GW COLONIAL ONE

CCAS and SEAS Computing Facility

THE GEORGE
WASHINGTON
UNIVERSITY

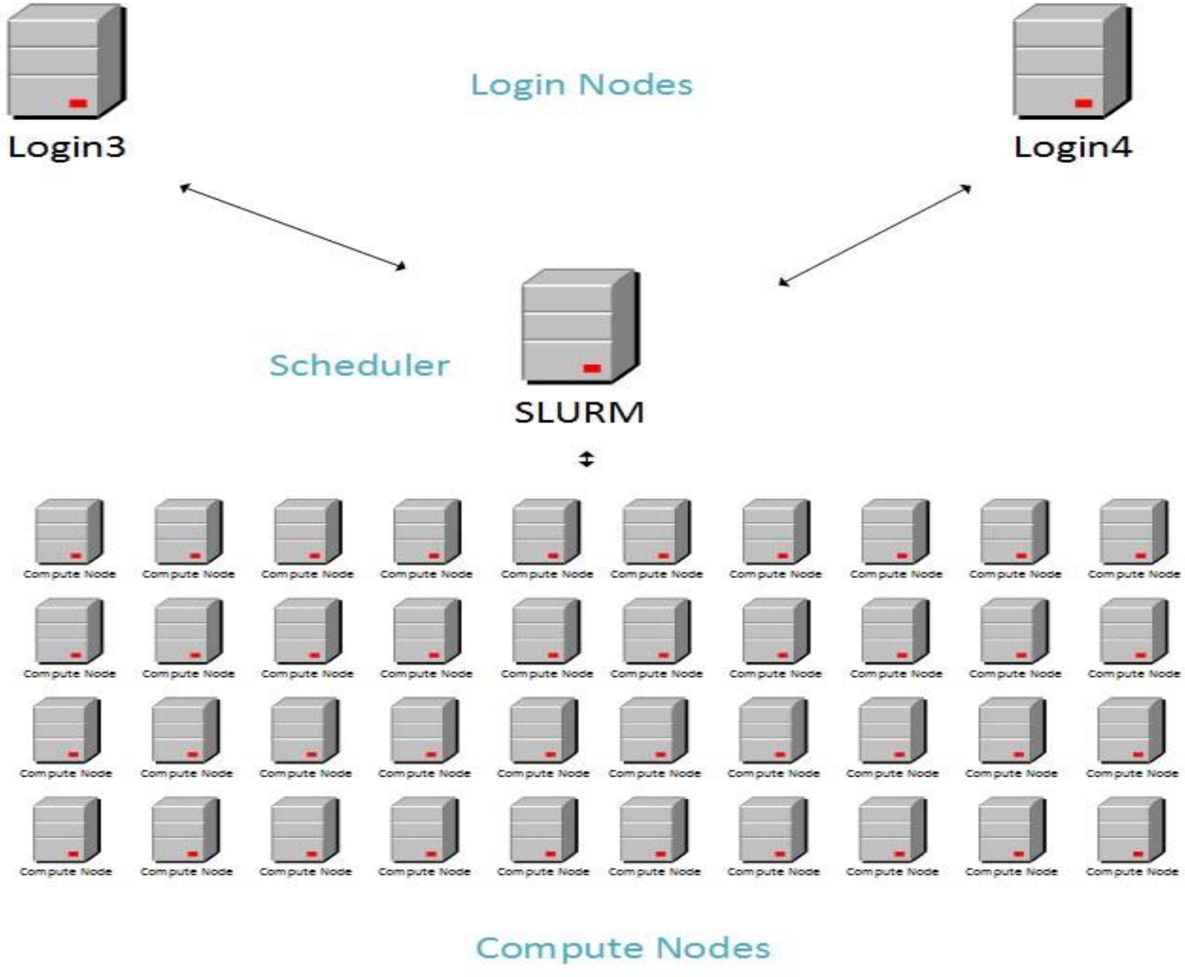
WASHINGTON, DC

HPC Workshop 2

What we're covering:

- Review Cluster Architecture
- Working with SLURM
- Simple job submission script
- How to submit job script
- sinfo, salloc, squeue, scancel, sbatch, srun
- Tips for scripting submit files
- Reporting Job Errors

