemem     up 7-00:00:00      1   idle a16-04
```

What partition should I use?

https://carc.usc.edu/user-information/user-guides/hpc-basics/discovery-resources

- **debug –** small, short or test jobs; short queue
- **main** (default) – most jobs (serial and small-to-medium), can utilize older K40 gpus
- **epyc-64 –** medium-to-large parallel jobs
- **gpu –** jobs that require GPUs (P100, V100, A100, A40)
- **largemem –** jobs requiring lots of memory (up to 1TB)
- **oneweek –** long-running jobs

What partition should I use? (limits)

https://carc.usc.edu/user-information/user-guides/hpc-basics/discovery-resources

Queue (or partition)	Maximum run time	Maximum concurrent CPUs	Maximum concurrent GPUs	Maximum concurrent memory	Maximum concurrent jobs running	Maximum number of jobs queued
main	48 hours	1,200	36	---	500	5,000
epyc-64	48 hours	1,200	N/A	---	500	5,000
gpu	48 hours	400	36	---	36	100
oneweek	168 hours	208	N/A	---	50	50
largemem	168 hours	120	N/A	1000GB	3	10
debug	1 hour	48	4	---	5	5

sbatch

https://slurm.schedmd.com/sbatch.html

- Submit a job script for remote execution
- Use `module purge` to clear automatically loaded modules
- Use `--mem=0` to request all available memory on a node
- Pack short-running jobs together as job steps
- By default, output log files are named slurm-<jobid>.out and saved to the submit directory with both standard output and standard error messages
- Use `--output` and/or `--error` options to customize them
- Formatting options can be used (e.g., %x = job name -> %x.out)

sbatch (continued)

Option	Default value	Description
--nodes=<number>	1	Number of nodes to use
--ntasks=<number>	1	Number of processes to use
--cpus-per-taks=<number>	1	Number of cores per task
--mem=<number>	2GB	Total memory (single node)
--mem-per-cpu=<number>	2GB	Memory per processor core
--constraint=<attribute>		Node property to request (e.g., xeon-2640v4)
--partition=<partition_name>	main	Request nodes on specified partition
--time=<D-HH:MM:SS>	1:00:00	Maximum run time
--account=<account_id>	Default project account	Account to charge resources to
--mail-type=<value>		Email notifications type; can be: begin, end, fail, all
--mail-user=<address>		Email address
--output=<filename>		File for standard output redirection
--error=<filename>		File for standard error redirection

Create and submit a simple job script

- Use a text editor to create a file sample_job.sh that contains as follows:

```
#!/bin/bash
#SBATCH --nodes 1
#SBATCH --ntasks 1
#SBATCH --partition debug
#SBATCH --time=00:05:00
#SBATCH --chdir /home1/ttrojan/slurm-workshop-2022
#SBATCH --account=<account_id>
module purge
module load gcc/9.2.0
echo "Example start"
echo `date`
sleep 30
echo "Example end"
```

- Then submit it

```
$ sbatch sample_job.sh
Submitted batch job 154837
```

sbatch (continued)

Variable	Description
SLURM_JOB_ID	The ID of the job allocation
SLURM_JOB_NODELIST	List of nodfes allocated to the job
SLURM_JOB_NUM_NODES	Total number of nodes in the job's resource allocation
SLURM_NTASKS	Number of tasks requested
SLURM_CPUS_PER_TASK	Number of CPUs requested per task
SLURM_SUBMIT_DIR	The directory from which sbatch was invoked
SLURM_ARRAY_TASK_ID	Job array ID (index) number

Variables example for a job script

- Use a text editor to create a file sample_var_job.sh that contains as follows:

```
#!/bin/bash
#SBATCH --nodes 1
#SBATCH --ntasks 1
#SBATCH --partition debug
#SBATCH --time=00:05:00
#SBATCH --chdir /home1/ttrojan/slurm-workshop-2022
#SBATCH --account=<account_id>
module purge
module load gcc/9.2.0
echo "Job ID: $SLURM_JOB_ID"
echo "Nodelist: $SLURM_JOB_NODELIST"
cd $SLURM_SUBMIT_DIR
echo `pwd`
```

- Then submit it

