LCI workshop
on high performance clustered computing

Linux Clusters Institute: Scheduling with PBSPro

Ben Matthews, Software Engineer, NCAR

NCAR
NATIONAL CENTER FOR ATMOSPHERIC RESEARCH

What does a batch scheduler do?

- Large scale, high-performance Tetris!
- Divide up a shared resource “fairly”
  - “fair” may depend on politics/business logic
  - Jobs should never “starve”
- Prevent users from stepping on each other
- Ensure system is utilized as much as possible
- Record statistics/track usage
- Assist middleware [MPI] with multi-node job launch

PBSPro

- Developed at NASA Ames (Mountainview CA/Moffett Airforce Base)
- Acquired by Altair Engineering in the early 00's
- Dual commercial/Open (Affero GPL v3)
- Support for various UNIX and Windows (mostly Linux + Windows)
- Various forks have been developed over the years
  - TORQUE (Adaptive Computing – Commercial)
  - OpenPBS (Open,ish)
- Reasonably Performant and Scalable

PBSPro: Features

- Rich “hook” infrastructure for customization
- Fairshare
- Backfill
- Compatibility with a wide variety of MPI implementations
- Well understood (if not well documented) accounting log
- Optional analysis components (commercial add-on only)

PBSPro: Basic Components

- Server
  - Runs on one or two, typically dedicated, servers
  - Mediates between other components and maintains the queues
- Scheduler
  - Takes a list of jobs from the server, tells the server which to run
- MoM
  - Runs on each compute node, starts and supervises user code. Optional job-setup on the compute node.
- Com
  - Facilitates communication between components (only needs configuration at scale)

Hardware Requirements

- For failover
  - Two servers
  - Shared filesystem (must support POSIX locking, but NFS ok)
- Server software is not well threaded yet: prefer higher clock frequency over many cores
- Database performance matters (SSD would be nice)
- Queues are stored in RAM, so memory usage scales with queue length. More RAM = better

System Software Setup

- One user account for PBS to run under (typically “pbsdata”)
- UID<>username mapping should be consistent across the cluster
- Optionally, MUNGE can be used to authenticate the cluster
- ssh (or rsh), allowing passwordless connections between cluster nodes (use ssh keys or host trust) strongly recommended
- scp or rcp (or similar) must work (passwordless) between submit hosts and cluster nodes (for file staging)
- shared filesystem on compute nodes is **not** required, but is strongly recommended

Installation

- RPMs provided to commercial customers for SLES and RHEL
- Can also build from source (and optionally produce RPMs)
- Four install types:
  - Server
  - Execution Host
  - “commands only” (head-node)
  - Everything (direct install from source)
- RPMs are relocatable (see the documentation for details)

Installation: pbs.conf

- Present on all nodes
- Specifies which components to start and where the servers are
- Used to generate the initial configuration

/etc/pbs.conf

```
PBS_EXEC=/opt/pbs
PBS_HOME=/gpfs/pbs
PBS_START_SERVER=0
PBS_START_MOM=0
PBS_START_SCHED=0
PBS_START_COMM=0
PBS_SERVER=laadmin1.ib0.laramie.ucar.edu
PBS_PRIMARY=laadmin1.ib0.laramie.ucar.edu
PBS_SECONDARY=laadmin2.ib0.laramie.ucar.edu
PBS_SCP=/usr/bin/scp
PBS_RSHCOMMAND=ssh
PBS_CORE_LIMIT=unlimited
PBS_MAIL_HOST_NAME="ucar.edu”
PBS_AUTH_METHOD=MUNGE
```

Other places to look for configuration

- $PBS_HOME/{sched,server}_priv/{sched,server}_config

- “qmgr”
- Per-component configuration typically generated during the first startup

Starting PBS

- `systemctl start pbs` #>= version 14, systemd systems
- `/etc/init.d/pbs start` #<=version 13, other init types
- Must be done on the server node(s) and all execution nodes

PBSPro: Commands

- qmgr
  - Configuration
- qsub
  - Submit Jobs
- qstat
  - View Status of Jobs/Queues/Servers
- qrls/qhold
  - Hold/Release Jobs
- pbs_rsub/pbs_rstat/pbs_rdel
  - Manipulate Reservations