Cluster Architecture



Login3

Login Nodes

Login4

Scheduler

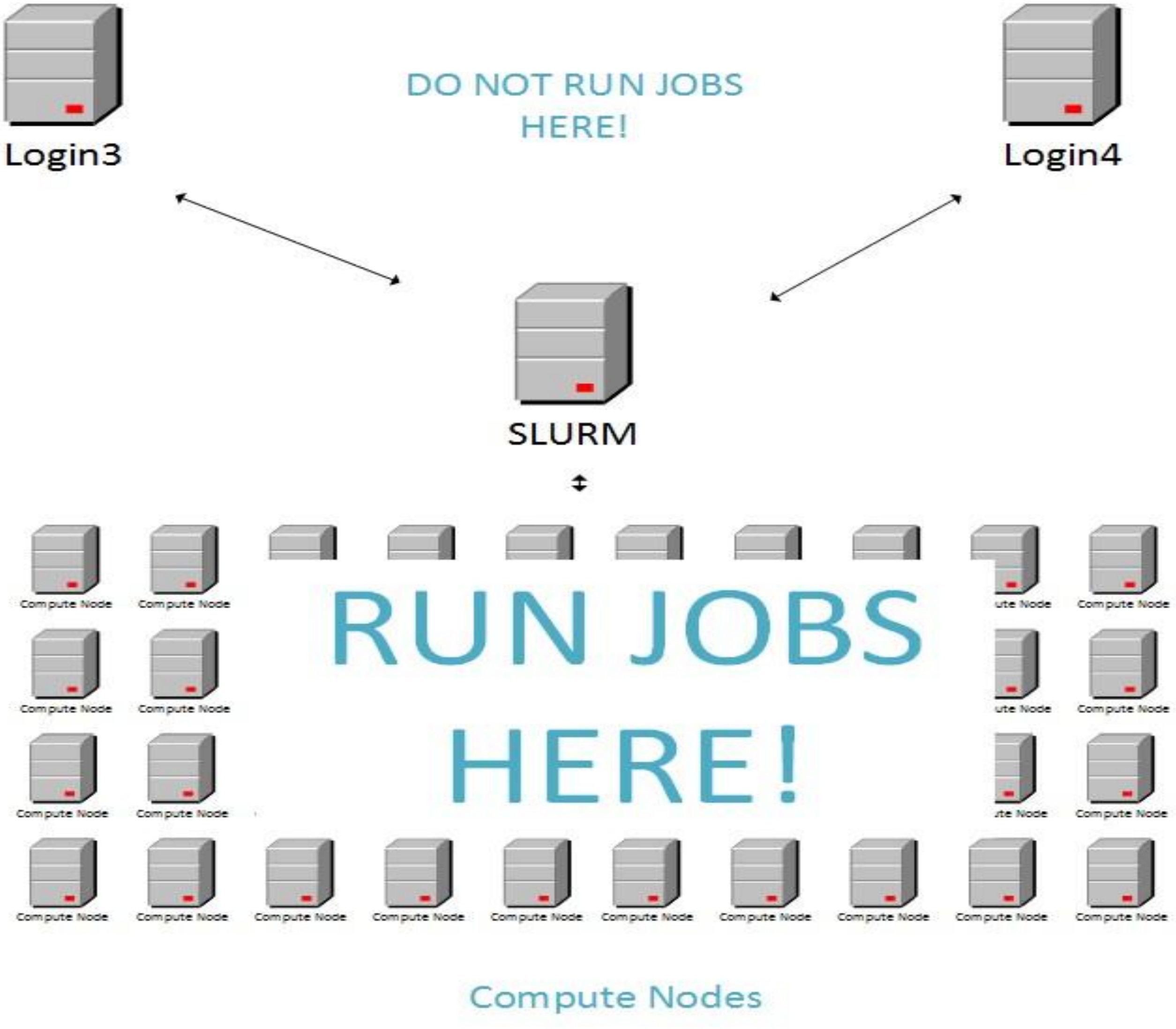
SLURM

Compute Nodes

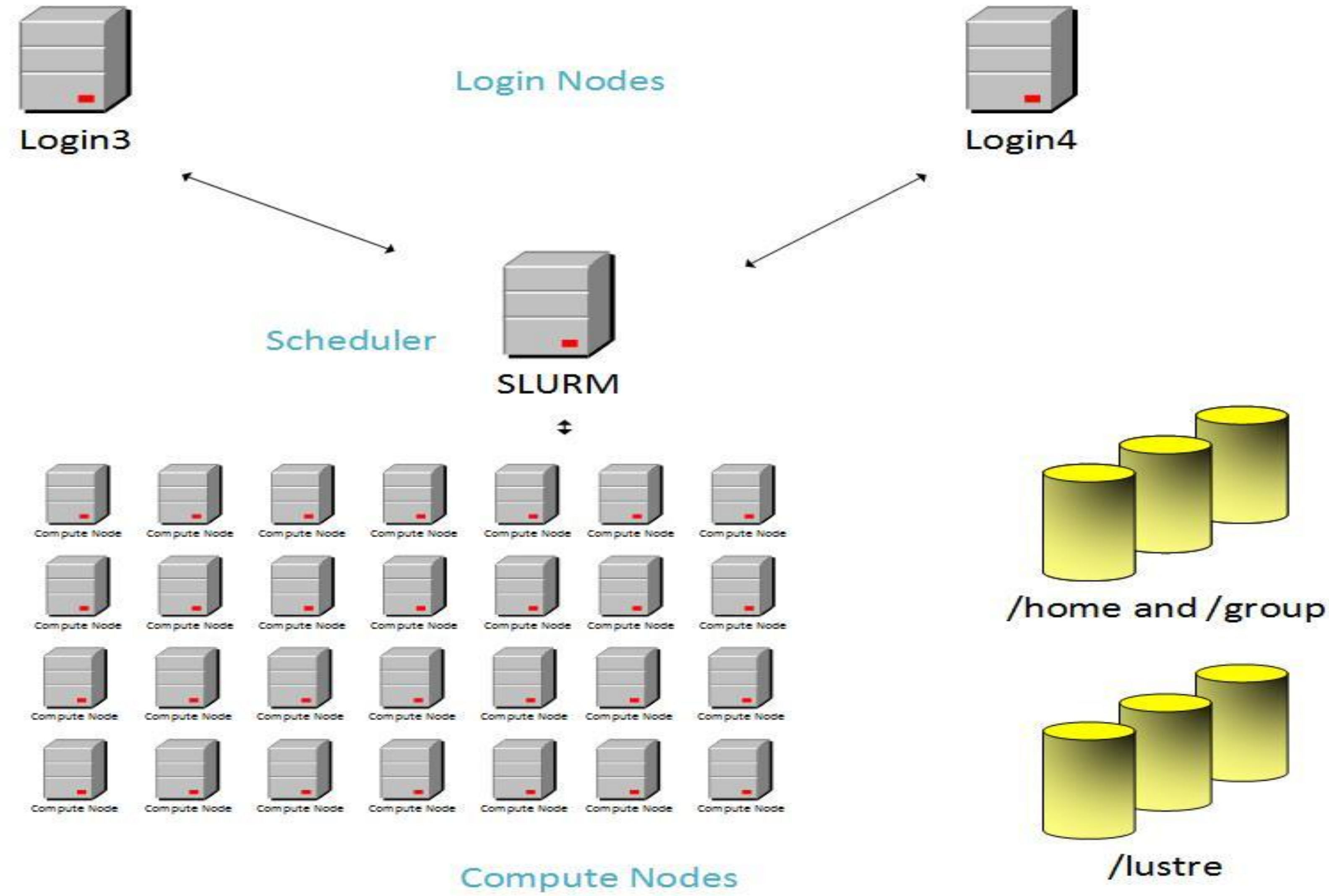
Cluster Architecture

- Login Node - Server that acts as your interface to the cluster
- Scheduler - Server that schedules jobs
- Compute Nodes - Servers that run jobs

Cluster Architecture



Cluster Architecture (Storage)