```
$ sbatch sample_var_job.sh
Submitted batch job 154837
```

srun

https://slurm.schedmd.com/srun.html

- Launch parallel tasks or job steps for MPI jobs
- More details on using MPI: https://carc.usc.edu/user-information/user-guides/software-and-programming/mpi
- Use `srun --help` for more options

Variables example for a job script

- Use a text editor to create a file sample_mpi_job.sh that contains as follows:

```
#!/bin/bash
#SBATCH --nodes 3
#SBATCH --ntasks 30
#SBATCH --partition main
#SBATCH --time=00:10:00
#SBATCH --chdir /home1/ttrojan/slurm-workshop-2022
#SBATCH --account=<account_id>
#SBATCH --exclusive
module purge
module load gcc/8.3.0
module load openmpi/4.0.2
module load pmix/3.1.3
ulimit -s unlimited
srun --mpi=pmix_2 --ntasks $SLURM_NTASKS ./mpi_app
```

- Then submit it

```
$ sbatch sample_mpi_job.sh
Submitted batch job 154837
```

salloc

https://slurm.schedmd.com/salloc.html

- Allocates resources for an interactive job
- Shares most options with `sbatch`
- Example interactive session with the use of K40 GPUs:

```
[osinski@discovery1 ~]$ salloc --time=2:00:00 --cpus-per-task=8 --gres=gpu:k40:2 --partition=main
salloc: Granted job allocation 5919107
salloc: Waiting for resource configuration
salloc: Nodes e16-03 are ready for job
[osinski@e16-03 ~]$ hostname
e16-03.hpc.usc.edu
[osinski@e16-03 ~]$ nvidia-smi -L
GPU 0: Tesla K40m (UUID: GPU-1f625725-19f5-b4f7-ad27-1901ee9b12f5)
GPU 1: Tesla K40m (UUID: GPU-3ed86dc4-3046-74e0-4983-9b8bd01a0671)
[osinski@e16-03 ~]$ exit
exit
salloc: Relinquishing job allocation 5919108
[osinski@discovery1 ~]$
```

squeue

https://slurm.schedmd.com/squeue.html

- Displays status of jobs and job steps
- `squeue --help`
- All jobs:

```
[osinski@discovery1 ~]$ squeue | head
           4679566      main discover  sunwool  R    2:19:33      8 d23-[13,15-16],e21-14,e22-[08-09,12],e23-01
           4680126      main discover  sunwool  R      39:11      8 d23-[13-16],e22-[05-06,08-09]
           4678655      main job.slur liukuang  R   11:09:20      1 d14-08
           4679445      main  1086-7B   asareh  R    4:18:00      1 d11-46
           4679444      main  1086-7B   asareh  R    4:19:31      1 d05-40
```

- Just your jobs:

```
[ttrojan@discovery1 ~]$ squeue -u ttrojan
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
           3678639   epyc-64   test_1  ttrojan PD       0:00      4 (Resources)
           3678721   epyc-64   test_2  ttrojan PD       0:00      4 (Priority)
           3675759   epyc-64   test_3  ttrojan  R 1-01:48:12      2 b22-[29-30]
```

Codes for common job states

https://slurm.schedmd.com/squeue.html

- **PD PENDING –** Job is awaiting resource allocation
- **R RUNNING –** Job currently has an allocation
- **CD COMPLETED –** Job has terminated on all nodes with an exit code of zero
- **CG COMPLETING –** Job is in the process of completing. Some processes on some nodes may still be active
- **CA CANCELLED –** Job was explicitly cancelled by the user or system administrator. The job may or may not have been initiated

Codes for common pending reason

https://slurm.schedmd.com/squeue.html

- **Resources** – Job is waiting for resources to become available
- **Priority** – One or more higher priority jobs exist for this partition or advanced reservation
- **ReqNodeNotAvail** – Some node specifically required by the job is not currently available
- **QOSMaxCpuPerUserLimit** – The job has reached the maximum CPU per user limit
- **QOSMaxGresPerUser** – The job has reached the maximum GPU per user limit
- **AssocGrpCPUMinutesLimit** – The project account has run out of CPU time
- **InvalidAccount** – the job's account is invalid

squeue (continued)

https://slurm.schedmd.com/squeue.html

- Useful options: `--start` and `--partition`
- Formatting options with `--format` or `--Format`
- Can use environment variable (`export SQUEUE_FORMAT="..."`)
- Create an alias `alias myq="squeue -u $USER"`
- And add it to your .bashrc file

Job priorities

https://slurm.schedmd.com/fair_tree.html

- Based on fairshare algorithm and job age
- Fairshare values depend on a number of factors:
  - Number of jobs submitted
  - Resources used
  - Resources requested
  - project account activity

sprio

https://slurm.schedmd.com/sprio.html

- Display job priority information
- Can be difficult to interpret
- After normalizing, a priority value closer to 1 means a higher priority

