Agave User Environment

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MAE 598/ APM 525

August 29, 2018

ASU Knowledge Enterprise Development

ARIZONA STATE UNIVERSITY

Outline

- Get an account
- System information
- Initial login
- Transferring files
- Modules
- Compiling
- Batch System
- Job Monitoring
- Interactive mode
- Good citizenship

Anti-outline

- Shell scripting
- Installing software
- Debugging (parallel or otherwise)

For any assistance with these – please contact us at any time:

support@hpchelp.asu.edu

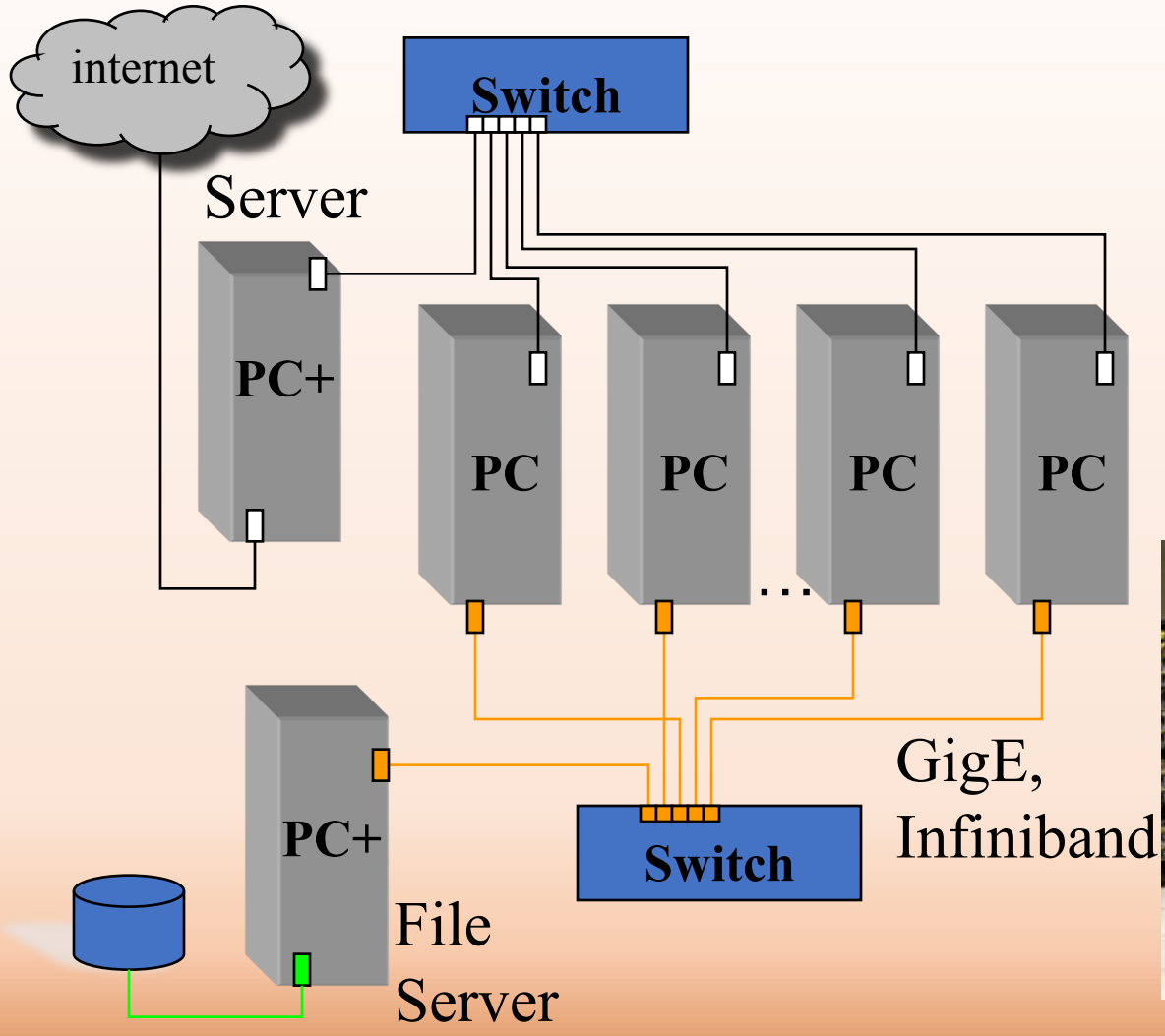
Office hours: GWC546 1-4pm Tues, Wed (during academic year)

