!(intergalactic popular beverage)

SLURM: Workload manager for HPC batch cluster

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Agenda

- To introduce the SLURM scheduler/resource manager batch system replacing the current PBS job scheduler
  - Why the change?
- Key SLURM commands
  - Compare with PBS
- Couple of examples using SLURM

What is SLURM

- **S**imple **L**inux **U**nified **R**esource **M**anager
  - Written in C (half a million-lines of code)
- Linux utility for Resource management for job scheduling and resource management
- Open source utility widely used in other computing centers
  - Research centers, across the globe

Why Enterprise Information Technology is migrating to SLURM?

- Make the new batch system compatible with CIT's Beowulf computing cluster
- Linux distribution OS will change from Ubuntu to CentOS in the next six months
- The proprietary Moab/Torque scheduler/resource manager will be replaced by SLURM during the migration

New System aiming to bring a large performance boost

Information gleaned from Dr. Doug O'Neal's email

- Servers
  - HPE DL360 Gen 14 servers (no hyper-threading)
- System
  - 2 Intel Skylake processors
  - 18 physical cores each running at 2.7GHz.
  - 768GB memory, SSD system disk, and a 960GB SSD scratch disk.
- Few systems
  - 2 Nvidia GTX 1080Ti graphics cards
    - Support image processing and machine learning efforts
- Contact x 5115 for any questions on the new batch

Useful commands

- sinfo: View information & status of SLURM nodes and partitions
  - pbsnodes -a
- sbatch/scancel: Submit/cancel a batch (script) to SLURM
  - qsub/qdel
- sacct: To display accounting data for all jobs
- squeue: To view information about all jobs located in SLURM scheduling queue
  - squeue –u username

https://slurm.schedmd.com/

sinfo: information on nodes & partitions

```
bash-4.2$ sinfo
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
quick        up    4:00:00      7   idle fr-s-hpc-a2-[02-08]
norm*        up 10-00:00:0      6   idle fr-s-hpc-a2-[03-08]
unlimited    up   infinite      2   idle fr-s-hpc-a2-[07-08]
```

- **PARTITION**
  - quick partition contains 7 nodes (for now, each node = 16 cores)
  - normal partition contains 6 nodes
  - unlimited partition contains 2 nodes

- **TIMELIMIT**
  - 4:00:00 means hr:min:sec

Examples

How to submit a job using AMBER as an example

PBS → SLURM

PBS	SLURM	What it means?
qsub <job-file>	sbatch <job-file>	Submit the script to queue
qsub –I	salloc <options>	Request interactive job
showstart	squeue –start	Display estimated start time
qstat <-u username>	squeue <-u username>	Check jobs for username
qstat <queue>	squeue –p <partition>	Display queue/partition information
qstat –f <job-id>	scontrol show job <job-id>	Display detailed job details (WorkDir, .e or .o output file dir location etc.)
qdel <job-id>	scancel <job-id>	Delete <job-id>

```
#PBS -S /bin/csh -N  VINA-1 -r n -c n
#PBS -l pvmem=2gb
#PBS -l walltime=18:10:00
#PBS -l nodes=1:ppn=16
```

```
#!/usr/bin/tcsh
#SBATCH --export=NONE
#SBATCH --partition=norm
#SBATCH --job-name=VINA-1
#SBATCH --output=VINA-1.out
#SBATCH --nodes=1
#SBATCH --ntasks=16
#SBATCH --time=18:10:00
#SBATCH --mem-per-cpu=2gb
```

sinfo

```
bash-4.2$ sinfo
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
quick        up    4:00:00      7   idle fr-s-hpc-a2-[02-08]
norm*        up 10-00:00:0      6   idle fr-s-hpc-a2-[03-08]
unlimited    up   infinite      2   idle fr-s-hpc-a2-[07-08]
```

sbatch

scancel 532

```
[ravichandrans@fr-s-hpc-a2-01 Amber_SLURM]$ sbatch amber16_tutorial_3.batch
Submitted batch job 532
```

squeue

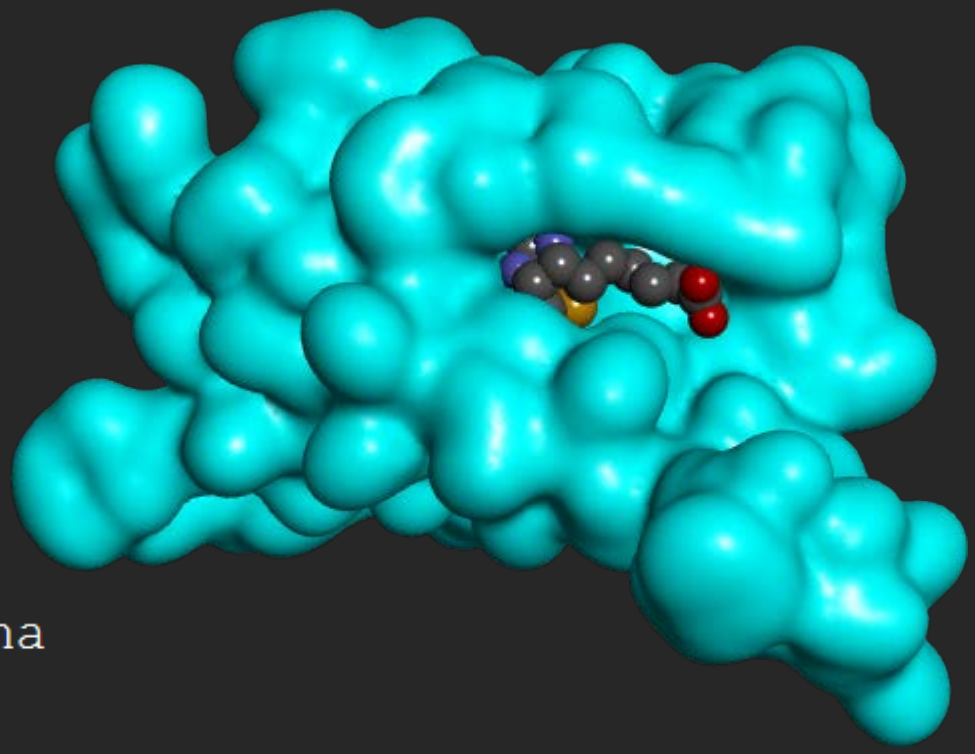
squeue –u ravichandrans

```
[ravichandrans@fr-s-hpc-a2-01 Amber_SLURM]$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
               532      norm AMBER16  ravichan  R       0:50      1 fr-s-hpc-a2-03
```