```
[osinski@discovery1 ~]$ sprio -j 5918718
          JOBID PARTITION   PRIORITY       SITE        AGE  FAIRSHARE    JOBSIZE  PARTITION        QOS                TRES
        5918718 main            1142          0          5        136          1       1000          0          cpu=0,mem=1
[osinski@discovery1 ~]$ sprio -j 5918718 -n
          JOBID PARTITION PRIORITY   AGE        FAIRSHARE  JOBSIZE    PARTITION  QOS        TRES
        5918718 main      0.00000026 0.0048570  0.0135671  0.0010957  1.0000000  0.0000000  cpu=0.00,mem=0.00
```

scancel

https://slurm.schedmd.com/scancel.html

- Cancel pending or running jobs
- `scancel --help`

```
[ttrojan@discovery1 ~]$ scancel 2918718

[ttrojan@discovery1 ~]$ scancel -u ttrojan
```

sstat

https://slurm.schedmd.com/sstat.html

- Display status information for running jobs
- `sstat --help`

```
[ttrojan@discovery1 ~]$ sstat -j <jobid>

[ttrojan@discovery1 ~]$ sstat -j <jobid> --format=JobID,MaxRSS,AveCPUFreq,MaxDiskRead,MaxDiskWrite
```

sacct

https://slurm.schedmd.com/sacct.html

- Display accounting information for past jobs
- `sacct --help`
- By default only jobs from past day
- Useful options `--starttime`, `--endtime`, --brief, and `--state`

```
[ttrojan@discovery1 ~]$ sacct -j <jobid>

[ttrojan@discovery1 ~]$ sacct -j <jobid> --format=JobID,MaxRSS,AveCPUFreq,MaxDiskRead,MaxDiskWrite,State,ExitCode
```

Job exit codes

https://slurm.schedmd.com/job_exit_code.html

- Exit status, 0-255
- 0 -> success, completed
- Non-zero -> failure
- Codes 1-127 indicate error in job
- Exit codes 129-255 indicate jobs terminated by Unix signals
- `man signal`

seff

- Display job efficiency information for past jobs (CPU and memory use)
- Is used to optimize resource requests
- `sacct --help`
- By default only jobs from past day
- Useful options `--starttime`, `--endtime`, --brief, and `--state`

```
$ seff 5919108
Job ID: 5919108
Cluster: discovery
User/Group: osinski/osinski
State: COMPLETED (exit code 0)
Nodes: 1
Cores per node: 8
CPU Utilized: 00:00:01
CPU Efficiency: 0.13% of 00:12:24 core-walltime
Job Wall-clock time: 00:01:33
Memory Utilized: 2.53 MB
Memory Efficiency: 0.02% of 16.00 GB
```

scontrol

https://slurm.schedmd.com/scontrol.html

- Display or modify slurm configuration and state
- Mostly for admins, some commands for users
- `scontrol --help`
- Examples:

```
scontrol show partition <partition>

scontrol show node <nodeid>

scontrol show job <jobid>

scontrol hold <jobid>

scontrol release <jobid>
```

Job dependencies

- Are allowing to submit at once a set of jobs from a larger pipeline
- Defer the start of a job until the specified dependencies have been satisfied
- Examples:
  - `-d depend=afterok:jobid[:jobid...]`
    Starts after jobid has finished without errors.
  - `-d depend=afternotok:jobid[:jobid...]`
    Starts after jobid has finished with errors.
  - `-d depend=afterok:jobid,before:jobid2`
    Starts after jobid is finished, but not until jobid2 has started.
  - `-d depend:afterok:jobid -d depend:afterok:jobid2`
    Starts after both jobid and jobid2 have finished.
  - `-d depend=afterokarray:jobid`
    Starts after the job array jobid has finished without errors.
  - `-d depend=after:jobid[+time][:jobid[+time]...]`
    Starts after the job array jobid in minutes specified in 'time' or without delay if no 'time' is given
  - `-d depend=afterany:jobid`
    Starts after the job jobid has finished regardless of exit code.

Job dependencies

Example:

- **Step 1:**

```
[ttrojan@discovery1 ~]$ sbatch preprocessing-step.sh
Submitted batch job 18866
```

- **Step 2:**

```
[ttrojan@discovery1 ~]$ sbatch -d after:18866 job-array-step.sh
Submitted batch job 18870
```

- **Step 3:**

```
[ttrojan@discovery1 ~]$ sbatch -d afterok:18870 postprocessing-step.sh
Submitted batch job 18867
```

Job Arrays

- A way to run the same commands on many (hundreds, thousands) of datasets/samples.
- A variable called `$SLURM_ARRAY_TASK_ID` is used to determine the element of the array being run.
- `#SBATCH --array=1-1000`
- `$SLURM_ARRAY_TASK_ID` becomes 1 in first job, 2 in second job, etc…
- Modify job or application to use index

Without Job Arrays – Numbered Files

```
#!/bin/bash
#SBATCH --nodes 1
#SBATCH --ntasks 1
#SBATCH --partition main
#SBATCH --time 00:05:00
#SBATCH --chdir /home1/ttrojan/slurm-workshop-2022
#SBATCH --account=<account_id>
module purge
module load gcc/9.2.0
module load fastqc
echo "Starting FastQC job"
fastqc -o results/fastqc-rawseq-ordered raw-seq-ordered/yeast_1_50K.fastq
fastqc -o results/fastqc-rawseq-ordered raw-seq-ordered/yeast_2_50K.fastq
fastqc -o results/fastqc-rawseq-ordered raw-seq-ordered/yeast_3_50K.fastq
fastqc -o results/fastqc-rawseq-ordered raw-seq-ordered/yeast_4_50K.fastq
fastqc -o results/fastqc-rawseq-ordered raw-seq-ordered/yeast_5_50K.fastq
fastqc -o results/fastqc-rawseq-ordered raw-seq-ordered/yeast_6_50K.fastq
echo "Finish FastQC job"
```

Job Arrays – Numbered Files

- Here is an example SLURM script for a job array. Save as `fastqc_numbered_array.job`

```
#!/bin/bash
#SBATCH --nodes 1
#SBATCH --ntasks 1
#SBATCH --partition main
#SBATCH --time 00:05:00
#SBATCH --array=1-6
#SBATCH --chdir /home1/ttrojan/slurm-workshop-sep2021
#SBATCH --account=<account_id>
module purge
module load gcc/9.2.0
module load fastqc
echo "Starting FastQC job“
sleep 20
fastqc -o results/fastqc-rawseq-ordered-arr raw-seq-
ordered/yeast_${SLURM_ARRAY_TASK_ID}_50K.fastq
echo "Finish FastQC job"
```

View Job Array

squeue -u uscnetid

```
[ttrojan@disocvery1 slurm-workshop-2021]$ squeue -u ttrojan
JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
1152 main     bash ttrojan  R    2:17:32      1 d05-40
1153 main     bash ttrojan  R    2:17:12      1 d05-40
1207_1 main numbered ttrojan  R       0:02      1 d05-41
1207_2 main numbered ttrojan  R       0:02      1 d05-40
1207_3 main numbered ttrojan  R       0:02      1 d05-42
1207_4 main numbered ttrojan  R       0:02      1 d05-45
1207_5 main numbered ttrojan  R       0:02      1 d05-44
1207_6 main numbered ttrojan  R       0:02      1 d05-44
```

Job Arrays – Unnumbered Files

- Start by creating a list of all of the unnumbered filenames
- Then create slurm array script for fastqc jobs that have unnumbered filenames