Get an account

- researchcomputing.asu.edu - "Create an account"
- Faculty and students get 25K hours every month. Students link to faculty (PI) account
- For assistance installing/using software on the cluster: support@hpchelp.asu.edu
- Login via ssh, putty (Windows).

```
ssh userid@agave.asu.edu
```

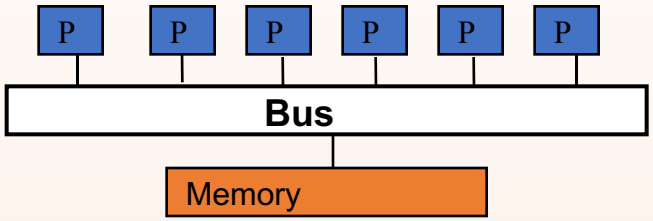
Generic Cluster Architecture

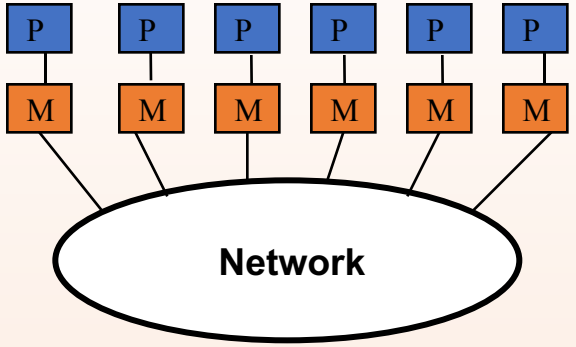


(Adv. HPC System)

lonestar.tacc.utexas.edu

Shared and Distributed Memory





Shared memory (SMP): single address space. All processors have access to a pool of shared memory. Agave normal and phi nodes have 28 and 64 cores per node, respectively.

