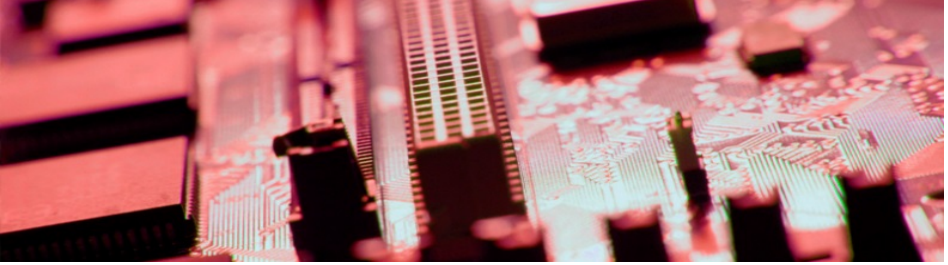

LCI workshop
on high performance clustered computing

Linux Clusters Institute: Scheduling

David King, Sr. HPC Engineer
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University of Illinois

NCSA

About me

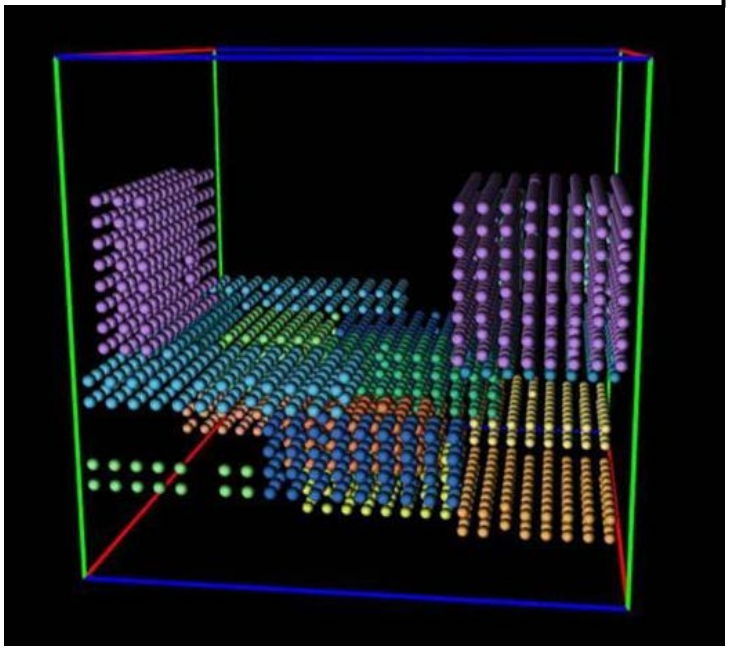
- Worked in HPC since 2007
- Started at Purdue as a Student
  - Initially fixing nodes
  - Moved on to bigger projects
- Sysadmin at Idaho National Laboratory for a year
- Sr. HPC Engineer at Northwestern University for 5 years
  - Scheduling with Moab and Torque
  - Condo Cluster of 1000 nodes
- Sr. HPC Engineer at NCSA for about a year
  - Scheduling on Blue Waters
  - 27k node system using Torque/Moab

Scheduling Schedule

- Introduction
- Workload Management Overview
  - What is the goal?
- Review of Fundamentals of Workload Managers
    - Queues
    - Priority
    - FIFO
    - Fairshare
    - QOS
    - Reservations
- Feature Set Survey
  - PBS Pro
  - Torque
  - Moab/Maui
  - LSF
  - Other Open Source Tools
- Cloud and Scheduling
- Break
- Slurm Deep Dive
  - Components
  - Interface
- Limiting Resources
  - Overview
  - Cgroups
  - Processor affinity
  - Containers
- Cloud and Scheduling
- Accounting
  - Xdmod
  - Gold/Mam
  - Slurm
- Lunch
- Slurm Hands-on

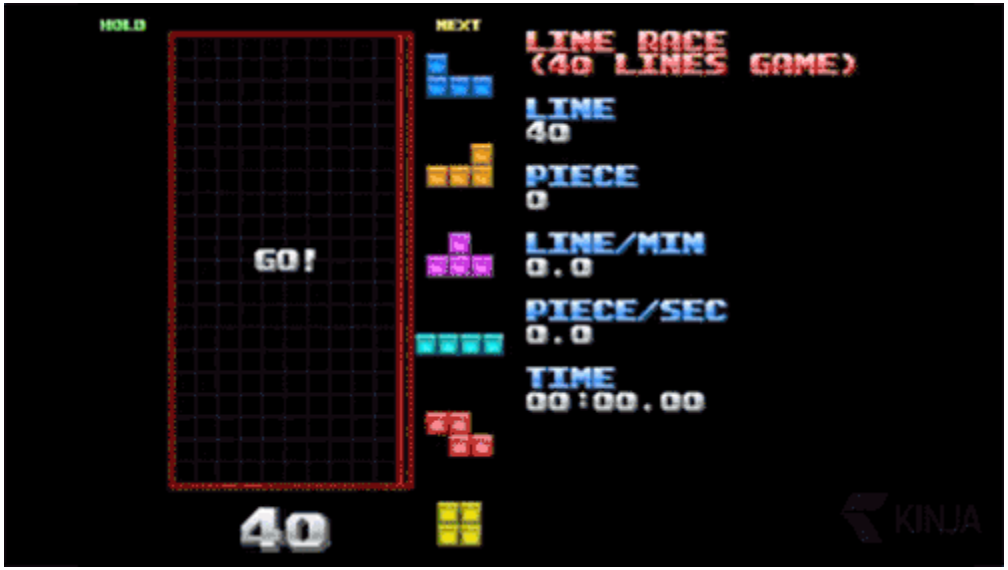
Workload Management Overview

- What is the goal of workload management?
  - Efficient, effective use of all resources by the user community under normal use
  - Ability to accommodate unusual circumstances and special requests



Workload Management Overview

- What it looks like in practice to the admin:



Workload Management

- Workload management is software that “fairly” manages jobs running on an HPC system.
- Most can apply many different policies and many inputs including past usage and available allocation to determine priorities.
- What is deemed “fair” depends a great deal upon the point of view!
  - Top complaint: “Bob is hogging the system by submitting [too many|too big|too long running] jobs.”
- Generates the number one question from users:
  - “Why doesn’t my job start?”
- You can’t please all of the people all of the time!