PBS Objects

- Queues – collect jobs
- Nodes – run jobs
- Resources – generic properties

Queues

- Two types:
  - Execution
  - Routing
- Routing queues accumulate jobs and pass them on to execution queues based on resource requests
- Execution queues store jobs and dispatch them to nodes
- May be fixed length or unrestricted (up to the amount of memory on your PBS server)
- May impose various restrictions/access controls

Manipulating Queues

- qmgr -c ‘create queue new_queue’ #create a queue
- qmgr -c ‘set queue new_queue your_resource = foo’ #set a resource
- qmgr -c ‘set queue new_queue started=true’ #run jobs
- qmgr -c ‘set queue new_queue enabled=true’ #accept new jobs
- qmgr -c ‘print queue @default’ #list queues

Resources

- Used to control the flow of jobs through PBS
  - Typically used much less extensively by non-PBS schedulers (SLURM)
- Can be requested by the user, a hook, or required by a queue
- Static (set by an admin) or Dynamic (collected by the server/MoM)

Resources

- Things your job needs
- Could be strings, numbers, etc
- Can be a thing that a specific node or queue provides
- Could be provided by something external (like a license server) but tracked by the scheduler
- Could be a simple property of a job

Adding Custom Resources

- Make an entry in $PBS_HOME/server_priv/resourcedef
- If you are going to schedule based on your resource, add it to the "resources" list in $PBS_HOME/sched_priv/sched_config
- Attach the resource to nodes/queues/etc in qmgr

Nodes

- Physical Hardware to run on (where MoM runs)
- Can be subdivided into vnodes which can be independently scheduled
- Can be assigned resources that can then be used to control which jobs will run
- Can be assigned dynamic resources, which are periodically measured by user provided or built-in scripts (load average, memory usage, etc).

Nodes

- May be in various states – see the output of “pbsnodes –a”
- Common States:
  - offline – node is broken or marked down by an administrator
  - job-exclusive – node is completely allocated to a job
  - free – node is available for use
  - down – Server and MoM aren’t communicating
  - resv-exclusive – node is completely reserved
- Nodes can be in multiple states, for example, reserved and running a job

Built-in Node resources

- Memory
- CPUs
- Free Disk
- Load Average
- Hostname
- OS
- Vnode
- System specific details (Cray, etc)

Manipulating Nodes

- qmgr -c ‘create node node001’ #create a new node
- qmgr -c ‘print node @default’ #list nodes
- pbsnodes -o -c “this node is broken” node001 #offline node001
- pbsnodes -r node001 #online node001
- pbsnodes -a –F dsv #list nodes, parseable

ACLs and Security

- Currently apply to user-id or a user's **primary** group
- Can be used to restrict who may run how many jobs in which queue
- Can be supplemented with user-supplied python-scripts for additional flexibility ("hooks")
- Configured as queue properties via qmgr
- Kernel provided user information is trusted, however MUNGE can be used to provide some level of authentication
- Users can be granted limited administrative privileges (killing other user's jobs, running qmgr, etc)

Hooks

- Short python scripts that are run at various points in the scheduling process
- Can be used to implement additional business logic or functionality
- Need to be **fast** and **robust**
  - Run by the Server or MoM and can therefore break the Server or MoM
- Newish feature with some rough edges but very flexible
  - Avoid them if you can
- Configured via qmgr

Components of a Job

- Resources you need? `-l select=1:ncpus=1:mpiprocs=1`
- For how long? `-l walltime=1:00:00`
- Where? `-l place=scatter`
- Which Queue? `-q workq`
- Where to put the output? `-o stdout.log –e stderr.log`
- See the qsub manpage for other options

Placement

- Placement statement is three colon delimited (optional) clauses:
  - -l place=arrangement:sharing:grouping
- Arrangement determines where the resources are allocated
  - free: use any free vnodes
  - pack: try to use vnodes from one (or as few as possible) hosts
  - scatter: one chunk per host
  - vscatter: one chunk per vnode
- Sharing
  - excl: vnodes aren't shared (but hosts might be)
  - exclhost: hosts aren't shared
  - group= group by some resource

Select

- Request a number of “chunks” containing some resources
- Chunks are plus delimited
- Resources are colon separated
- First part of a chunk is the number of copies
- qsub -l select=2:ncpus=4:mem=1gb+1:ncpus=2:mem=5gb
  - Give me 2 vnodes, with 4 cpus and 1gb of ram
  - Also 1 vnode with 2 cpus and 5gb of ram
- Can be quite complex – see the documentation for details