Login Nodes

Login3

Login4

Scheduler

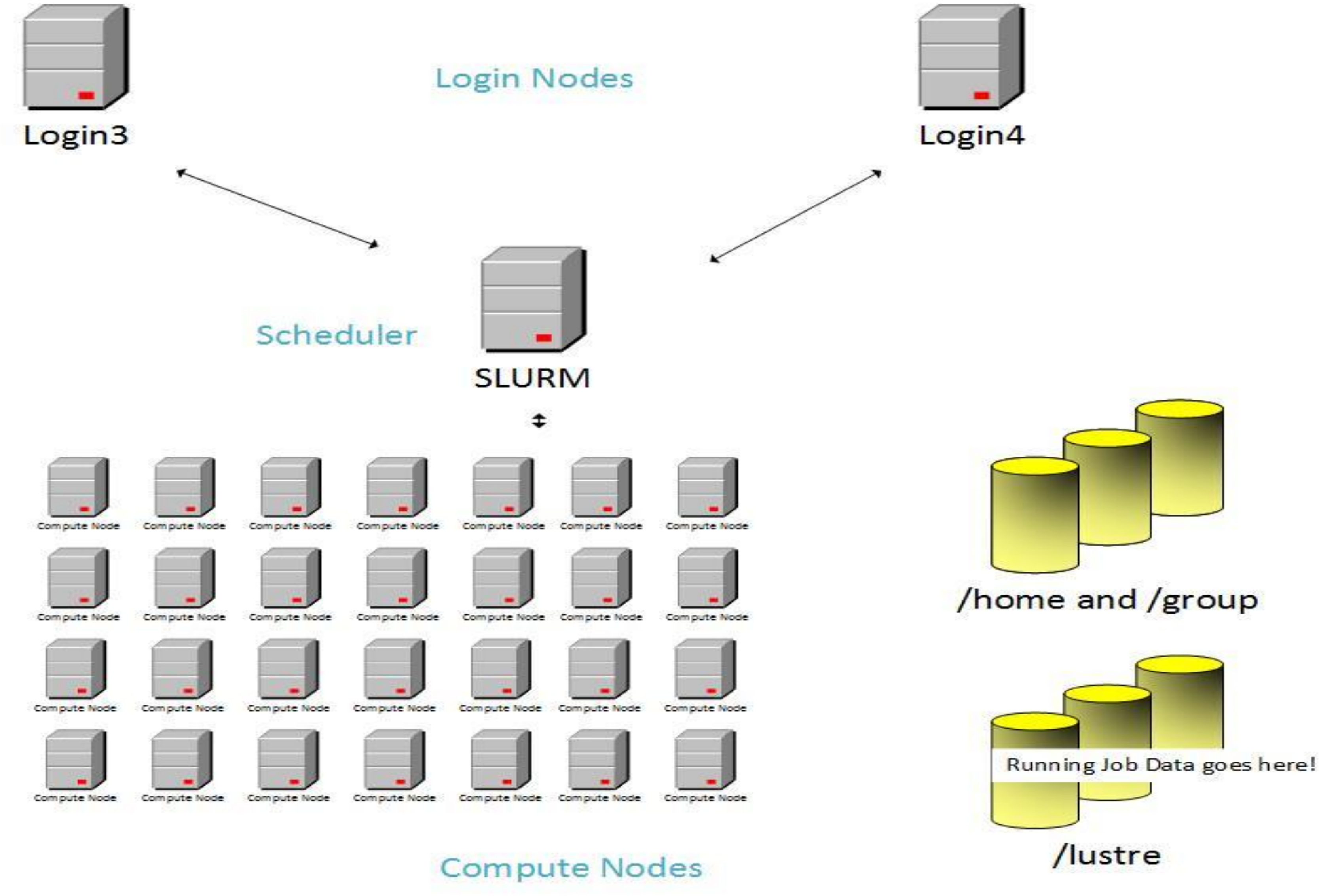
SLURM

Compute Nodes

/home and /group

/lustre

Cluster Architecture (Storage)



Login3

Login Nodes

Login4

Scheduler

SLURM

/home and /group

Running Job Data goes here!

/lustre

Compute Nodes

Working with SLURM

Overview: Slurm is an open source, fault-tolerant, and highly scalable cluster management and job scheduling system for large and small Linux clusters.

- Slurm requires no kernel modifications for its operation and is relatively self-contained. As a cluster workload manager, Slurm has three key functions:
    - First, it allocates exclusive access to resources (compute nodes) for users for some duration of time so they can perform work.
    - Second, it provides a framework for starting, executing, and monitoring work (normally a parallel job) on the set of allocated nodes.
    - Finally, it arbitrates contention for resources by managing a queue of pending work.

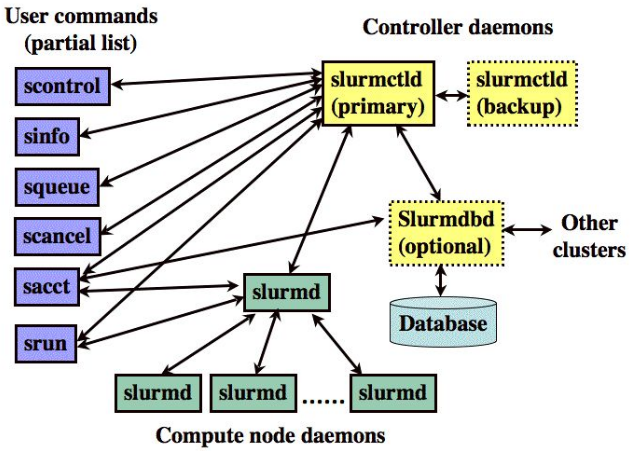
Working with SLURM

Why use SLURM?