```
#!/bin/bash
#SBATCH --nodes 1
#SBATCH --ntasks 1
#SBATCH --partition main
#SBATCH --time 00:05:00
#SBATCH --array=1-6
#SBATCH --chdir /home1/ttrojan/slurm-workshop-2022
#SBATCH --account=<account_id>
module purge
module load gcc/9.2.0
module load fastqc echo "Starting FastQC job"
sleep 20
ls raw-seq/ > unnumbered-filenames.txt
line=$(sed -n -e "$SLURM_ARRAY_TASK_ID p" unnumbered-filenames.txt)
fastqc -o results/fastqc-rawseq-unordered raw-seq/${line}
echo "Finish FastQC job"
```

Important Things to Note

- Job length
  - If over 24 hours, can this be split up, can threads be increased?
- Many small files
  - To be avoided!
  - Group into larger files
- Data
  - Save space by removing temp files
  - Archive data as soon as reasonable
  - Let us know if you are adding several TB of data
  - Use /scratch or /scratch2 whenever possible for temporary files

Important Things to Note

- Make sure you are not on the login node when you launch an application
  - You can check the system you are on by typing `hostname`
- Make sure you reserve as many processors as you need
  - A mismatch here can increase your runtime or wait time
- Make sure you reserve as much RAM as needed
  - Overestimating increases wait time, underestimating crashes
- Know which resources work the best
  - Sometimes using a debug or epyc-64 is better

Resources

- CARC home page
  - https://carc.usc.edu
- CARC User Forum
  - https://hpc-discourse.usc.edu/categories
- SLURM tutorials
  - https://slurm.schedmd.com/tutorials.html
- SLURM quick reference
  - https://slurm.schedmd.com/pdfs/summary.pdf

Resources

- CARC home page
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Review: Interactive Jobs

- When you need to provide unpredictable input

```
[ttrojan@discovery1 ~]$ hostname
discovery1.usc.edu
[ttrojan@discovery1 ~]$ salloc -p debug
[ttrojan@a02-26 ~]$ hostname
a02-26.hpc.usc.edu
[ttrojan@a02-26 ~]$ exit
exit
[ttrojan@discovery1 ~]$ hostname
discovery1.usc.edu

[ttrojan@discovery1 ~]$
```

Review: Bash Scripts

- Bash scripts are a series of commands that can be grouped together within files to accomplish a series of tasks
- This allows you to run one command instead of several successive commands

Exercise:

- Start an interactive job to the debug queue
- This program sleeps for 10 seconds and then prints out “Hello World”
- Make this file, give it execute permissions, and run

```
#!/bin/bash
# This program: sleeps for 10 seconds, then prints "Hello World"
sleep 10
echo "Hello World"
```

Prepare to Run Jobs

- Copy example data to your home directory

```
[ttrojan@discovery1 ~]$

[ttrojan@discovery1 ~]$ git clone https://github.com/uschpc/slurm-workshop-2022.git

[ttrojan@discovery1 ~]$ cd slurm-workshop-2022

[ttrojan@discovery1 ~]$ ls
```

Example: Create the FastQC Job Script

- Use a text editor to create a file name samplefastqc.sh that contains what follows:

```
#!/bin/bash
#SBATCH --nodes 1
#SBATCH --ntasks 1
#SBATCH --partition debug
#SBATCH --chdir /home1/ttrojan/slurm-workshop-sep2021
#SBATCH --account=<account_id>
module purge
module load gcc/9.2.0
module load fastqc
echo “Example FastQC start”
sleep 20
fastqc -o results/fastqc-rawseq raw-seq/yeast_1_50K.fastq
echo “Example FastQC end”
```

Example: Run the FastQC Job Script

- Submit the job