Methods of memory access :
- Bus
- Crossbar

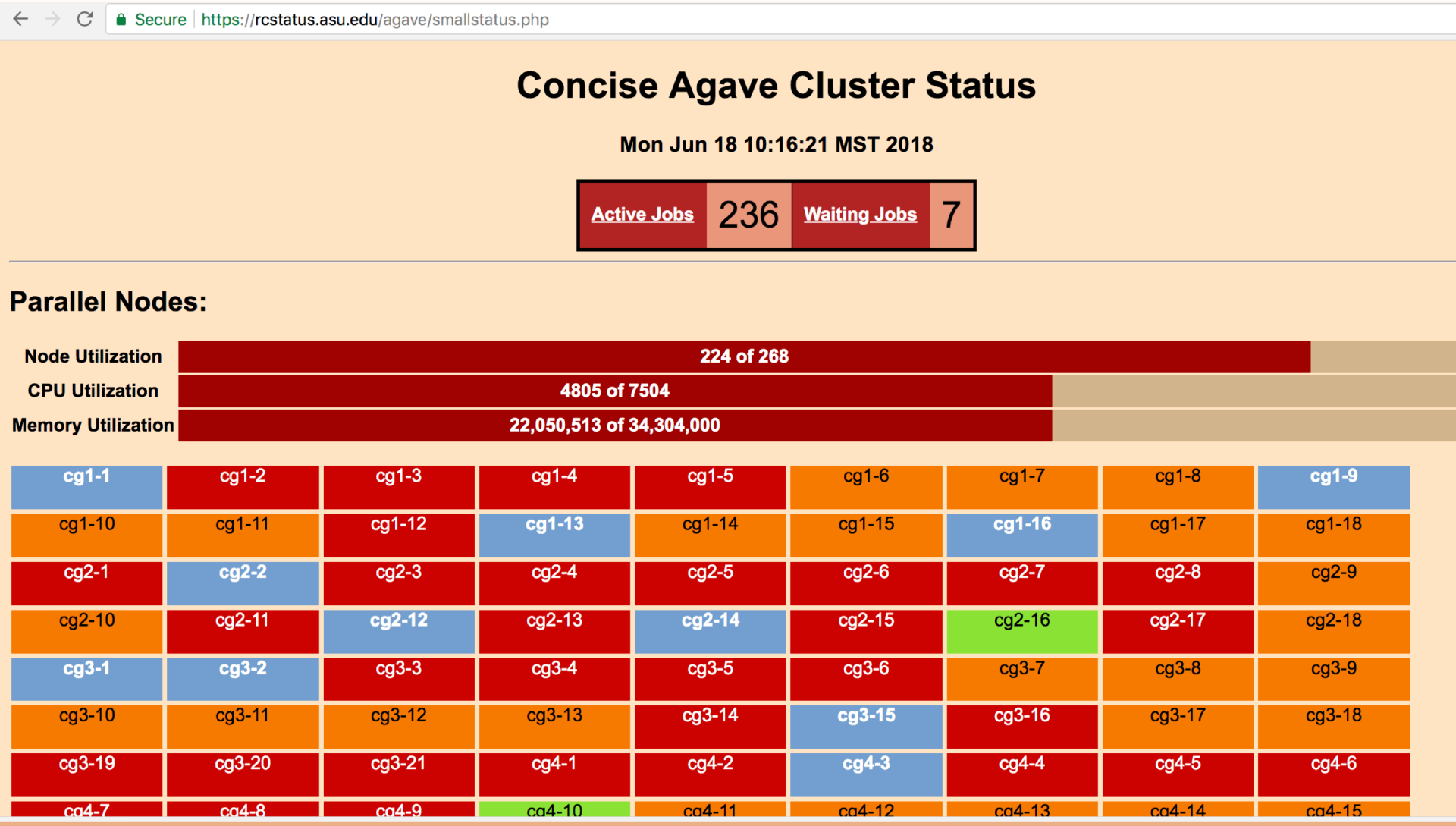
API: OpenMP

Distributed memory (MPP): each Processor has its own local memory. Must do message passing to exchange data between processors. (examples: Clusters)

Methods of memory access :
- various topological interconnects

API: Message Passing Interface (MPI)

Graphical View of Agave



Agave system Information

- **Agave ~7.5K Broadwell cores**
  - **>300 trillion floating point operations per second (TFLOPs)**
  - **>34TB aggregate RAM**
  - **>6PB aggregate disk**
  - **Omnipath Interconnect – 100Gb/s**
  - **Located in ISTB1**
- **~5K Xeon Phi cores**
- **GPU partition(s)**
- **Agave is a true *cluster* architecture**
  - **Each Broadwell node has 28 processors and 128GB of RAM (~4.5GB/CPU).**
  - **Programs needing more resources *must* use parallel programming**
  - **Normal, single processor applications *do not go faster* on Agave**

Initial Login

- Login with SSH
  `ssh agave.asu.edu`
- Connects you to a login node
- Don't overwrite ~/.ssh/authorized_keys
  - Feel free to add to it if you know how to use it:
    - `ssh-keygen`
    - `ssh-copy-id -i ~/.ssh/id_rsa.pub userid@agave.asu.edu`
  - SSH is used for job start up on the compute nodes. Mistakes can prevent your jobs from running
- For X forwarding, use `ssh -X`
- Nomachine: rcstatus.asu.edu/agave/howto
  - Click on "Logging in to Agave cluster with NoMachine Remote Desktop"
  - Get nomachine client and nomachine profile
- Xming
- **From outside ASU campus, use VPN**: download from sslvpn.asu.edu

Transferring files

- Secure copy

```
scp projectfile
 user1@agave.asu.edu:/home/user1/projectdir
scp –r projectdir
 user1@agave.asu.edu:/home/user1/projectdir
```

- **`rsync -e ssh`** for large file transfers
- **`rsync –avtr bigfiledir user1@agave.asu.edu:/home/user1/projectdir`**
- Winscp
- ftp: Filezilla

Packages

- Modules are used to setup your PATH and other environment variables
- They are used to setup environments for packages & compilers

```
[user1@agave1 ~]$ module          {lists options}
[user1@agave1 ~]$ module avail    {lists available packages}
[user1@agave1 ~]$ module load <package> <…> {add one or more packages}
[user1@agave1 ~]$ module unload <package> {unload a package}

[user1@agave1 ~]$ module list     {lists loaded packages}

[user1@agave1 ~]$ module purge    {unloads all packages}
```

- Multiple compiler families available, so make sure you are consistent between libraries, source and run script!