sacct

```
[ravichandrans@fr-s-hpc-a2-01 ~]$ sacct
       JobID    JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
532          AMBER16 M+       norm                    16    RUNNING      0:0
```

```
[ravichandrans@fr-s-hpc-a2-01 Vina_SLURM]$ cat Vina2018-1.pbs
#!/usr/bin/tcsh
#SBATCH --export=NONE
#SBATCH --partition=norm
#SBATCH --job-name=VINA-1
#SBATCH --output=VINA-1.out
#SBATCH --nodes=1
#SBATCH --ntasks=16
#SBATCH --time=18:10:00
#SBATCH --mem-per-cpu=2gb

setenv VINA autodock_vina_1_1_2_linux_x86/bin/vina

cd /users/priapp/$USER/SLURM/Vina_SLURM
$VINA/vina --config vina_conf.txt
```



```
[ravichandrans@fr-s-hpc-a2-01 Vina_SLURM]$ sbatch VINA.batch
Submitted batch job 534
[ravichandrans@fr-s-hpc-a2-01 Vina_SLURM]$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
               534      norm   VINA-1 ravichan  R       0:08      1 fr-s-hpc-a2-03
```

```
[ravichandrans@fr-s-hpc-a2-01 Vina_SLURM]$ tail VINA-1.out
   2          -6.4       1.455       2.465
   3          -6.3       1.316       2.442
   4          -6.2       1.264       2.253
   5          -5.8       1.192       1.791
   6          -5.5       1.762       3.063
   7          -4.6       2.734       6.611
   8          -4.1       1.185       2.521
   9          -3.8       1.485       2.275
  10          -3.6       1.751       2.158
Writing output ... done.
```

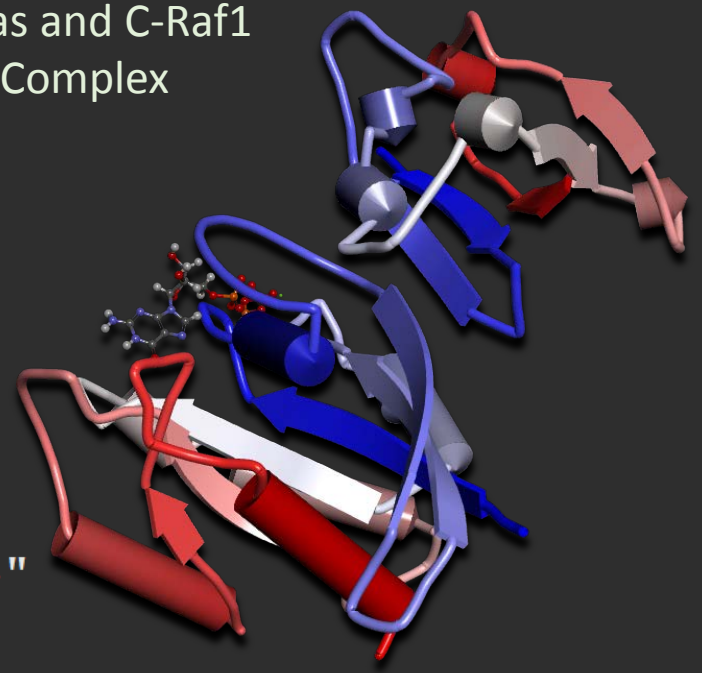
Thanks to Dennis Foley for providing the script

```
#SBATCH --export=NONE
#SBATCH --partition=norm
#SBATCH --job-name=AMBER16_MPI_T3
#SBATCH --output=res_amber16_t3.txt
#SBATCH --nodes=1
#SBATCH --ntasks=16
#SBATCH --time=18:10:00
#SBATCH --mem-per-cpu=10gb

set NODE = "`hostname -s`"
module load amber
set AMBER_TUTORIAL_3_DATA = "$HOME/SLURM/Amber_SLURM/Tutorial_3"
# Please make sure the NCPUS match the "--ntasks" key value
set NCPUS = 16

setenv MYHOME /scratch/cluster_tmp/$USER/Amber16-Test
set P_SANDER  = "$AMBERHOME/bin/sander.MPI"
cp $AMBER_TUTORIAL_3_DATA/* .

mpirun -n $NCPUS ${P_SANDER} -O -i min.in -o min.out -p ras-raf_solvated.prmtop \
       -c ras-raf_solvated.inpcrd -r min.rst -ref ras-raf_solvated.inpcrd

module unload amber
module unload intel_parallel
```

Partition key says where to run

Example: 18 hours and 10 minutes

H-Ras and C-Raf1 Complex



Additional Information

- https://slurm.schedmd.com/

- HPC NIH
  - https://hpc.nih.gov/docs/pbs2slurm.html

Thanks

Ravi & Dennis