- SLURM allows jobs to be scheduled so a user does not have to wait until a node is free to begin work. SLURM does the waiting for you!
- SLURM allows resources to be prioritized for groups that purchase shares on Colonial One.
- SLURM enables efficient use of the cluster since it constantly monitors resources in use and schedules jobs on unallocated resources as they free up
- SLURM runs a job based on a submit script.
- A submit script calls your job script to execute your calculations.

Architecture I

As depicted in Figure 1, Slurm consists of a **slurmd** daemon running on each compute node and a central **slurmctld** daemon running on a management node (with optional fail-over twin). The **slurmd** daemons provide fault-tolerant hierarchical communications. The user commands include: **sacct**, **salloc**, **sattach**, **sbatch**, **sbcast**, **scancel**, **scontrol**, **sinfo**, **smap**, **squeue**, and **srun**. All of the commands can run anywhere in the cluster.



Architecture II

The entities managed by these Slurm daemons, shown in Figure 2, include **nodes**, the compute resource in Slurm, **partitions**, which group nodes into logical (possibly overlapping) sets, **jobs**, or allocations of resources assigned to a user for a specified amount of time, and **job steps**, which are sets of (possibly parallel) tasks within a job. The partitions can be considered job queues, each of which has an assortment of constraints such as job size limit, job time limit, users permitted to use it, etc. Priority-ordered jobs are allocated nodes within a partition until the resources (nodes, processors, memory, etc.) within that partition are exhausted. Once a job is assigned a set of nodes, the user is able to initiate parallel work in the form of job steps in any configuration within the allocation. For instance, a single job step may be started that utilizes all nodes allocated to the job, or several job steps may independently use a portion of the allocation.

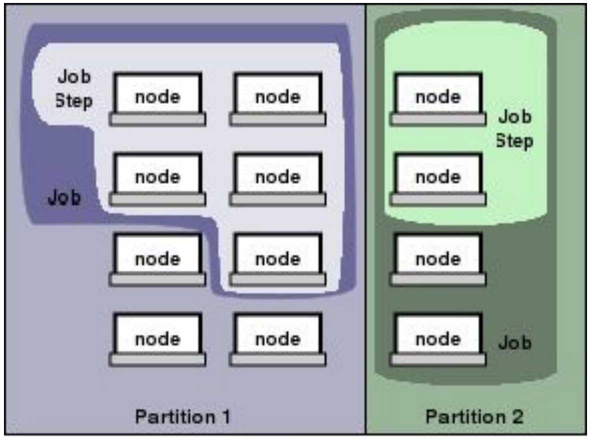


Figure 2. Slurm entities

Software, Modules & Login

- Common software is available to all users via the “module” system
- Can I install my own software?
    - Yes, provided it runs from your home/group directory
    - Users cannot use a package manager (yum) to install software
    - Colonial One users do not have root on Colonial One

Login to Colonial One using your GW NetID/email address & password

```
$ ssh <netid>@login.colonialone.gwu.edu
```

SLURM Commands

sinfo

- lists node and partition information for the cluster
- useful for finding unallocated nodes

Example: type "sinfo" at the prompt

```
PARTITION    AVAIL  TIMELIMIT  NODES  STATE NODELIST
defq*           up 14-00:00:0    128  alloc node[033-160]
short           up 2-00:00:00     95  alloc node[097-191]
128gb           up 14-00:00:0     24  alloc node[041-064]
256gb           up 14-00:00:0      8  alloc node[033-040]
2tb             up 14-00:00:0      1  alloc node901
gpu             up 7-00:00:00     22  alloc node[003-020,029-032]
gpu             up 7-00:00:00     10   idle node[001-002,021-028] ← Free nodes!
gpu-noecc       up 7-00:00:00     22  alloc node[003-020,029-032]
gpu-noecc       up 7-00:00:00     10   idle node[001-002,021-028] ← Free nodes!
ivygpu          up 7-00:00:00     21   idle node[333-353] ← Free nodes!
ivygpu-noecc    up 7-00:00:00     21   idle node[333-353]   ← Free nodes!
allgpu-noecc    up 7-00:00:00     22  alloc node[003-020,029-032]
allgpu-noecc    up 7-00:00:00     31   idle node[001-002,021-028,333-353] ← Free
nodes!
debug           up    4:00:00      2  alloc node[991-992]
debug-cpu       up    4:00:00      1  alloc node992
debug-gpu       up    4:00:00      1  alloc node991
```

SLURM Commands

salloc - Obtain a Slurm job allocation (a set of nodes), execute a command, and then release the allocation when the command is finished. You can use salloc to run interactive jobs:

```
salloc -N 1 -p ivygpu -t 5
```

srun - Run a parallel job on cluster managed by Slurm. Use srun to identify your allocated nodes after running salloc:

```
srun hostname #or
squeue -u <netid>
ssh nodename
```

SLURM Commands

squeue - view information about jobs located in the Slurm scheduling queue.