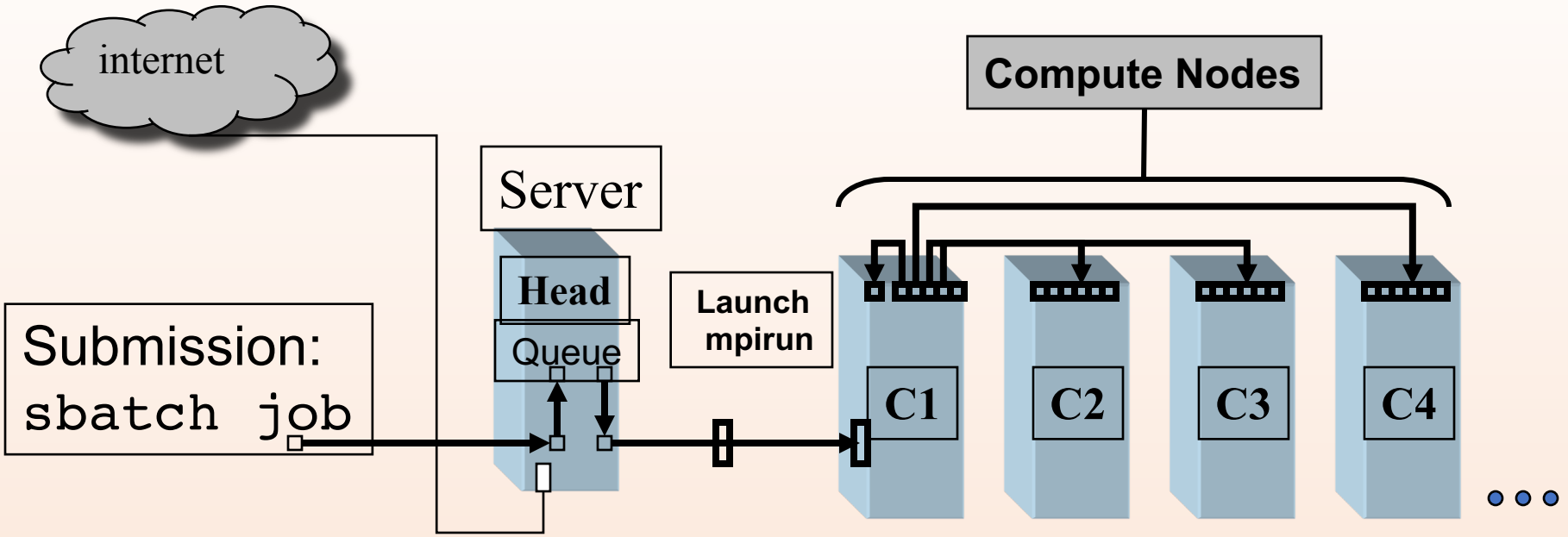
Compile

- After linking (via `module` command)
- Different compilers unfortunately means different flags

```
[user1@agave1 ~]$ module load intel/2018x
[user1@agave1 ~]$ icc -qopenmp -o program program.c

[user1@agave1 ~]$ module purge
[user1@agave1 ~]$ module load gcc/8x
[user1@agave1 ~]$ gcc -fopenmp -o program program.c
[user1@agave1 ~]$ gfortran -fopenmp -o program
program.f
[user1@agave1 ~]$ export OMP_NUM_THREADS=28
```

- Multiple compiler families available, so make sure you are consistent between libraries, source and run script!