Resource Managers

- Manage the sharing of the available resources on your system
  - At a minimum resources are managed at the granularity of a node.
  - You may also want to manage global resources such as licenses and shared file system space and node level resources such as memory and CPU cores.
- Keep track of requests
  - Requested resources, priority related fields, account, etc
- Provide tools to start/stop and monitor jobs
  - Ideally providing a highly scalable process launching/management capability.
- Automate Submission of Jobs
  - Define workflows and/or Job dependencies
- Prioritization or Queues to control execution order

Schedulers

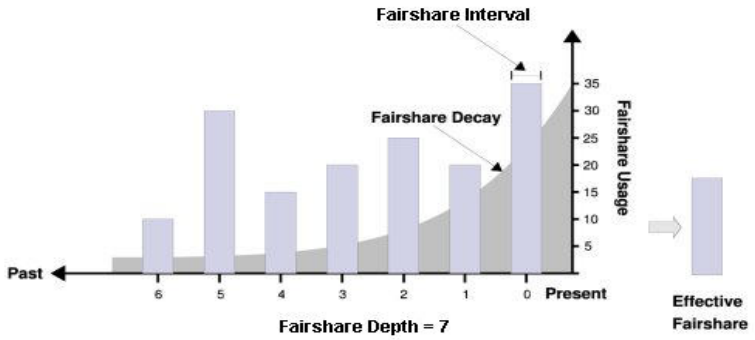
- The scheduler takes the information on available resources and requests to “optimize” the order and mapping of requests to the resources.
  - Many possible inputs and tunable settings can impact the scheduling algorithm
  - Resource related – amount, type, duration
  - Account – user, group, project
  - Policies – size of job, project, fair share, duration of job, required turnaround time, etc
- Tuning the scheduler is an art!
  - Know what your goals are first!
  - Ongoing process to tune the policy adapting to actual use!
  - Scheduling is not “set it and forget it”

Features Set

- Job Priority Factors
  - Fairshare
  - QOS
  - Multi-factor Priority
  - Backfill
  - Preemption/Gang Scheduling
- Reservations
- Job Arrays
- Topology Aware
- GPU/Intel Phi Support
- Power Capping

Fairshare

- Takes historical resource utilization as a factor in job priority.
- The more you use, the less priority you get.
- If Bob uses the entire cluster on Monday, his priority will be less for the rest of the week.
- Can be set for users, groups classes/queues, and QoS.
- Multi-level targets
- Highly tunable for interval (duration of window), depth (number of days), decay (weighting of contribution of each day) and what metric to use.



QOS

- QoS is Quality of Service
- Provides special treatment for jobs based on specified criteria
- Examples are:
  - Give a group access to special resources or bump priority to specific jobs within the group
- A QOS can be used to:
  - Modify job priorities based on QOS priority
  - Configure preemption
  - Allow access to dedicated resources
  - Override or impose limits
  - Change “charge rate” (a.k.a. UsageFactor)

Multi-factor Priority

- Multi-factor priority is the use of multiple factors to determine the order in which a job will start compared to others
- Uses a weighted equation
- Allows for tunable parameters
- Slurm uses the following:
  - Job priority = (PriorityWeightAge) * (age_factor) +
    (PriorityWeightFairshare) * (fair-share_factor) +
    (PriorityWeightJobSize) * (job_size_factor) +
    (PriorityWeightPartition) * (partition_factor) +
    (PriorityWeightQOS) * (QOS_factor) +
    SUM(TRES_weight_cpu *TRES_factor_cpu, TRES_weight_<type> *
    TRES_factor_<type>, ...)

Backfill

- If jobs were started in strict priority order, system utilization would be significantly lower and there would be less throughput.
- Backfill allows lower priority jobs to be started without affecting the start time of **any** higher priority jobs
- Example: Short small jobs that can fill in and finish before a large full system job
- Different schedulers handle backfill different ways
  - Moab looks at backfill on every iteration
  - Slurm has a special backfill iteration
- Highly tunable
- Time consuming as every job is taken into consideration
  - Use of limits highly suggested on clusters with lots of small jobs that are running into performance issues

Preemption/Gang Scheduling

- Preemption is stopping a "low-priority" job(s) to let a "high-priority" job run.
- Lower priority job can be cancelled, suspended or requeued
- A grace period should be implemented before preemptions to allow for check pointing
- Gang Scheduling is time slicing and oversubscribing a node to multiple workloads
  - Suspends jobs and balances between various workloads
  - Increases workload efficiency
  - Can create indeterminate workload times
  - Difficult to predict start of future jobs

Reservations

- Allows the ability to reserve advanced resources for users, accounts or groups
- Can also be used for future system maintenance
- Reservations can be standing such that they occur on a regular basis
- Can be used for cores, nodes, licenses and other resources
- Does not work with gang scheduling due to unpredictable end times of jobs

Reservation Examples

- Have a PM for 14 days out from 0800-1700, need to ensure no jobs are still running – **system reservation**
- Have a training event on Thursday, and the teacher/guest accounts will need 5 nodes reserved for 3 hours so that they can practice submitting jobs – **user reservation**
- Node 10 needs to be reserved for interactive jobs (devel & testing) M-F 0800-1800, but can do general work the rest of the time – **standing reservation**
- Need to troubleshoot a cluster-wide issue and am willing to let running work continue, but don't want new jobs to start while troubleshooting

Job Dependencies

- The workflow may require the output/results of Job1 to be available before Job2 can run successfully.
- The scheduler will not normally force jobs to run in submission order due to other priority factors
- Job Dependency support allows the user to indicate that one job must finish before another can start.
  - Can be tricky to implement if trying to submit many jobs at once

Job Arrays

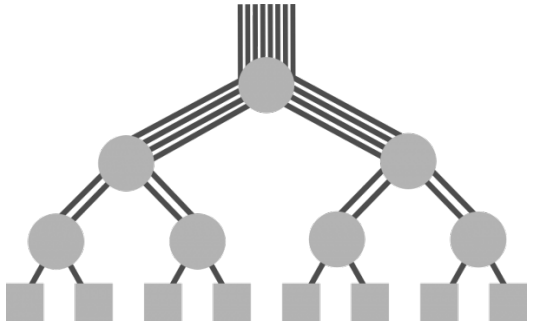
- Mechanism for submitting and managing collections of similar jobs quickly and easily
- Quickly submits thousands of jobs in seconds
- Used for jobs that have the same time limit, size and only small variations in executables or datasets
- Uses environment variables to implement variation within job