```
[ttrojan@discovery1 ~]$ sbatch fastqc1.job

Submitted batch job 33723
```

- Check the status of the job

```
[osinski@discovery1 ~]$ squeue –u osinski
JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
33723 debug fastqc.s osinski  R       0:02      1 a02-26
```

Example: Check Output File for Errors

- Check Output File for Errors

```
[ttrojan@discovery1 ~]$ cat slurm-33723.out
Started analysis of yeast_1_50K.fastq
Approx 5% complete for yeast_1_50K.fastq
Approx 10% complete for yeast_1_50K.fastq
Approx 15% complete for yeast_1_50K.fastq
Approx 20% complete for yeast_1_50K.fastq
Approx 25% complete for yeast_1_50K.fastq
Approx 30% complete for yeast_1_50K.fastq
Approx 35% complete for yeast_1_50K.fastq
Approx 40% complete for yeast_1_50K.fastq
Approx 45% complete for yeast_1_50K.fastq
Approx 50% complete for yeast_1_50K.fastq
Approx 55% complete for yeast_1_50K.fastq
Approx 60% complete for yeast_1_50K.fastq
Approx 65% complete for yeast_1_50K.fastq
Approx 70% complete for yeast_1_50K.fastq
Approx 75% complete for yeast_1_50K.fastq
Approx 80% complete for yeast_1_50K.fastq
Approx 85% complete for yeast_1_50K.fastq
Approx 90% complete for yeast_1_50K.fastq
Approx 95% complete for yeast_1_50K.fastq
Approx 100% complete for yeast_1_50K.fastq
Analysis complete for yeast_1_50K.fastq
```

Example: Create the BLAST Job Script

- Replace swissprot with the path to the v5 of swissprot db obtained from https://carc.usc.edu/user-information/bio-resources/genbank

```
#!/bin/bash
#SBATCH --nodes 1
#SBATCH --ntasks 10
#SBATCH --partition debug
#SBATCH --chdir /home1/ttrojan/slurm-workshop-2022
#SBATCH --account=<account_id>
#SBATCH -time 00:05:00
module purge
module load gcc/9.2.0
module load blast-plus
echo "Start BLAST Job"
blastp -db swissprot -query blast/query.txt -out results/blast/results.txt -num_threads
$SLURM_NTASKS
echo "Finish BLAST Job"
```

Example: Run the BLAST Job Script

- Submit the job

```
[ttrojan@discovery1 ~]$ sbatch blast1.job

Submitted batch job 4773117
```

- Check the status of the job

```
[ttrojan@discovery1 ~]$ squeue –u ttrojan
JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
4773117      Main   blast1.j  ttrojan  R       0:02      1 a02-d11
```

Example: Check BLAST Job Stats with sacct

- sacct can get stats for a job after its completed

https://slurm.schedmd.com/sacct.html

```
[ttrojan@discovery1 ~]$ sacct -j 4773117 --format=JobID,State,Elapsed,NCPUS,MaxRSS
```

```
[ttrojan@discovery1 ~]$ sacct -j 4773117 --format=JobID,State,Elapsed,NCPUS,MaxRSS
       JobID      State    Elapsed      NCPUS     MaxRSS
------------ ---------- ---------- ---------- ----------
4773117       COMPLETED   00:00:09         10
4773117.bat+  COMPLETED   00:00:09         10      1228K
4773117.ext+  COMPLETED   00:00:09         10       832K
```

What is Wrong

```
#!/bin/bash
# ----------------SLURM Parameters----------------
#SBATCH --partition main
#SBATCH --ntasks 1
#SBATCH --mem=1g
#SBATCH --nodes 1
#SBATCH --chdir /home1/ttrojan/slurm-workshop-2022
#SBATCH --account=<account_id>
# ----------------Load Modules--------------------
# ----------------Commands------------------------
python3 /home1/ttrojan/script.py
```

What is Wrong

- The module is not loaded

```
#!/bin/bash
# ----------------SLURM Parameters----------------
#SBATCH --partition main
#SBATCH --ntasks 1
#SBATCH --mem=1g
#SBATCH --nodes 1
#SBATCH --chdir /home1/ttrojan/slurm-workshop-2022
#SBATCH --account=<account_id>
# ----------------Load Modules--------------------
module purge
module load gcc/9.2.0
module load python/3.7.6
# ----------------Commands------------------------
python3 /home1/ttrojan/script.py
```

What is Wrong II