Batch Submission Process



Queue: Job script waits for resources on Server
Compute nodes execute the job script, launching MPI processes

Launch: contact each compute node to start executable (e.g. a.out)

Batch Systems

- *Agave* systems use slurm for batch queuing and scheduling
- Batch jobs are submitted on the front end and are subsequently executed on compute nodes as resources become available
- Order of job execution depends on a variety of parameters:
  - Submission Time
  - Resources requested
  - Backfill Opportunities: small jobs may be back-filled while waiting for bigger jobs to complete
  - Advanced Reservations: jobs my be blocked in order to accommodate advanced reservations (for example, during maintenance windows)
  - Number of Actively Scheduled Jobs: there are limits on the maximum number of concurrent processors used by each user

SLURM Commands

sbatch, srun, salloc	Submit a job
squeue	Check on the status of jobs
sinfo	Get info on nodes/partitions
scancel	Delete running and queued jobs
scontrol	Alter/hold/release jobs

man pages for all of these commands

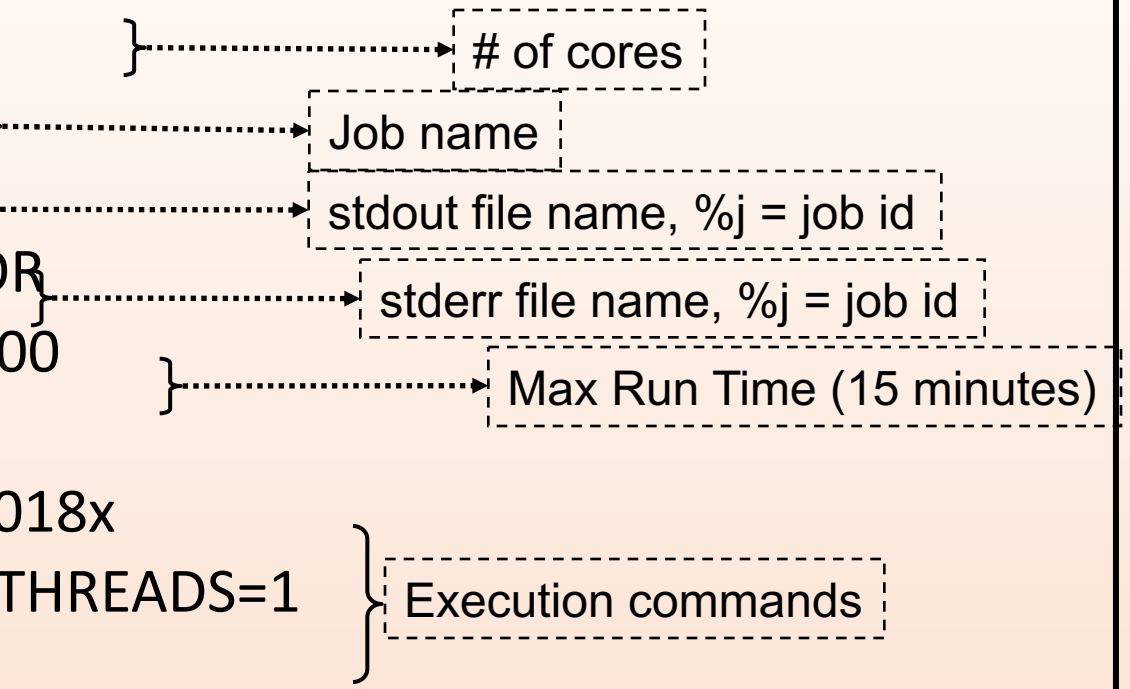
showjobs	Running jobs with queue info
longjob <jobid>	Details on job

Batch System Concerns

- Submission (* need to know)
  - Required Resources*
  - Estimated runtime*
  - Run-time Environment
  - Directory of Submission/Execution
  - Files for stdout/stderr Return
  - Email Notification
- Job Monitoring
- Job Deletion
  - Queued Jobs
  - Running Jobs