Topology Aware

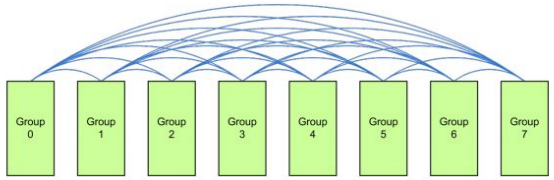
- Network Topology aware scheduling can improve application performance and increase workload throughput
- Applications that are communication (latency or bandwidth) sensitive can improve with proper job placement
- Job locality can cause less cluster fragmentation and less communication contention between jobs

Hierarchical Topology Aware

- Most common network configuration is Fat-Tree
  - Nodes are at the edge
  - Switches are hierarchically
  - Uplink bandwidth between switches is higher
  - Bisection bandwidth could be less than within switch due to switch limitation or cost
  - Placing workload within a switch provides full bandwidth for workload
  - Placing workload as close as possible will reduce latency decreasing the amount of hops required between nodes

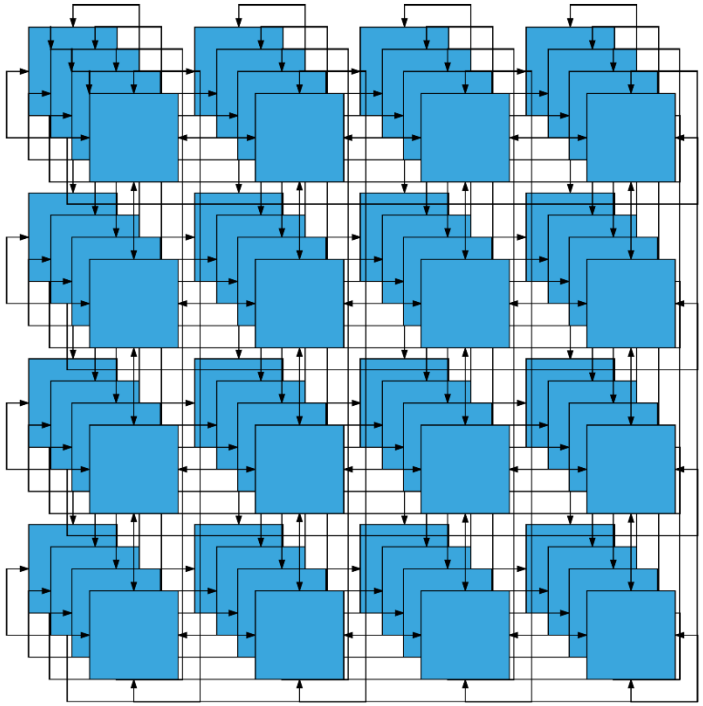


- Dragonfly networks are similar to fat-tree in grouping of nodes on edge
  - Groups of switches interconnected connected
  - Generally uses the same interface as Fat-Tree with a slightly different algorithm



3-D Torus Interconnect Topology Aware

- A 3-D Torus is a mesh network with no switches
- All sides are connected to each other
- Blue Waters at NCSA uses this topology
- Job placement is critical for throughput
- Network Congestion can be a problem if jobs are placed where communication is flowing through each other
- Locality is important for performance
- Not all links have to be the same speed



Accelerator Support

- Specialized hardware such as GPUs, FPGAs and Intel PHIs are increasing in demand
- Workload managers can monitor and assign these resources just like CPUs or memory
  - The difference is that some nodes may not have any of these resources

Power Capping and Green Computing

- The idea to limit the work done by a specific job to a fixed of total power consumed
- The implementation is usually a resource manager (RM) throttle of local cpu performance per node
  - May not account for MB power from DIMM's, networking & any GPU's
- Alternately, the RM may be able to monitor the total power consumed at the power supply (usually through BMC hooks) and simply terminate the job at the requested amount
- Node can also be shutdown while not in use
- Not all schedulers support this

Common Open Source and Commercial Schedulers and Workload Managers

- There are several commercial and open source choices for workload management
  - Portable Batch System derived
    - PBS Pro – commercial and open source product supported by Altair Engineering
    - Torque – open source maintained by Adaptive Computing
      - Very limited built-in scheduler
      - Can utilize the Maui Scheduler – open source
        - In maintenance mode
      - Moab scheduler is a commercial fork of Maui developed by Adaptive
  - Univa Grid Engine (UGE) (formally Sun Grid Engine) supported by Univa
  - Platform LSF – IBM Commercial product
  - SLURM – Open source with commercial support

PBS Pro

- Both a scheduler and Workload Manager
- Continued Development from the original PBS at NASA Ames
- Commercially Released in 2000
- Joined Altair Engineering in 2003
- Open Sourced in 2016

Torque

- Torque (Terascale Open-source Resource and Queue)
  - A fork of OpenPBS started in 2003
  - OpenPBS is itself a fork of the commercial PBS in 1998, but hasn't seen continued development.
    - PBSPro also derived from this code base and has seen continued commercial development.
  - PBS (Portable Batch System) was started in 1991
    - Note that this is prior to the rise of large scale distributed memory systems. In certain ways these products all still show some shortcomings based on this original design!
  - Actively developed and commercially supported by Adaptive Computing
- The included scheduler for the open source variants has always been quite simple.
  - FIFO + backfill (no reservations)

Maui

- Open Source Scheduler
- Maui development was started in the mid-1990's by David Jackson working as a contractor to develop a better scheduler to run on top of LoadLeveler on the IBM SP at the Maui High-Performance Computing Center.
- Fairly quickly he developed the interfaces needed to run on top of PBS/OpenPBS.
- The key feature is use of reservations for all jobs as well as for blocking out sets of resources for sets of users along with Backfill.
- Unfortuately, support for Maui has been deprecated- last update was in 2015

Moab

- Commercially available from Adaptive Computing
- Moab (named for a location in Utah where David Jackson lives) is a commercial fork of Maui started in 2001.
  - Pretty much all enhancements since then have went into Moab.
- Keeps most all of the Maui features and adds more.
- One recent feature added specifically for Blue Waters is topology aware scheduling – very relevant for the Cray 3D torus, less so for typical InfiniBand clusters.
- Interfaces with multiple workload managers including Slurm, Torque and PBS Pro.
- Highly customizable.

