O2 for Orchestra Users

HMS Research Computing

Welcome to O2!

- HMS Research Computing's new High-Performance Compute cluster to enhance the compute capacity available to HMS Researchers
- Newer, faster cores with high memory allocation to facilitate multi-core and parallelized workflows
- SLURM scheduler to efficiently dispatch jobs

O2 Tech Specs

- 7000 cores
- 32 or 28 cores per node
- 256/224 GB RAM per node (8GB/core)
- 24 GPUs (8 M40 / 16 K80)
- Login/load balancer 5 VM (8 cores/16GB memory)
- InfiniBand connectivity between nodes available
- CentOS 7

Storage on O2

- Mounts all Orchestra storage
- Isilons: /home, /n/groups, /n/data1, /n/data2
- research.files: transfer partition, /n/files
- Lustre: /n/scratch2

Storage Mount Points

- /home, /n/data1, /n/data2 same
- /groups = /n/groups
- /files= /n/files on transfer partition (ask us)
- /n/scratch2

slurm

- slurm is an open-source scheduler
- Rich, user-contributed community of questions and answers
- Simpler partition structure and management of fairshare (partition, user, group)
- Optimization for MPI and GPU
- Better resource allocation
- Advanced job accounting

Login/transfer

- Login Nodes (5 Virtual Machines)
  $ ssh eCommons@o2.hms.harvard.edu
- With X11:

  $ ssh –XY eCommons@o2.hms.harvard.edu
- Transfer Server (sFTP/port 22, 10 nodes):

  transfer.rc.hms.harvard.edu

Class Practical

- Login to O2 via

```
$ ssh eCommons@o2.hms.harvard.edu
```

- Copy the class files and scripts to your /home

```
$ cp -r /n/groups/rc-training/o2 ~
```

.bashrc

- Orchestra and O2 both source the same ~/.bashrc
- Perl local::lib from Orchestra will not work on O2
- Module files are not synonymous between systems, and module loads will break
- Modify .bashrc as follows:

```
if [[ "$HMS_CLUSTER" = o2 ]]
then
    # O2-specific settings
elif [[ "$HMS_CLUSTER" = orchestra ]]
then
    # Orchestra-specific settings
fi
```

Interactive Job:

- Interactive session: up to 20 cores, 12 hours

```
$ srun --pty -p interactive -t 0-12:00 bash
```

- Can add cores (up to 20)
  `-c`
- Can add total memory (default 1G, max 250G):
  `--mem 8G`

Jobs: bsub -> sbatch

- All in one line: --wrap="command here" #not recommended
- `sbatch –p partition –t 0-1:00 --wrap="command"`

```
$ sbatch –p short –t 0-1:00 --wrap="cp file.txt .."
```

- Complete shell script #recommended
- `$ sbatch completeSlurmJob.run`

```
#!/bin/bash
#SBATCH –p short
#SBATCH –t 0-1:00
 cp file.txt ..
```

Partitions (queues): -q -> -p

Partition	Priority	Max Runtime	Max Cores	Limits
short	16	12 hours	20	
medium	6	5 days	20	
long	4	30 days	20	
interactive	14	12 hours	20	2 job limit
priority	14	30 days	20	2 job limit
mpi	12	5 days	640	20 core min
highmem	12	5 days	28	750G
gpu		72 GPU hours	20cpu	
transfer		5 days	4	

Walltime: -W -> -t

- -t days-hours:minutes
- -t hours:minutes:seconds
- Need to specify how long you estimate your job will run for
- Aim for 125% (over)
- Subject to maximum per partition
- Excessive runlimits (like partition max) take longer to dispatch, and affect fairshare

CPU: -n -> -c

- `-c X` to designate CPU: max 20
- `-N X` to constrain all cores to X nodes
- CPU time: wall time (-t) * (-c) CPUs used
- Unable to use CPU not requested (no overefficient jobs): cgroups constraint

Memory: -Rusage -> --mem

- Only 1G is allocated by default
- `--mem=XG` #total memory over all cores
- `--mem-per-cpu=XG` #total memory per CPU requested, use for MPI
- No unit request (G) defaults to Megabytes
  - 8G ~= 8000