SLURM: OpenMP “job” Script

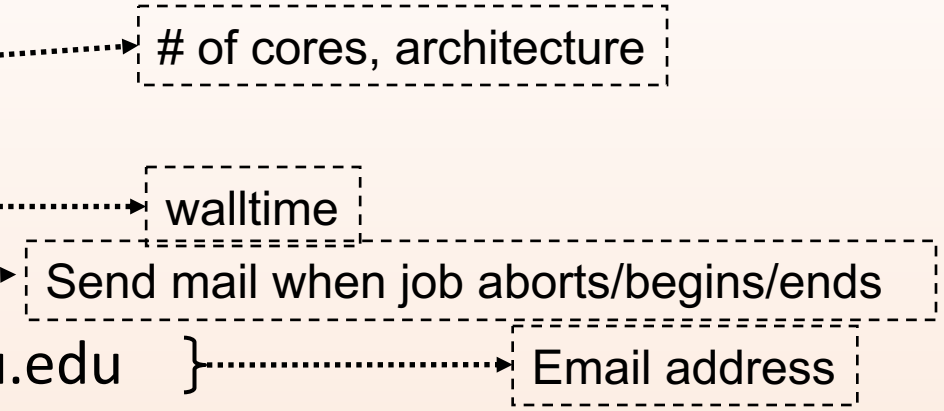
```
#!/bin/bash
#SBATCH -n 1
#SBATCH -J hello
#SBATCH -o %j.OUT
#SBATCH -e %j.ERROR
#SBATCH -t 0-00:15:00

module load intel/2018x
export OMP_NUM_THREADS=1
./hello
```




```
[user1@agave1 ~]$ sbatch job
```

SLURM: OpenMP Job Script II

```
#!/bin/bash
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=28
#SBATCH --time=96:00:00
#SBATCH --mail-type=ALL
#SBATCH --mail-user=user1@asu.edu

module load openmpi/3.0.0-gnu-7x
export OMP_NUM_THREADS=28
export OMP_DYNAMIC=TRUE
time srun –mpi=pmi2 lmp_g++_openmpi –in in.eam –v x 2
```



Batch Script Debugging Suggestions

- Echo issuing commands
  - (“set -x” or “set echo” for bash or csh).
- Abort job when a critical command fails.
- Print environment
  - Include the "env" command if your batch job doesn't execute the same as in an interactive execution.
- Use “./” prefix for executing commands in the current directory
  - The dot means to look for commands in the present working directory. Not all systems include "." in your $PATH variable. (usage: ./a.out).
- Track your CPU time

Normal and wildfire queues

- The mybalance command:

```
[user1@agave1 ~]$ mybalance

User                    : user1
CPU Hours Allocated     : 25000
CPU Hours Used          : 526.36
CPU Hours Available     : 24473.63
```

- If the resource request for your submitted job (#CPUs X walltime requested) fits within your available CPU hours, the job is **non-preemptable**, i.e. will run uninterrupted in the **normal** queue.
- If your resource request exceeds the available CPU hours, the job is **preemptable**, and will run in the **wildfire** queue.
- Limit of 50 running jobs per user

SLURM partitions and environment

- Serial and parallel partitions
  - No need to specify – automatically determined based on requested resources
- `#SBATCH -p phi`
- `#SBATCH -p physicsgpu1 # Use physicsgpu1 partition`
- `#SBATCH -p cidsegpu1 # Use cidsegpu1 partition`

```
#SBATCH -q wildfire # Run job in wildfire QOS queue
#SBATCH --gres=gpu:2
```

Variable	Purpose
SLURM_JOB_ID	Batch job id
SLURM_SUBMIT_DIR	Directory where job was submitted
SLURM_JOB_NODELIST	Filename containing list of nodes
SLURM_ARRAY_TASK_ID	Slurm array index (next slide)

SLURM arrays and small jobs

- Arrays can loop to submit many jobs: `--array`
- `sbatch --array=0-20 job`

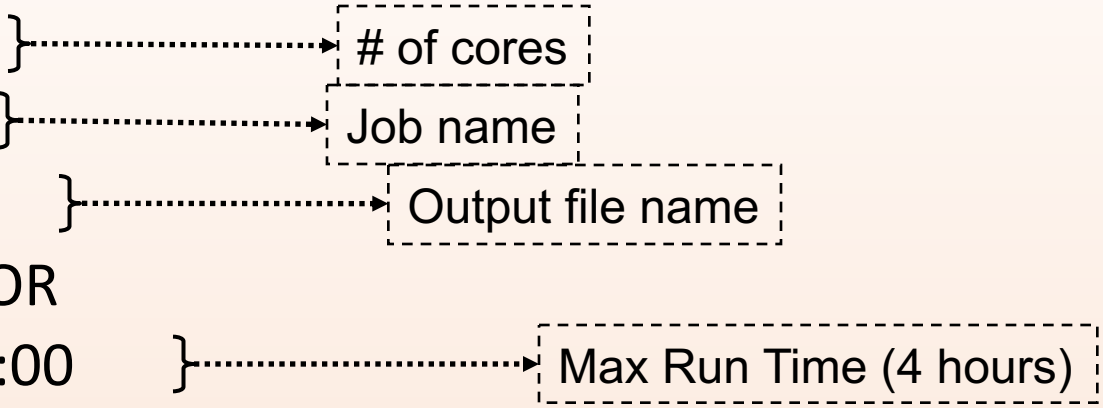
```
(in job) ./executable.x < $SLURM_ARRAY_TASK_ID.inp
 or ./executable2.x $SLURM_ARRAY_TASK_ID
```