```
#!/bin/bash
# ----------------SLURM Parameters----------------
#SBATCH --partition main
#SBATCH --ntasks 20
#SBATCH --mem=10g
#SBATCH --nodes 1
# ----------------Load Modules--------------------
module purge
module load gcc/9.2.0
module load blast-plus
# ----------------Commands------------------------
blastn -query fasta.file -db database_name -outfmt 6 \
-num_alignments 1 -num_descriptions 1 -out output_file
```

What is Wrong II

- Number of processors and no working directory

```
#!/bin/bash
# ----------------SLURM Parameters----------------
#SBATCH --partition main
#SBATCH --ntasks 20
#SBATCH --mem=10g
#SBATCH --nodes 1
#SBATCH --chdir /home1/ttrojan/slurm-workshop-2022
#SBATCH --account=<account_id>
# ----------------Load Modules--------------------
module purge
module load gcc/9.2.0
module load blast-plus
# ----------------Commands------------------------
blastn -query fasta.file -db database_name -outfmt 6 num_alignments 1 \ -num_descriptions 1 -out
output_file -num_threads 20
```

What is Wrong II

- Number of processors and no working directory
- Better to use $SLURM_NTASKS

```
#!/bin/bash
# ----------------SLURM Parameters----------------
#SBATCH --partition main
#SBATCH --ntasks 20
#SBATCH --mem=10g
#SBATCH --nodes 1
#SBATCH --chdir /home1/ttrojan/slurm-workshop-2022
#SBATCH --account=<account_id>
# ----------------Load Modules--------------------
module purge
module load gcc/9.2.0
module load blast-plus
# ----------------Commands------------------------
blastn -query fasta.file -db database_name -outfmt 6 num_alignments 1 \ -num_descriptions 1 -out
output_file -num_threads $SLURM_NTASKS
```

What is Wrong III

```
#!/bin/bash
# ----------------SLURM Parameters----------------
#SBATCH --partition main
#SBATCH --ntasks 1
#SBATCH --mem=200g
#SBATCH --nodes 1
#SBATCH --chdir /home1/ttrojan/slurm-workshop-2022
#SBATCH --account=<account_id>
# ----------------Load Modules--------------------
module purge
module load gcc/8.3.0
module load R
# ----------------Commands------------------------
Rscript /home1/ttrojan/R_example.R
```

What is Wrong III

- Wrong partition/mem requirements too high

```
#!/bin/bash
# ----------------SLURM Parameters----------------
#SBATCH --partition epyc-64
#SBATCH --ntasks 1
#SBATCH --mem=200g
#SBATCH --nodes 1
#SBATCH --chdir /home1/ttrojan/slurm-workshop-2022
#SBATCH --account=<account_id>
# ----------------Load Modules--------------------
module purge
module load gcc/8.3.0
module load R
# ----------------Commands------------------------
Rscript /home1/ttrojan/R_example.R
```

What is Wrong IV

```
#!/bin/bash
# ----------------SLURM Parameters----------------
#SBATCH --partition main
#SBATCH --nodes 1
#SBATCH --mem=4g
#SBATCH --ntasks 1
#SBATCH --chdir /home1/ttrojan/slurm-workshop-2022
# ----------------Load Modules--------------------
module purge
module load gcc/8.3.0
Module load cuda/10.0.130
module load motioncor2
# ----------------Commands------------------------
python /home1/ttrojan/motioncor2.job
```

What is Wrong IV

- GPU resources not specified

```
#!/bin/bash
# ----------------SLURM Parameters----------------
#SBATCH --partition main
#SBATCH --nodes 1
#SBATCH --mem=4g
#SBATCH --ntasks 1
#SBATCH --gres=gpu:p100:1
#SBATCH --chdir /home1/ttrojan/slurm-workshop-2022
#SBATCH --account=<account_id>
# ----------------Load Modules--------------------
module purge
module load gcc/8.3.0
Module load cuda/10.0.130
module load motioncor2
# ----------------Commands------------------------
python /home1/ttrojan/motioncor2.job
```

What is Wrong V

