Job Scheduling with Moab Cluster Suite

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Some terminology..

- **Resource Manager**
  - Manages a queue of jobs for a cluster of resources
  - Launches job to a simple FIFO job queue
  - The Resource Manager is Torque

- **Workload Manager**
  - A scheduler that integrates with one or more Resource Managers to schedule jobs across domains of resources (servers, storage, applications)
  - Prioritizes jobs
  - Provides status of running and queued jobs
  - Implements fair-share mechanism and achieving efficient utilization of resources
  - Enforces established policy
  - Collects and reports resource usage statistics
  - The workload manager is Moab
User submits job request

Moab Workload Manager

Control jobs

Torque Resource Manager

Query jobs, resources & policies

iDataPlax dx360 M2 node001,…node168

x3950 M2 servers smp001, ... smp007
Moab / Torque scheduler

- Moab Cluster Suite
  - Initially started as the commercial derivative of Maui Cluster Scheduler when the open source job scheduler was maintained and supported by Adaptive Computing (formerly Cluster Resources, Inc) mid-90s for use on clusters and supercomputers with contributions from several academic institutions and national research labs.
  - The Maui Workload Manager is NOT a resource manager.
    - The scheduler tells the resource manager what to do, when and where to run jobs
    - Can be integrated with several resource managers, including Torque
  - Capable of supporting multiple scheduling policies, dynamic priorities, extensive reservations and fair-share capabilities
  - Users typically submit jobs and query state of resources and jobs through the resource manager.
    - Users will submit the job script for the resource manager.
- **Torque Resource Manager**
  - An open source resource manager providing control over batch jobs and distributed compute nodes
  - Community effort based on the original PBS project with enhancement in scalability, fault tolerance and feature extensions over standard OpenPBS
  - Fault Tolerance Additional failure conditions checked/handled Node health check script support
  - Aggressive development with new capabilities – advanced diagnostics, job arrays, high-throughput support
  - **Scalability**
    - Significantly improved server to MOM communication model
    - Ability to handle larger clusters (over 20,000 cores)
    - Ability to handle tens of thousands of jobs
    - Ability to support larger server messages
- Documentation on Moab and Torque resource manager at Adaptive computing
  - Links from the url:
    http://www.clusterresources.com/resources/documentation.php

- Tutorials / User Guide from computing centers, such as
  - https://computing.llnl.gov/tutorials/moab/
Moab commands

- Majority of Moab commands are for use by the scheduler administrators. For command details, access links from:
  

<table>
<thead>
<tr>
<th>Moab end user commands</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>checkjob</td>
<td>Provide detailed status report for specified job</td>
</tr>
<tr>
<td>mjobctl</td>
<td>Control and modify job</td>
</tr>
<tr>
<td>e.g. mjobctl –c JOBid</td>
<td>cancels a job with ID JOBid</td>
</tr>
<tr>
<td>showbf</td>
<td>Show resource available for jobs with specific resource requirements</td>
</tr>
<tr>
<td>showq</td>
<td>Display all jobs in active, idle and non-queued states. The flags to display extended details can only be used by level 1, 2, or 3 scheduler administrators</td>
</tr>
<tr>
<td>showstart</td>
<td>Show estimates of when job can/will start</td>
</tr>
<tr>
<td>showres</td>
<td>Show existing reservations</td>
</tr>
</tbody>
</table>
Submitting jobs

- If Moab is configured to run as root, users can submit jobs to Moab directly using `msub`

  `msub` [-a datetime] [-A account] [-c interval] [-C directive_prefix] [-d path]
  [-S path_list] [-u user_list] [-v variable_list] [-V] [-W additional_attributes]
  [-z][script]

- Jobs submitted by msub can run on any of the resources of the resources managers managed by Moab

- Jobs submitted to a resource manager (e.g. qsub for Torque) can only run resources managed by the resource manager.
Building Torque job script

- Users build job scripts and submit the job using the qsub command for scheduling
  
  ```
  ```


- The job script is a plain text file
  - Includes shell scripting, comment lines
  - Command, directives specific to the batch system
    - The directive is an alternative to command line option to specify job attributes
    - All directive lines must precede shell script command

- Shell scripting is parsed at runtime

- The job script may be specified as qsub command line argument [script] or may be entered via STDIN or piped to qsub.
  
  ```
  cat job.script | qsub
  ```
Torque job script..