Univa Grid Engine

- Originally Developed by Genias Software in 1999 as CODINE and GRD
- Acquired by Sun Microsystems and renamed Sun Grid Engine (SGE) and released the software as open source
- Oracle acquired Sun in 2010 and SGE became Oracle Grid Engine (OGE)
- In 2011, Univa started a fork of the open source SGE and later acquired all commercial rights to Grid Engine now Univa Grid Engine (UGE)

Platform LSF (Load Sharing Facility)

- Originally based on the Utopia Project at the University of Toronto
- Commercialized by Platform Computing
- Acquired by IBM in 2012
- Easy to upgrade with in place patching
- Lots of add support for analytic, dashboards, submission portals
- Supports multiple APIs for submitting jobs
  - Python, Perl, DRMAA, SAGA

Slurm

- Simple Linux Utility for Resource Management
  - No longer all that simple!
  - Started out as a collaborative effort between LLNL, Linux NetworX, HP and BULL in 2001.
  - Designed with distributed memory parallel systems as the primary target to address some of the short comings at the time with systems like PBS and Torque.
  - Open-source code with commercial support/development provided by SchedMD.
  - Extendible architecture means there are many plugins available to modify the default SLURM behavior.
  - SLURM use has grown dramatically over the past five years at all system sizes.
    - Partly as a result there is a large and active community engaged in the development of the product and add-ons.

Choosing the right Scheduler and Workload Manager

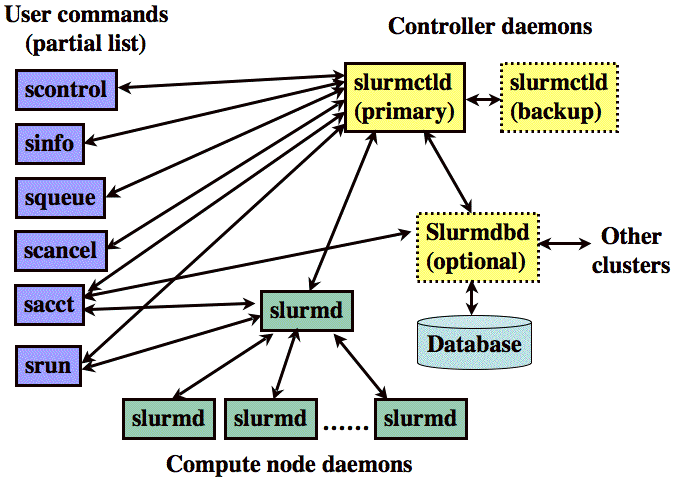
- What is your budget?
- What support level do you need?
- What is your experience with various scheduler?
- What is your workload?
  - High-throughput computing?
  - Number of jobs?
- Feature set needed

SLURM In Depth

- Architecture
- Daemons
- Configuration Files
- Key Configuration Items
- Node Configuration
- Partition Configuration
- Commands
- Test Suite

SLURM Architecture

- SLURM is designed with scalability and reliability as key goals.
- Optional redundancy for the management daemon.
- Node daemons form a hierarchical communication tree
- Optional database to manage accounting and other restrictions.



SLURM Daemons

- Daemons
  - slurmctld – controller that handles scheduling, communication with nodes, etc – One per cluster (plus an optional HA pair)
  - slurmdbd – (optional) communicates with MySQL database, usually one per enterprise
  - slurmd – runs on a compute node and launches jobs
  - slurmstepd – run by slurmd to launch a job step
  - munged – authenticates RPC calls (https://code.google.com/p/munge/)
    - Install munged everywhere with the same key
- Slurmd
  - hierarchical communication between slurmd instances (for scalability)
- slurmctld and slurmdbd can have primary and backup instances for HA
  - State synchronized through shared file system (StateSaveLocation)

Slurm Prerequisites

- Each node in cluster must be configured with a MUNGE key and have the daemons running
- MUNGE generated credential includes
  - User id
  - group id
  - time stamp
  - whatever else it is asked to sign and/or encrypt
    - names of nodes allocated to a job/step
    - specific CPUs on each node allocated to job/step, etc.

SLURM Configuration Files

- Config files are read directly from the node by commands and daemons
- Config files should be kept in sync everywhere
- Exception slurmdbd.conf: only used by slurmdbd, contains database passwords
- DebugFlags=NO_CONF_HASH tell Slurm to tolerate some differences. Everything should be consistent except maybe backfill parameters, etc that slurmd doesn't need
- Can use “Include /path/to/file.conf” to separate out portions, e.g. partitions, nodes, licenses
- Can configure generic resources with GresTypes=gpu
- man slurm.conf
- Easy: http://slurm.schedmd.com/configurator.easy.html
- Almost as easy: http://slurm.schedmd.com/configurator.html

Key Configuration Items

- ClusterName can be set as desired, will need to use it later for accounting.
  - Prefer lower case names.
- On the head node where slurmctld will run:
  - Set ControlMachine to “hostname –s” output.
  - SlurmUser=slurm NodeName
- All nodes run slurmd:
  - SlurmdUser=root

Partition Configuration

- Partitions are configured in slurm.conf. Specify the nodes associated with each partition along with limits.
  - PartitionName=batch Nodes=n[001-072],g[01-18] Default=YES MaxTime=INFINITE State=UP RootOnly=YES
  - PartitionName=cpus Nodes=pp[05-16] MinNodes=1 MaxNodes=4 MaxTime=24:00:00 STATE=UP
- Nodes can be in multiple partitions. Each partition can specify min and max nodes and times.

Commands

- squeue – view the queue
- sbatch – submit a batch job
- salloc – launch an interactive job
- srun – two uses:
- outside of a job – run a command through the scheduler on compute node(s) and print the output to stdout
- inside of a job – launch a job step (i.e. suballocation) and print to the job's stdout
- sacct – view job accounting information
- sacctmgr – manage users and accounts including limits
- sstat – view job step information
- sreport – view reports about usage
- sinfo – information on partitions and nodes
- scancel – cancel jobs or steps, send arbitrary signals (INT, USR1, etc)
- scontrol – list and update jobs, nodes, partitions, reservations, etc

A Simple Sequence of Jobs

- sbatch –ntasks=1 –time=10 preprocess.batch

  submitted batch job 100

  - Run the preprocess.batch script on 1 task with a 10 minute time limit, resulting job has an id of 100
- sbatch –ntasks=128 –time=60 --depend=100 work.batch

  submitted batch job 101

  - Run the work.batch script on 128 tasks with a 60 minute time limit after job 100 completes.
- sbatch –ntasks=1 –time=10 --depend=101 post.batch

  submitted batch job 102

  - Run the post.batch script on 1 tasks for up to 10 minutes after job 101 completes.