- For single line short jobs: `--wrap`

```
sbatch -n 2 --wrap="module load gcc/7x;gcc -fopenmp
hello_world.c;export OMP_NUM_THREADS=2;./a.out"
```

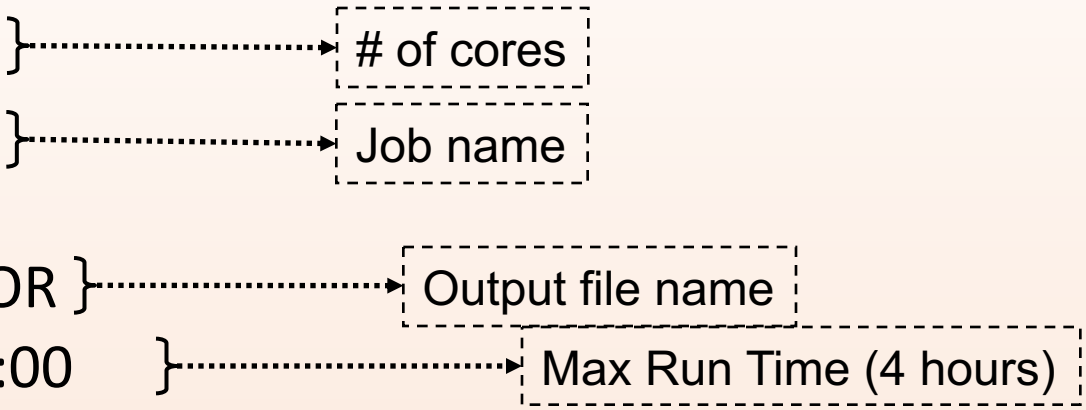
Matlab Job Script

```
#!/bin/bash
#SBATCH -n 1
#SBATCH -J hello
#SBATCH -o %j.OUT
#SBATCH -e %j.ERROR
#SBATCH -t 0-04:00:00

module load matlab/R2018a
matlab –nodisplay –nodesktop –nosplash < hello.m
matlab –nodisplay –nodesktop –nosplash –r “hello, quit”
```



R Job Script

```
#!/bin/bash
#SBATCH -n 1
#SBATCH -J hello
#SBATCH -o %j.OUT
#SBATCH -e %j.ERROR
#SBATCH -t 0-04:00:00

module load r/3.5.1
R --no-save --quiet --slave < regression.r
Rscript regression.r 20000
```



Job Monitoring (*squeue* utility)

```
[user1@agave1 ~]$ squeue
      JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
   208952_[0-199]    serial   COLD_3   mrline PD       0:00      1 (BeginTime)
          207709    serial R-px-OSa epopplet PD       0:00      1 (AssocMaxJobsLimit)
          207710    serial R-px-OSa epopplet PD       0:00      1 (AssocMaxJobsLimit)
          207711    serial R-px-OSa epopplet PD       0:00      1 (AssocMaxJobsLimit)
          207712    serial R-px-OSa epopplet PD       0:00      1 (AssocMaxJobsLimit)
          207713    serial R-px-OSa epopplet PD       0:00      1 (AssocMaxJobsLimit)
        .
        .
        .
```

Basic *squeue* options:

-u username Display jobs belonging to specified user

-l, --long Display extended job information

SLURM Job Manipulation/Monitoring

- To kill a running or queued job (takes ~30 seconds to complete):

```
scancel <jobID>
```

- To suspend a queued job:

```
scontrol hold job <jobId>
```

- To resume a suspended job:

```
scontrol release job <jobID>
```

- To alter job information in queue:

```
scontrol update job <jobID> NumNodes=6-6
NumCPUs=6 NumTasks=6
```