Sample Job

```
#!/bin/bash
#PBS -l walltime=1:00
#PBS -lselect=2:ncpus=1:mpiprocs=2
#PBS -A SSSG0001
#PBS -N test_job
#PBS -q share

cd PBS_O_WORKDIR
mpirun ./a.out
```

Sample Job - Running

```
chmod +x job_script.sh
qsub ./job_script.sh
```

Scheduling Features: backfill

- Scan lower priority jobs for tasks that can be fit between larger/longer jobs
- Expensive, but can significantly improve utilization
- Most effective when jobs make accurate walltime requests
- The number of jobs to schedule around is configurable (may have a significant impact on your scheduling time)
  - `backfill_depth`

Scheduling Features: Fairshare

- Jobs are prioritized by a configurable per-user (or per-project) importance score (potentially hierarchical)
- Jobs are de-prioritized by historical usage (subject to some half-life)
- Users who are “important” and/or haven’t used much CPU*time recently run first
- Prevent any one user from monopolizing the system
- Give those who are more important a little more priority while still preventing starvation

Scheduling Features: Fairshare

- Priority = usage/allocated_percentage_of_system
- Usage is decayed by a configurable factor every configurable unit of time
- Default decay is a 24 hour half-life
- Usage is a configurable expression, often cpu*seconds
- Percentage is based on “shares”
  - Configure 10 users with 100 shares each, each user gets 10%
  - Shares are in arbitrary units
  - Defined in $PBS_HOME/sched_priv/resource_group
- Smaller priority = run sooner

Scheduling Features: Placement Sets

- Special resources attached to nodes
- Scheduler will try to keep each job in the smallest possible placement set
- Ensure locality – try to keep a job's assigned nodes within a switch/rack/datacenter/etc

Array Jobs

- An optimized way to run N of the same job
- Each job is passed its index (useful to specialize)
- Potentially faster to schedule than individual jobs
- qsub –J “1-100”

Job Sort

- Which job should we run next?
- Configurable. Can be based on a user-defined python expression, fairshare, or static queue based priority
- Many schedulers allow you to use multiple scaled factors – PBS does **not** (yet)
  - Secondary factors used only to break ties – if two jobs have exactly equal fairshare priority, only then will queue priority take effect
  - Can turn off fairshare completely
- Can use a site-specific python function, but can't integrate fairshare score

Additional Configuration: Health Check

- Verify that a node is healthy right before launch
  - Filesystems mounted
  - All the RAM present
  - CPUs present and at a reasonable frequency/temperature
  - Network up
  - OS correct
  - Daemons running
- If not, requeue the job and mark the node offline

Additional Configuration: Health Check

- Example hook provided with PBS: $PBS_EXEC/unsupported/NodeHealthCheck.py
- NHC was presented yesterday – can be integrated with PBS via hooks
- Good idea to run something right before and/or right after each job
- Details tend to be site specific – track what your users break and check for that

Additional Configuration: cgroups

- Contain each job to the resources that it requested
- Prevent out-of-memory events or other buggy code from breaking your compute nodes
- Newer OS may require integration with systemd instead of cgroups directly
- No direct support in PBS, but can be accomplished with hooks. Altair can provide a sample upon request

Troubleshooting: Why won't my job run??

- Because you asked for something silly!
  - qstat -f jobid
  - Check the comments field
  - Check that the job needs <= sizeof(cluster)
- Because too many nodes are broken
  - pbsnodes -l
- Because the system is otherwise broken
  - Filesystem mounted?
  - Network up?
- Because the system is busy
  - qstat -a

Troubleshooting: Why did X's job run before mine?

- Because you're unimportant or you've been hogging the system (fairshare)
- Because their job was smaller/shorter and was backfilled
- Because your job asked for something that was unavailable
  - Consumable resources
  - Special nodes
  - Placement sets