Tasks versus Nodes

- Tasks are like processes and can be distributed among nodes as the scheduler sees fit.
- Nodes means you get that many distinct nodes.
  - Must add –exclusive to ensure you are the only user of the node!

- Run hostname as two tasks:
  - srun --ntasks=2 --label hostname

- Same on two whole nodes:
  - srun --nodes=2 --exclusive –label hostname

Interactive Jobs

- salloc uses a similar syntax to sbatch, but blocks until the job is launched and you then have a shell within which to execute tasks directly or with srun.
- salloc --ntasks=8 --time=20 --pty bash

  salloc: Granted job allocation 104
- Try hostname directly.
- Try srun --label hostname

srun

- srun can be used as a general purpose task launcher.
- Inside of a job it can be used to launch your tasks from a master script
- srun support launching multiple executables at once using a simple config file.

- Many MPI implementations either use srun directly or the mpirun ties into srun.

sacct

- sacct provides accounting information for jobs and steps
- Many filtering and output options
- Works with the accounting file or optional database
- Return accounting information on user bob

  sacct –u bob
- Return accounting information on the debug partition

  sacct –p debug

sacctmgr

- Manages the accounting database
  - Add/delete users, accounts, etc
  - Get/Set resource limits, fair share allocations, etc
- sprio – view factors comprising a jobs priority
- sshare – view current hierarchical fair share information
- sdiag – view stats on the scheduling module operation (execution time, queue length)

scancel Command

- Cancel a running or pending job or step
- Can send arbitrary signal to all processes on all nodes associated with a job or step
- Has filtering options (state, user, partition, etc)
- Has an interactive (verify) mode

scancel 101.2

scancel 102

scancel –user=bob –state=pending

sbcast

- Copy a file to a local disk on allocated nodes
  - Execute within an allocation
  - Data is transferred using hierarchical slurmd daemons
- Might be faster than a shared file system.

strigger

- SLURM can run an arbitrary script with certain events occur
  - Node goes down
  - Daemon stop or restarts
  - Job is close to time limit

- strigger command can be used to create, destroy or list event triggers.

Host Range Syntax

- Host range syntax is more compact, allows smaller RPC calls, easier to read config files, etc
- Node lists have a range syntax with [] using “,” and “-”
- Usable with commands and config files
- n[1-10,40-50] and n[5-20] are valid
- Comma separated lists are allowed:
    - a-[1-5]-[1-2],b-3-[1-16],b-[4-5]-[1-2,7,9]

squeue

- Want to see all **running jobs** on **nodes n[4-31]** submitted by all users in **account acctE** using **QOS special** with a certain set of **job names** in **reservation res8** but only show the **job ID** and the **list of nodes** the jobs are assigned then sort it by **time remaining then descending by job ID**?
- There's a command for that!
- squeue -t running -w n[4-31] -A acctE -q special -n name1,name2 -R res8 -o "%.10i %N" -S +L,-i
- Way too many options to list here. Read the manpage.

sbatch,salloc,srun

- sbatch parses #SBATCH in a job script and accepts parameters on CLI
  - Also parses most #PBS syntax
- salloc and srun accept most of the same options
- **LOTS** of options: read the man page!

sbatch,salloc,srun

- Short and long versions exist for most options
- **-N 2** # node count, same as **--nodes=2**
  - In order to get exclusive access to a node add **--exclusive**
- **-n 8** # task count, same as **--ntasks=8**
  - default behavior is to try loading up fewer nodes as much as possible rather than spreading tasks
- **-t 2-04:30:00** # time limit in d-h:m:s, d-h, h:m:s, h:m, or m
- **-p p1** # partition name(s): can list multiple partitions
- **--qos=standby** # QOS to use
- **--mem=24G** # memory per node
- **--mem-per-cpu=2G** # memory per CPU
- **-a 1-1000** # job array

Job Arrays

- Used to submit homogeneous scripts that differ only by an index number
  - $SLURM_ARRAY_TASK_ID stores the job's index number (from **-a**)
  - An individual job looks like 1234_7 where ${SLURM_JOB_ID}_${SLURM_ARRAY_TASK_ID}
- "scancel 1234" for the whole array or "scancel 1234_7" for just one job in the array
- **Prior** to 14.11
  - Job arrays are purely for convenience
  - One sbatch call, scancel can work on the entire array, etc
  - Internally, one job entry created for each job array entry at submit time
  - Overhead of job array w/1000 tasks is about equivalent to 1000 individual jobs
- **Starting in** 14.11
  - "Meta" job is used internally
  - Scheduling code is aware of the homogeneity of the array
  - Individual job entries are created once a job is started
  - Big performance advantage!

scontrol

- scontrol can list, set and update a lot of different things
  - scontrol show job $jobid # checkjob equiv
  - scontrol show node $node
  - scontrol show reservation
- scontrol <hold|release> $jobid # hold/release (“uhold” allows user to release)
- Update syntax:
  - scontrol update JobID=1234 Timelimit=2-0 #set 1234 to a 2 day timelimit
  - scontrol update NodeName=n-4-5 State=DOWN Reason=”cosmic rays”
- Create reservation:
  - scontrol create reservation reservationname=testres nodes=n-[4,7-10] flags=maint,ignore_jobs,overlap starttime=now duration=2-0 users=root
- scontrol reconfigure #reread slurm.conf
- LOTS of other options: read the man page

Reservations

- Slurm supports time based reservations on resources with ACLs for users and groups.
- A system maintenance reservation for 120 minutes:
  - scontrol create reservation starttime=2009-02-06T16:00:00 duration=120 user=root flags=maint,ignore_jobs nodes=ALL
- A repeating reservation:
  - scontrol create reservation user=alan,brenda starttime=noon duration=60 flags=daily nodecnt=10
- For a specific account:
  - scontrol create reservation account=foo user=-alan partition=pdebug starttime=noon duration=60 nodecnt=2k,2k
- To associate a job with a reservation:
  - sbatch --reservation=alan_6 -N4 my.script
- To review reservations:
  - scontrol show reservation

Node Configuration

- All compute nodes are defined in slurm.conf in the form:
- NodeName=n[001-080] CPUs=12 RealMemory=48260 Sockets=2 CoresPerSocket=6 ThreadsPerCore=1 State=UNKNOWN
- Sockets, Cores, Threads help define the NUMA domains to aid in pinning processes to cores
- RealMemory defines the “configured” memory for the node.
- Can add “GRES=gpu:2” for a GPU resource

SLURM Test Suite

- SLURM includes and extensive test suite that can be used to calibrate proper operation
- include over 300 test programs
- executes thousands of jobs
- executes tens of thousands of steps
- change directory to testsuite/expect
- create file “globals.local” with installation specific information
- set slurm_dir “/home/moe/SLURM/install.linux”
- set build_dir “/home/moe/SLURM/build.linux”
- set src_dir “/home/moe/SLURM/slurm.git”
- Execute individual tests or run regression for all tests

Plugins

- Dynamically linked objects loaded at run time based upon configuration file and/or user options
- 80 plugins of 20 different varieties currently available
- Accounting storage: MySQL, PostgreSQL, text file
- Network topology: 3D-torus, tree
- Different versions of MPI:
  - OpenMPI, MPICH1, MVAPICH, MPICH2, etc.
- There is an API that is available for you to write your own plugin to make Slurm perform how you would like.