- The job script will be executed from the user’s home directory
- For parallel jobs, the job script will be staged to and executed on the first allocated compute node.
- The job script will use the default user environment variables (set in the shell startup script e.g. .bashrc) unless the ‘-V’ or ‘-v’ flags are specified to include all current environment variables (-V), or selected environment variables (-v)
- qsub will pass the value of the environment variables HOME, LANG, LOGNAME, PATH, MAIL, SHELL and TZ to the job script and be assigned to a new name prefixed with PBS_O
- qsub will process a line as a directive is the string of characters starting with the first non white space character on the line and of the same length as the directive prefix matches the directive prefix.
- The directive prefix is determined in order of preference:
  - value of command line option “-C”
  - Value of environment variable PBS_DPREFIX if defined
  - The string “#PBS”
Resources are requested at job submission with:

- with command line option –l for qsub. For example: -l walltime=1:00:00 –l nodes=4:ppn=4
- Directives in the job script. For example,
  #PBS –l walltime=1:00:00
  #PBS –l nodes=4:ppn=4

A few frequently requested resources:

- `-l mem=<size>` is maximum amount of physical memory used by the job
  where `<size>` is defined in form of number of bytes (suffix b) or words (suffix w)
  The multiplier is k=1024, m=1,048,576, g=1,073,741,824, t=1,099,511,627,776
  e.g. –l mem=1gb

- `-l vmem=<size>` is maximum amount of virtual memory used by all concurrent processes in the job

- `-l walltime=<seconds>` or `[HH:]MM:[SS]` is the maximum amount of real time during which the job is in run state

- `-l cput=<seconds>` or `[HH:]MM:[SS]` is the maximum amount of CPU time used by all processes in the job
-l nodes={<node_count> <hostname>}[<ppn<ppn>][<property>]<property>][+]

is the number and/or type of nodes to be reserved for use by the job. The value is one or more node_specs joined with the ‘+’ character, “node_spec[+node_spec...]”.

Each node_spec is an number of nodes required of the type declared in the node_spec and a name or one or more property or properties desired for the nodes. The number, the name, and each property in the node_spec are separated by a colon ‘:’. If no number is specified, one (1) is assumed. The name of a node is its hostname. The properties of nodes are:

ppn=# - specifying the number of processors per node requested. Defaults to 1.
property - a string assigned by the system administrator specify a node’s features

For example:

-l nodes=2:ppn=4+4:ppn=2 : requesting 2 nodes with 4 cores per node and 4 nodes with 2 cores per node, a total of 6 nodes with 16 cores
-l nodes=node001+node003+node005 : requesting 3 specific nodes by hostname
-N name : Declares a name for the job. If –N is not specified, the job name is the base name of the job script.

Running interactive jobs:
- -I option specified on the command line
- script include the –I directive
- Job attributed interactive declared to be true: -W interactive=true
- During execution of the interactive job, input to and output from the job is passed through the qsub.
- Useful for debug while building and testing applications
### Job Script Environment Variables

- Exported batch environment variables that can be used in job script:

<table>
<thead>
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<tr>
<td>PBS_JOBNAME</td>
<td>user specified jobname</td>
</tr>
<tr>
<td>PBS_JOBID</td>
<td>Job identifier assigned by the batch system</td>
</tr>
<tr>
<td>PBS_ARRAYID</td>
<td>value of job array index for this job</td>
</tr>
<tr>
<td>PBS_NODEFILE</td>
<td>Name of file containing the list of node(s) assigned</td>
</tr>
<tr>
<td>PBS_QUEUE</td>
<td>Name of queue from which the job will be executed</td>
</tr>
<tr>
<td>PBS_O_HOST</td>
<td>Name of the host upon which the qsub command is running</td>
</tr>
<tr>
<td>PBS_O_QUEUE</td>
<td>Name of original queue to which job was submitted</td>
</tr>
<tr>
<td>PBS_O_WORKDIR</td>
<td>Absolute path of current working directory of qsub</td>
</tr>
<tr>
<td>PBS_O_LOGNAME</td>
<td>name of submitting user</td>
</tr>
<tr>
<td>PBS_O_HOME</td>
<td>Home directory of submitting user</td>
</tr>
<tr>
<td>PBS_O_PATH</td>
<td>Path variable user to locate executables within job script</td>
</tr>
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</table>