List jobs for your user account:

```
squeue -u <username>
```

Estimate when a job will start:

```
squeue -u username --start
```

List by job status:

```
squeue -u username -t RUNNING or PENDING
```

SLURM job status

Check Status of Job by User

```
[user@login4 ~]$ squeue -u <username>
    JOBID     PARTITION  NAME            USER ST        TIME  NODES NODELIST(REASON)
    2325403   defq       job_OpenMP.sh   user PD     0:00   1      (Resources)
```

Jobs typically pass through several states in the course of their execution. The typical states are PENDING, RUNNING, SUSPENDED, COMPLETING, and COMPLETED. An explanation of each state follows.

CA = CANCELLED

CD = COMPLETED

CG = COMPLETING

F = FAILED

NF = NODE_FAIL

PD = PENDING

R = RUNNING

S = SUSPENDED

TO = TIMEOUT

SLURM Commands

sbatch - Submit a batch script to Slurm

```
    sbatch <sumbit_script.sh>
```

scancel - used to signal or cancel jobs, job arrays or job steps.

```
    scancel <jobid>
```

sinfo - view information about Slurm nodes and partitions.

SLURM COMMANDS (cont.)

- salloc - Obtain a Slurm job allocation (a set of nodes), execute a command, and then release the allocation when the command is finished.
- squeue - view information about jobs located in the Slurm scheduling queue.
- scancel - Used to signal jobs or job steps that are under the control of Slurm.
- sbatch - Submit a batch script to Slurm.
- srun - Run parallel jobs

hello-mpi.py

This small Python program will list an mpi process number and the node it is running on. Copy the text into a document called "hello-mpi.py" and save it.

```
#hello.py
from mpi4py import MPI
import socket

comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = MPI.COMM_WORLD.Get_size()
thishost = socket.gethostname()

print "hello world from process ", rank, " of ",size, "
on ", thishost   < ------ THIS IS ALL ONE LINE
```

How to submit job script I

Load the current MPI module so we can run our program correctly:

```
module load openmpi/1.8/gcc/4.9.2/cpu
module load python/2.7.6
```

Check your home directory to make sure your compiled program is there:

```
ls -la hello*
```

How to submit job script I

Create a SLURM script using an editor such as vi or emacs using steps 1 through 3. The script (or file) can be called anything you want but should end in .sh (i.e. submit.sh).

Step 1: Resource Specification

```
[user@login4 ~]$ nano submit.sh

#!/bin/sh
#SBATCH --time 5:00
#SBATCH -o testing%j.out
#SBATCH -e testing%j.err
#SBATCH -p defq -N 1
#SBATCH --mail-user=<username>@gwu.edu
#SBATCH --mail-type=ALL
module load openmpi/1.8/gcc/4.9.2/cpu
module load python/2.7.6
mpirun -n 8 python /home/<username>/hello.py
```

Step 2: Submit job

```
module load slurm
[user@login4 ~]$ sbatch submit.sh
Submitted batch job 2325403
```

How to submit job script I

SLURM will email you when you job has finished. Once the job is finished, SLURM will place a .out file and a .err file (if there are errors) in the directory with your submit script.

```
$> ls slurm*
slurm-2333627.out  slurm-2333631.out  slurm-2333633.out
slurm-2333629.out  slurm-2333632.out  slurm-2333636.out
```

The .out file is the result of your job. `Cat` or `less` the file to show you the results.

```
$> cat slurm-2333636.out
Process 1 on node991.cm.cluster out of 8
Process 3 on node991.cm.cluster out of 8
Process 7 on node991.cm.cluster out of 8
Process 5 on node991.cm.cluster out of 8
Process 4 on node991.cm.cluster out of 8
Process 6 on node991.cm.cluster out of 8
Process 0 on node991.cm.cluster out of 8
Process 2 on node991.cm.cluster out of 8
```

Reporting Job Errors

- Email to hpchelp@gwu.edu
- Include .err file
- Include submit script
- Include what modules you loaded