Robust Accounting

- For more robust accounting we need to setup the database connection, slurmdbd.
- http://slurm.schedmd.com/accounting.html

- Likely want:
  - AccountingStorageEnforce=associations,limits,qos

- We will talk about this more later

Database Use

- Accounting information written to a database plus
  - Information pushed out to live scheduler daemons
  - Quality of Service (QOS) definitions
  - Fair-share resource allocations
  - Many limits (max job count, max job size, etc)
  - Based on hierarchical banks
    - Limits by user AND by banks

Setup Accounts

- Setup a couple accounts for testing:
  - sacctmgr add account none,test Cluster=gideontest Description="none" Organization="none”
  - Leaving off the cluster will add the account to all clusters in the slurmdbd
- Accounts are hierarchical
  - sacctmgr add account science Description="science accounts" Organization=science
  - sacctmgr add account chemistry,physics parent=science Description="physical sciences" Organization=science

Add Users to Accounts

- sacctmgr add user brett DefaultAccount=test
  - Adds user brett to the DB with a default account of test.
  - At this point user brett can run jobs again.
- sacctmgr add user brett account=chemistry
  - Add user brett to a second, non-default account
- sacctmgr modify account chemistry set GrpCPUMins=5000
  - Set a total usage limit
- sacctmgr show associations
  - Useful to inspect your account settings

Break Time

- Back in 30 minutes

Limiting and Managing Resources

- Cgroups
- Pam authentication modules
- Processor Affinity
- Containers

Control Groups (Cgroups)

- Cgroups are a Linux Kernel feature that limits, accounts for, and isolates the resource usage of a collection of processes
- Used to limit and/or track:
  - CPU
  - Memory
  - Disk I/O
  - Network
  - Etc…
- Features
  - Resource Limiting
  - Prioritization
  - Accounting
  - Control

Cgroup support within Workload managers

- Torque must be built using cgroups during configure time
  - Built using –enable-cgroups
  - Newer versions of hwloc is required which can be built locally
  - You must have cgroups mounted when compiling with cgroups
  - You cannot disable cgroup support on a live system
- Slurm Cgroup support is enable via multiple plugins
  - proctrack (process tracking)
  - task (task management)
  - jobacct_gather (job accounting statistics)

Pam module for compute node authentication

- A pluggable **authentication** module (**PAM**) is a mechanism to integrate multiple low-level **authentication** schemes into a high-level application programming interface (API). It allows programs that rely on **authentication** to be written independently of the underlying **authentication** scheme.
- Most schedulers have a PAM plugin module that can be used to restrict ssh access to compute nodes to only nodes where the user has an active job.
- This will not clean up any users that exist on the compute nodes

Pam_slurm

- Slurm provides a PAM plugin module that can be used to restrict ssh access to compute nodes to only nodes where the user has an active job.
- The pam_slurm PAM plugin is installed by the rpms.
- Need to add:

  auth include password-auth
  account required pam_slurm.so
  account required pam_nologin.so

  to /etc/pam.d/sshd
- Only do this on compute nodes! If you put it on the head node it will lock out users!

Processor Affinity

- Processor Affinity is binding of a process or thread to a CPU so that the process or thread will execute on the designated CPU or CPUs rather than any CPU.
- You are overriding the scheduling algorithm of the operating system
- Reasons to use Processor Affinity
  - Take advantage of remnants of a previous or existing process/thread may still reside in cache to speed up process by reducing cache misses
  - Varied tasks in a job might be scheduled on a single CPU that could be sped up if ran on 2 separate CPUs
  - Architecture of CPU such AMD Bulldozer
  - Multiple NUMA domains
- Issues with Processor Affinity
  - Does not solve load balancing issues
  - Challenging on non-uniform systems

Enabling Processor Affinity on Slurm

- The following are the parameters that need to be modified in the slurm.conf
  - SelectType=select/cons_res
  - SelectTypeParameters=CR_Core
  - TaskPlugin=task/affinity TaskPluginParam=sched
- An example would be:
  - srun --nodes=1-1 --ntasks=6 --cpu_bind=cores ...
  - Slurm allocates 3 CPUs on each socket of 1 node
  - Slurms distributes each task in a round robin configuration
- Many options to distribute tasks.

Containers

- Allow you to isolate applications with their entire runtime environments
- Uses the same kernel as host operating system
- Common container in HPC environments:
  - Docker
    - Mostly for DevOps, microservices, enterprise applications
    - Generally not great for HPC as requires escalated privileges
  - Shifter
    - Pulls images from Docker hub
    - No root escalation required
    - Compatible with Slurm via plugin and other workload managers
  - Singularity
    - Self-contained executable that is ran within a script
    - Allows importation of docker images
    - No root escalation or daemons required

Docker

- Leading container platform in the world
- Portable deployment across docker environments
- Easily local client install
- Images allow users to be root
- Create an image on your local machine and to cloud dock service
- Self contained image with bind-able host filesystems
- Large community of premade images on Dockerhub
- Not great in HPC environment as the docker daemon requires root with users having root equivalent permissions
- LSF, Torque integration

Shifter

- Developed by the National Energy Research Scientific Computing Center
- Leverages or integrates with public image repos such as Dockerhub
- Require no administrator assistance to launch an application inside an image
- Shared resource availability such as parallel filesystems and network interfaces
- Robust and secure implementation
- Localized data relieves metadata contention improving application performance
- “native” application execution performance
- Slurm integration via SPANK Plugin

Singularity

- Developed by Lawrence Berkeley Lab
- Packages entire application and environment within image
- No user contextual changes or root escalation allowed
- No root owned daemon processes
- Users can run Singularity containers just as they run any other program on the HPC resource
- No integration with scheduler required
- All standard input, output, error, pipes, IPC, and other communication pathways that locally running programs employ are synchronized with the applications running locally within the container.
- MPI integration