- To see more information on the partitions and their status:

```
sinfo
```

- To see a detailed info on job:

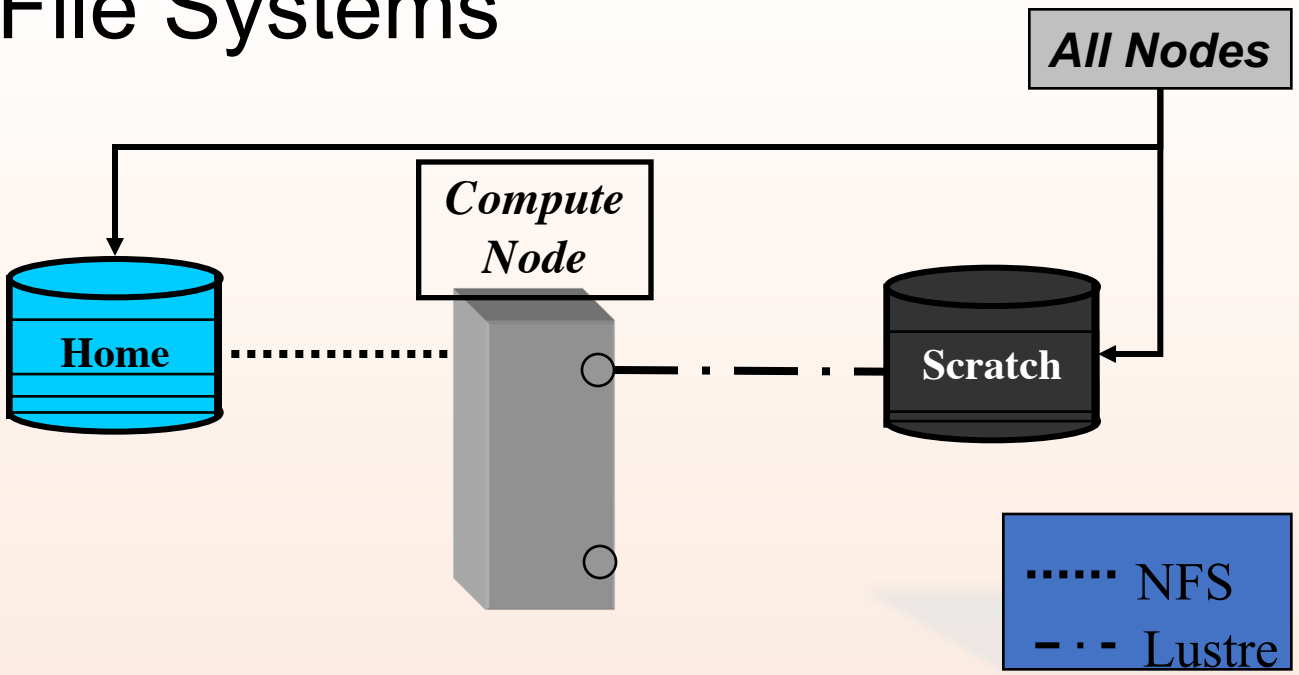
```
scontrol show job <jobID>
Scontrol show partition
```

Interactive Mode

- **`interactive`** Interactive mode
- **`interactive -p phi`** Interactive on Xeon phi
- **`screen`** Detach "`^ad`" interactive jobs.
  Reattach with **`screen -r`**. (Also **`tmux`**)
  1. **`screen`** (on login node)
  2. **`interactive`**

- **`interactive -N 1 -n 28`** Entire Broadwell node

Available File Systems



Mount point	User Access Limit	Lifetime
/home	500GB quota	Project
/scratch	no quota	30 days

Good citizenship

- Shared login node: Do not compute on the login nodes
- Shared filesystem: Run I/O intensive jobs on scratch
- Shared network: Do not start 20 scps
- Shared compute resource: Give good estimate of runtime. Test submission scripts before submitting them at large scale.
- Shared help desk: Do some homework before submitting ticket. Do not submit multiple tickets on same topic. Describe issue in detail (e.g. job ID, full path to failing sbatch script, etc.). Be patient.

Conclusion

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Info at: researchcomputing.asu.edu and rcstatus.asu.edu/agave