```
# ----------------SLURM Parameters----------------
#SBATCH --partition main
#SBATCH --ntasks 1
#SBATCH --mem=15g
#SBATCH --nodes 1
#SBATCH --chdir /home1/ttrojan/slurm-workshop-2022
#SBATCH --account=<account_id>
# ----------------Load Modules--------------------
module purge
module load gcc/9.2.0
module load samtools
# ----------------Commands-----------------------
samtools stats example.bam
```

What is Wrong V

- No bash shebang line, #!/bin/bash
- Can use long names for SBATCH parameters

```
#!/bin/bash
# ----------------SLURM Parameters----------------
#SBATCH --partition main
#SBATCH --ntasks 1
#SBATCH --mem=15g
#SBATCH --nodes 1
#SBATCH --chdir /home1/ttrojan/slurm-workshop-2022
#SBATCH --account=<account_id>
# ----------------Load Modules--------------------
module purge
module load gcc/9.2.0
module load samtools
# ----------------Commands------------------------
samtools stats example.bam
```

Mapping exercise: Answers

```
#!/bin/bash
#SBATCH --partition main
#SBATCH --nodes 1
#SBATCH --ntasks 20
#SBATCH --time 01:00:00
#SBATCH --chdir /home1/ttrojan/slurm-workshop-2022
#SBATCH --account=<account_id>
#SBATCH --mem 4g
module purge
module load gcc/9.2.0
module load bowtie2
module load samtools
module load bedtools2
mkdir results/read-mapping
cp data/R*.gz results/read-mapping
gunzip results/read-mapping/R1.fastq.gz
gunzip results/read-mapping/R2.fastq.gz
cp -v /project/biodb/genomes/Homo_sapiens/UCSC/hg19/Sequence/Chromosomes/chr21.fa results/read-mapping/
bowtie2-build --threads $SLURM_NTASKS results/read-mapping/chr21.fa results/read-mapping/chr21index
bowtie2 --threads $SLURM_NTASKS -x results/read-mapping/chr21index -q results/read-mapping/R1.fastq > results/read-mapping/R1.sam
bowtie2 --threads $SLURM_NTASKS -x results/read-mapping/chr21index -q results/read-mapping/R2.fastq > results/read-mapping/R2.sam
samtools view results/read-mapping/R1.bam | cut -f 6 | grep -c 'D' > results/read-mapping/R1.no_of_deletions.txt
samtools view results/read-mapping/R1.bam | cut -f 6 | grep -c 'I' > results/read-mapping/R1.no_of_insertions.txt
samtools view results/read-mapping/R2.bam | cut -f 6 | grep -c 'D' > results/read-mapping/R2.no_of_deletions.txt
samtools view results/read-mapping/R2.bam | cut -f 6 | grep -c 'I' > results/read-mapping/R2.no_of_insertions.txt
samtools view -bS results/read-mapping/R1.sam > results/read-mapping/R1.bam
samtools view -bS results/read-mapping/R2.sam > results/read-mapping/R2.bam
samtools sort results/read-mapping/R1.bam > results/read-mapping/R1_sorted.bam
samtools sort results/read-mapping/R2.bam > results/read-mapping/R2_sorted.bam
samtools view -h -b results/read-mapping/R1_sorted.bam "chr21:10000000-20000000" > results/read-mapping/R1_sorted_region.bam
samtools view -h -b results/read-mapping/R2_sorted.bam "chr21:10000000-20000000" > results/read-mapping/R2_sorted_region.bam
bamToBed -i results/read-mapping/R1_sorted_region.bam > results/read-mapping/R1_sorted_region.bed
bamToBed -i results/read-mapping/R2_sorted_region.bam > results/read-mapping/R2_sorted_region.bed
bedtools intersect -a results/read-mapping/R1_sorted_region.bed -b results/read-mapping/R2_sorted_region.bed > results/read-mapping/reads.bed
```