Scheduling and Cloud

- Using cloud resources can allow clusters to grow and shrink on demand.
- Can offer bursting or an independent self-contained cluster
- Moab, LSF, Slurm all support
- Slurm uses the power capping plugin to launch and shutdown nodes
- Reasons for using Cloud:
  - Limited resources
  - Cheaper compute during less demand
  - Some data is already in the cloud

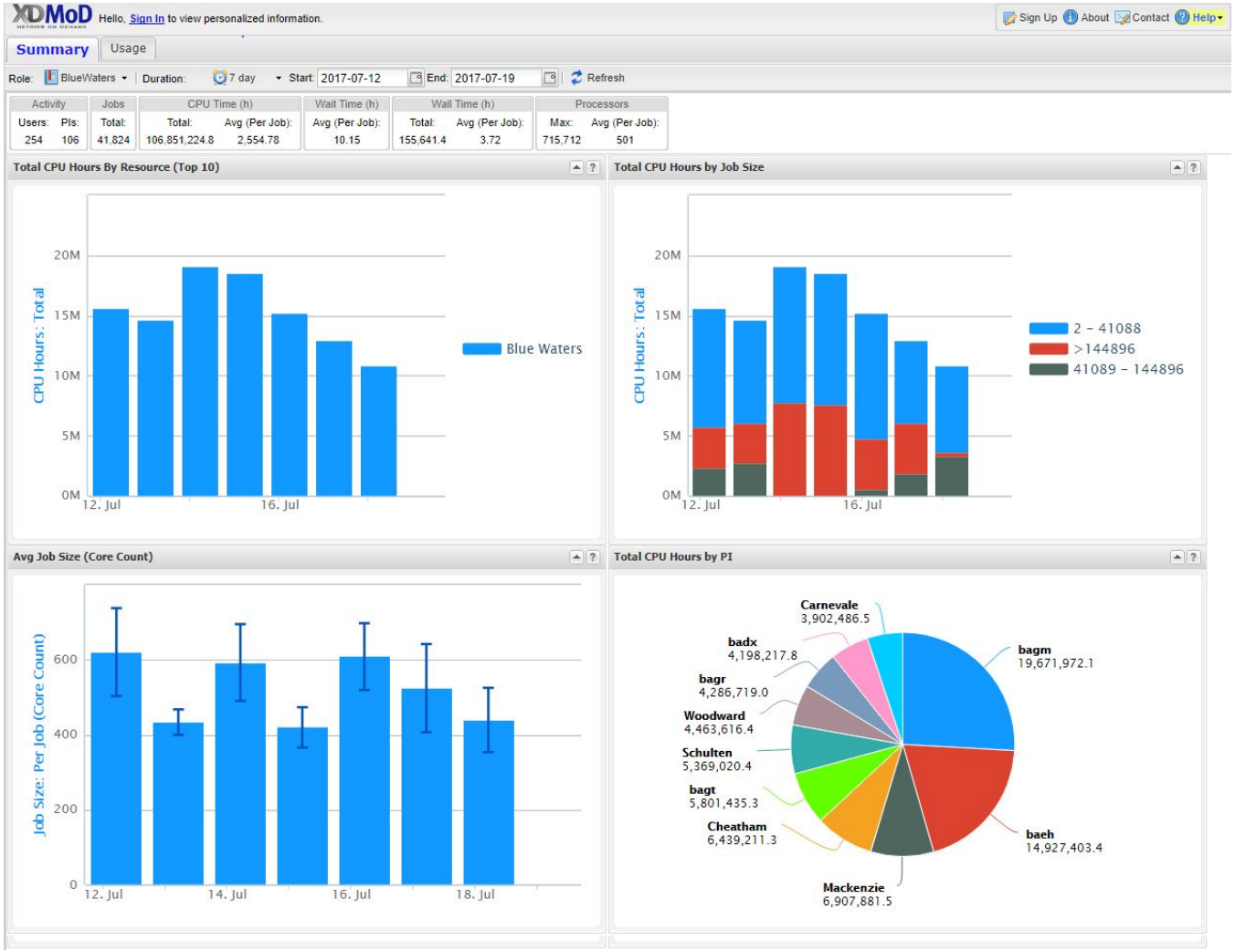
Accounting

- XDMod
- MAM/Gold

XDMod

- Open XDMoD is an open source tool to facilitate the management of high performance computing resource
- Support for SLURM, TORQUE/PBS, UGE and LSF
- Used to inform scheduler changes
  - Infer areas where jobs aren't getting through
  - Users that are 'gaming' the system
  - Users that are getting stuck
- Easy Reports
- Bluewaters XDmod

XDMod


XDMoD
Hello, Sign In to view personalized information.
Sign Up
About
Contact
Help
Summary
Usage
Role: BlueWaters
Duration: 7 day
Start: 2017-07-12
End: 2017-07-19
Refresh
Activity
Users: 254
PIs: 106
Jobs
Total: 41,824
CPU Time (h)
Total: 106,851,224.8
Avg (Per Job): 2,554.78
Wait Time (h)
Avg (Per Job): 10.15
Wall Time (h)
Total: 155,641.4
Avg (Per Job): 3.72
Processors
Max: 715,712
Avg (Per Job): 501
Total CPU Hours By Resource (Top 10)
CPU Hours: Total
20M
15M
10M
5M
0M
12. Jul
16. Jul
Blue Waters
Total CPU Hours by Job Size
2 - 41088
>144896
41089 - 144896
Avg Job Size (Core Count)
Job Size: Per Job (Core Count)
600
400
200
0
12. Jul
14. Jul
16. Jul
18. Jul
Total CPU Hours by PI
Carnevale
3,902,486.5
badx
4,198,217.8
bagr
4,286,719.0
Woodward
4,463,616.4
Schulten
5,369,020.4
bagt
5,801,435.3
Cheatham
6,439,211.3
Mackenzie
6,907,881.5
baeh
14,927,403.4
bagm
19,671,972.1