Job Construction

```
#!/bin/bash
#SBATCH -p #partition
#SBATCH -t 0-01:00 #time days-hr:min
#SBATCH -c X #number of cores
#SBATCH -N 1 #confine cores to 1 node, default
#SBATCH --mem=XG #memory per job (all cores), in GB
#SBATCH -o %j.out #out file
#SBATCH -e %j.err #error file
#SBATCH --mail-type=BEGIN/END/FAIL/ALL
#SBATCH --mail-user=mfk8@med.harvard.edu
```

Output/Error Files

- Can add jobid to filename with %j
- Sample:
  `-e %j.err`
  `-o %j.out`
- SLURM by default creates this outfile:
  `slurm-jobid.out`
- Additional Flags
- `%a` #job array id
- `%A` #master array job id
- `%N` #node name
- `%u` #user id

Mail

- Mail is not auto-generated upon completion/failure
- `#SBATCH --mail-type= NONE, BEGIN, END, FAIL, REQUEUE, ALL`
- `#SBATCH --mail-user=mfk8@med.harvard.edu`
- Not recommended, not a verbose output like LSF
- Use sacct instead

Practical: simple sbatch script

- From your `~/o2` directory,

```
$ sbatch submit.slurm
```

```
#!/bin/bash
#SBATCH -p short                    # Partition to submit to
#SBATCH -t 0-00:01                  # Time in minutes
#SBATCH -c 1                        # Number of cores requested
#SBATCH -N 1                        # Ensure that all cores are on one machine
#SBATCH --mem=2G                    # Memory total in GB
#SBATCH -o hostname.%j.out          #  Standard out goes to this file
#SBATCH -e hostname.%j.err          # Standard err goes to this file
srun hostname                       #command
```

Practical: checking result

- From `~/o2` directory:

```
$ less hostname.*.out
```

- This reads the file “hostname.%j.out”
- The host the job ran on is reported as:

`compute-a-16-X.o2.rc.hms.harvard.edu`

Job Master Allocations/Job Steps

- "sbatch" or "salloc" will create a master allocation of shared resources
- To run job steps or multiple commands in parallel with resources from the master allocation, use srun

```
#/bin/bash
#SBATCH -c 8
#SBATCH --mem 32000
srun -c 2 --mem=8000 COMMAND1 &
srun -c 4 --mem=8000 COMMAND2 &
srun -c 1 --mem=4000 COMMAND3 &
srun -c 1 --mem 12000 COMMAND4 &
wait #necessary

# starts 4 independent multicore tasks with
memory constraints
```

Practical: Job Parallelization

- From ~/o2:

```
$ sbatch date_parallel.sh
```

Contents:

```
#SBATCH -c 3
srun -c 1 date &
Srun -c 1 sleep 2m &
srun  -c 2 date &
srun  -c 3 date &
wait
```

- Output file can be read as

```
$ less parallel.*.out
```

Job Arrays

- `sbatch --array=1-30 submit.sh`
- `#SBATCH --array=1-30`
- slurm creates:
- `$SLURM_JOB_ID` #jobid of each job in array %j
- `$SLURM_ARRAY_JOB_ID` #jobid of entire array %A
- `${SLURM_ARRAY_TASK_ID}` #index of job %a

Example:

Files named: File1.txt File2.txt File3.txt ...File30.txt

Execution is:
myscript.sh File${SLURM_ARRAY_TASKID}.txt

Practical: Job Array

- From ~/o2

```
$ sbatch --array=1-4 fastqc_job_array.sh
```

- Relevant file pieces:

```
#SBATCH –o fastqc_%A_%a.out

module load fastqc/0.11.5

fastqc sample_”{SLURM_ARRAY_TASK_ID}” _R1.fastq
```

- Creates fastqc report for reach fastq file
- Creates output progress file named `fastqc_ArrayId_ArrayIndex.out`

Job Dependencies

- sbatch --dependency=
- after:jobid #(asynchronous)
- afterany:jobid #after exit or done
- afterok:jobid #success, exit code 0
- afternotok:jobid #failure
- singleton #after jobs with same name have terminated
- --kill-on-invalid-dep=<yes|no> #kill on unmet dependency (on by default)

Command Line Arguments

- slurm scripts can take command line arguments after them, unlike bsub
- Reference as $1, $2 etc
- sbatch submit.run 25 output.txt

```
#!/bin/bash
#SBATCH –p short
#SBATCH –t 0-1:00
python myscript.py $1 $2
```