Troubleshooting: Fairshare

pbs_fs

```
Fairshare usage units are in: cput
TREEROOT  : Grp: -1     cgrp: 0    Shares: -1     Usage:14141166288 Perc: 100.000%
facilities: Grp: 0      cgrp: 2    Shares: 100000 Usage: 14141165485 Perc: 99.990%
ASD       : Grp: 2      cgrp: 271  Shares: 5000000 Usage: 5301136879 Perc: 49.995%
A_ASDNCAR : Grp: 271    cgrp: 278  Shares: 5000000 Usage: 881376146 Perc: 24.997%
ACGD0005  : Grp: 278    cgrp: 284  Shares: 1      Usage: 791019631 Perc:  4.166%
ACGD0004  : Grp: 278    cgrp: 283  Shares: 1      Usage: 0      Perc:  4.166%
AACD0002  : Grp: 278    cgrp: 282  Shares: 1      Usage: 1854   Perc:  4.166%
ARAL0001  : Grp: 278    cgrp: 281  Shares: 1      Usage: 785    Perc:  4.166%
AHAO0001  : Grp: 278    cgrp: 280  Shares: 1      Usage: 421    Perc:  4.166%
```

Troubleshooting: No Output

- usecp
  - Was submission host alive?
- Check disks - is there space/quota available for output files?
- Is the job done? qstat -f [jobid]

Troubleshooting: Diagnostic collection

- $PBS_EXEC/unsupported/pbs_diag
  - Produces a tarball for PBS support
- tracejob [jobid]
  - Finds information about a job from the server log
  - Crippled if you're using syslog (only)
- Increase the log-level (different for each component – see docs)
- Look for core files in $PBS_HOME
- If the server is hung, "gstack [pid]" a few times to figure out what it's doing

Analytics

- Very limited support in PBS
- PBS Analytics
  - Web based reporting using the accounting data produced by PBS
  - Commercial product
- XDMoD
  - NSF sponsored web-based reporting tool
  - Some Limited PBS (and SLURM) support
  - Integration with other data sources
- Gold
  - Open (PNNL) or Commercial (Adaptive) but no recent releases

Reservations

- Two kinds: Standing and advanced
- Standing reservations reserve some resources on a regular basis
  - ical syntax
- Advanced reservations reserve some resources at a specific future time
- Reservations are queues
- Reservations will disappear if they can not be fulfilled
- Reservations for offline nodes may be reconfirmed on other nodes up to a configurable time before the start

Reservations

- Nodes that are offlined in a running reservation are **not** replaced
- Reservation queues are numerical and have a configurable prefix which indicates their type:
  - R123456
  - S123457
- Names can be attached to reservations, but they aren't really used
- Generally, reservation queues have an ACL that restricts who can submit to them

Reservations

- Common States:
  - Running – reservation can run jobs
  - Confirmed – resources are allocated, but the reservation hasn't started yet
  - Degraded – reservation is running, but some reserved resource is unavailable
  - Unconfirmed – scheduler is still looking for resources

Reservations

```
# pbs_rsub -l select=1:ncpus=72 -l place=free -R 1300 -E 1400
R311175.laadmin1.ib0.laramie.ucar.edu UNCONFIRMED
# pbs_rstat -f R311175.laadmin1.ib0.laramie.ucar.edu
Resv ID: R311175.laadmin1.ib0.laramie.ucar.edu
Reserve_Name = NULL
Reserve_Owner = pbsdata@laadmin1.ib0.laramie.ucar.edu
reserve_state = RESV_CONFIRMED
reserve_substate = 2
reserve_start = Thu Apr 27 13:00:00 2017
reserve_end = Thu Apr 27 14:00:00 2017
reserve_duration = 3600
queue = R311175
Resource_List.ncpus = 72
Resource_List.walltime = 01:00:00
Resource_List.nodect = 1
Resource_List.select = 1:ncpus=72
Resource_List.place = free
resv_nodes = (r1i0n1:ncpus=72)
Authorized_Users = pbsdata@laadmin1.ib0.laramie.ucar.edu
server = laadmin1.ib0.laramie.ucar.eductime = Thu Apr 27 11:48:43 2017
mtime = Thu Apr 27 11:48:43 2017
Variable_List =
PBS_O_LOGNAME=pbsdata,PBS_O_HOST=laadmin1.ib0.laramie.ucar.edu,PBS_O_MAIL=/var/spool/m
ail/pbsdata
```

Preemption

- If a more important job comes along, signal an existing job to make room
- Up to each user application to checkpoint (quickly) and terminate (or be kill -9'ed)
- Not used too much at academic HPC sites
  - Not much support from common applications

Support

- Commercial Support from Altair: http://www.pbsworks.com/SupportGT.aspx?d=Support,-Services-and-Support
- Community support forum on http://pbspro.org/
- PBS User's Group (This week in Las Vegas ;-( )
- Jira bug tracker: https://pbspro.atlassian.net/secure/Dashboard.jspa

Questions?