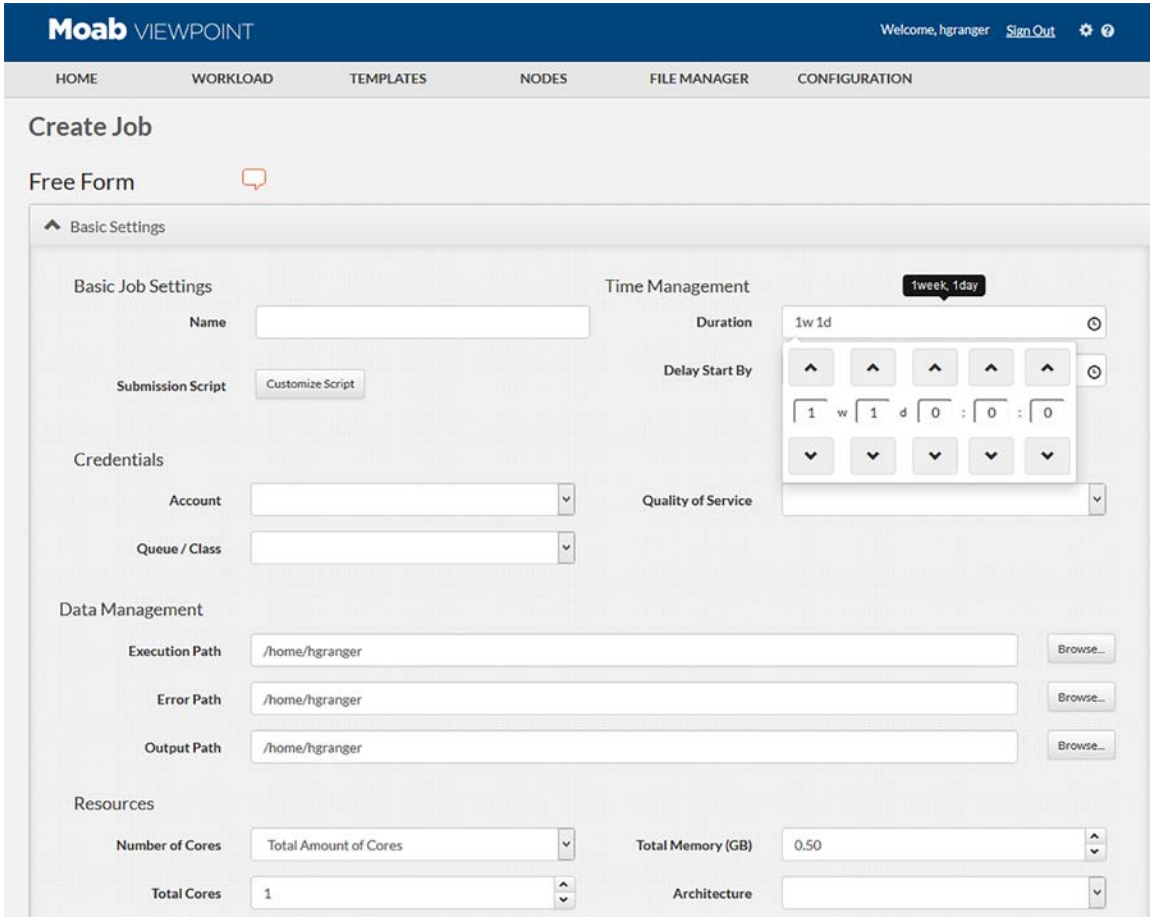
Moab Accounting Manager

- Originally called Gold as Open Source
- Uses Postgres as database
- Built by Scott Jackson (now at Adaptive Computing) at Pacific Northwest Laboratory
- Similar to SLURM accounting functionality
- Track usage per user, group, project, or account
- Pre-pay or pay-as-you-go models
- Charge rates per resource, action, or quality of service
- Lien-based model
- Enforce budgets

Job Submission Portals

- PBS Pro(Compute Manager), Moab (Viewpoint) and LSF have webportals for jobs submission
- Users can:
  - Submit jobs
  - Transfer files
  - Check status of jobs
  - Use job templates
- Some have administrative dashboard
  - Also ability to modify jobs
- Also can incorporate into authentication scheme

Moab Viewpoint



Lunch

Hands On with Slurm

- You are given a university community cluster of 2 nodes with 2 cores a piece
- It has the latest version of SLURM installed
- Software Environment modules are installed
- There are 4 departments
  - Math, Physics, Biology and Astronomy
- The scheduler is setup with 1 default queue (normal) and first in first out scheduler
  - The queue is limited to 20 minute jobs
- Accounting is setup with all of the users and groups
  - There is no enforcements of any limits

Getting Setup on Nebula

- Grab handout
- SSH to host
- Find all hosts
- Users and groups
- Exploring SLURM
  - Run a simple job
- After you are done exploring, users of the cluster will start submitting jobs

Things to know

- There is a NFS mounted home directory
- RPMs are installed
- All SLURM configs and binaries are in default locations on all nodes (/etc,/bin,/sbin)

Exercise 1: Enabling Fairshare

- Oh no! A professor Bob is complaining about the fairness of the cluster.
  - They only run 4 core jobs a few times a week and other are running a ton of single core jobs
- Enable Fairshare where all users are given an equal share of all of the resources
- Fairshare should be a very short period, 10 minute period with a depth of 6.
- Start up more jobs

Exercise 2: Enable Fairshare for Groups and Users

- The professors have decided that all departments need to share the cluster evenly
- They also want all users to share within the account
- Setup hierarchical fairshare between users and between accounts

Exercise 3: Issues with Priority

- Professor Bob is back to having issues getting high priority jobs through
- He has a deadline on a paper for a conference
- Create a reservation for the next 30 minutes for him on both of the nodes to help satisfy him temporarily
- For a more permanent fix create another partition with higher starting priority

Exercise 4: Limiting Groups with Accounting

- The IT department has decided they want to sell the resources to each department to help fund the machine
- Limit each project to 20 CPU hours
- Modify partitions so that the high priority is double the cost of the normal queue
- Follow the instructions on the handout

Exercise 5: Enable Preemption for a Low Queue

- Users want a the ability to submit low priority jobs to allow
- Make sure these jobs only backfill
- They should be half the cost of normal jobs

Extra Exercise 6: Singularity

- Biology wants to use a Docker image for their genomics project
- Follow the instructions on the hand out to pull a Ubuntu image from Dockerhub for Singularity

References

- Brett Bode
- https://en.wikipedia.org/wiki/Linux_PAM
- https://en.wikipedia.org/wiki/Platform_LSF
- http://www.nersc.gov/research-and-development/user-defined-images/
- http://singularity.lbl.gov/
- https://geekyap.blogspot.com/2016/11/docker-vs-singularity-vs-shifter-in-hpc.html
- http://clusterdesign.org/