X11 on O2

- To visualize or initiate plot devices, an X11 device must be active
- Mac: Xquartz installed and running
- Windows: Xming installed and running
- Login: ssh –XY
- SSH keys:

Host login.rc.hms.harvard.edu

ForwardX11 yes

ForwardX11Trusted yes

- To sbatch jobs add: --x11=batch
- To interactives, srun add: --x11

Fairshare -> Priority

- Dynamically assigned
- Factors contributing:
- Age, Fairshare, Partition, QOS, Nice
- Fairshare: 0-1 scale

Job Dispatch Order in O2

Sum of

- AGE = how long a job has been pending
- FAIRSHARE = fairshare of the user
- PARTITION = priority of the partition used
- QOS = quality of services, normally not used
- NICE = additional custom priority, normally not used

Notes:

- Jobs submitted to the partitions *interactive* and *priority* are evaluated before jobs in any other partitions, independently of the priority values.
- A lower priority job can be dispatched before an higher priority job if it does not impact the expect start time of the higher priority job *(job backfilling)*

Job Monitoring

- `$ squeue –u eCommons –t RUNNING/ PENDING`
- `$ squeue –u eCommons –p partition`
- `$ squeue –u eCommons --start`
- Detailed job info:
  `$ scontrol show jobid <jobid>`
- Completed job statistics:
  `$ sacct -j <jobid> --format=JobID,JobName,MaxRSS,Elapsed`

Job information: sacct

- Advanced job accounting options
- `$ sacct -j jobid`

Options:

`--name`

`-r/--partition`

`-s/--state`

`-o/--format`

- `$ sacct –u eCommons`
- `$ sacct --helpformat` #get available accounting features

sacct: basic information

- `sacct --helpformat` displays fields
- RC Recommends:

```
sacct –u eCommons --
format=jobid,Partition,state%22,MaxRSS,MaxVMSize,ReqTRES%20,Star
t%20,End%20,Timelimit%14,exitcode --units=G
```

- Gives jobid, partition, end state, Max Memory, Max Virtual Memory, Requested Cores/Mem, Start, Stop, Timelimit, Exit Code in GB format

sacct: state

- BF BOOT_FAIL
- CA CANCELLED
- CD COMPLETED
- CF CONFIGURING
- CG COMPLETING
- DL DEADLINE
- F FAILED
- NF NODE_FAIL
- PD PENDING
- PR PREEMPTED
- R RUNNING
- RS RESIZING
- S SUSPENDED
- TO TIMEOUT

Cancelling/Pausing Jobs

- `$ scancel <jobid>`
- `$ scancel -t PENDING`
- `$ scancel --name JOBNAME`
- `$ scancel jobid_[indices]` #array indices
- `$ scontrol hold <jobid>` #pause
- `$ scontrol release <jobid>` #resume
- `$ scontrol requeue <jobid>` #cancel and rerun

MPI on O2

- Message Passing Interface
- Distribute work over multiple nodes, allowing for the utilization of more cores
- openMPI-2.0.1 compiled against GCC 6.2.0
- MATLAB, Python, R, Perl, Java, C++, Fortran implementations
- Needs wrapper function “mpirun” to dispatch to compute nodes with SLURM
- Run in “mpi” partition –p mpi after being added to partition
- Core cap: 640 processors, 5 day runtime

LMOD: Software Modules

- LMOD system adds directory paths of software into $PATH variable, and resolves software dependencies and conflicts
- Most software compiled against gcc-6.2.0: load first
- `$ module load gcc/6.2.0` #note, no directories anymore
- `$ module spider` #software currently available
- `$ module load software/version` #load software, no directories
- `$ module unload software/version` #unload
- `$ module purge` #dump all modules
- `$ module help` <software> #displays run info

Programming langages

- Python: load module (2.7.12, conda2, 3.6.0)
  - use virtualenv to maintain packages (pip/easy install)
- R: load module (3.2.5, 3.3.3, 3.4.1)
  - Setup O2-specific personal R library, .Renviron (install.packages/biocLite)
- Perl: load module (5.24.0)
  - Setup O2-specific local::lib (cpan/cpanm) in .bashrc
- MATLAB: load module (2016b, 2017a)
  - Setup cluster profile, only use on 1 HPC at a time

For more direction

- http://hmsrc.me/O2docs
- http://rc.hms.harvard.edu
- RC Office Hours: Wed 1-3p Gordon Hall 500
- rchelp@hms.harvard.edu