Diffusion processes on complex networks

Torque/PBS systems

Janusz Szwabiński

Torque resource manager

- Homepage of the project:
  http://www.adaptivecomputing.com/products/open-source/torque/
- based on the original PBS projects
- provides control over batch jobs and distributed computer resources
- can integrate Maui/Moab (workload manager)

Job queues in Torque

- list of queues:

```
qstat -q
```

- detailed info on a queue:

```
qstat -Q -f
```

- job submission:
  - only on master node (with a running `pbs_server`)
  - submission command: `qsub`

Options of `qsub` command

Resource	Format	Description
`cput`	seconds or [[HH:]MM:]SS	Maximal time used by all processes of the job.
`file`	size	Total size of the disk space required for the job.
`host`	string	Name of the node on which the job should be executed.
`mem`	size	Total size of RAM space required for the job.
`nice`	integer number from -20 (highest priority) and 19 (lowest priority)	Priority of the executed process.
`nodes`	{<node_count> | <hostname>} [:ppn=<ppn>] [:<property>[:<property>]...] [+ ...]	Number and type of nodes required for the job. Hostname is the name of the node, ppn is the number of processors on given node (1 by default), property – a string assigned to the node by the cluster admin

Options of `qsub` command

Resource	Format	Description
`pcput`	seconds or [[HH:]MM:]SS	CPU time consumed by a single process within a task
`pmem`	size	Memory requirements of a single process
`pvmem`	size	Virtual memory requirements of a single process.
`vmem`	size	Virtual memory requirements of all processes running within a task.
`walltime`	seconds, or [[HH:]MM:]SS	Maximal real time required for completing the task.

Usage examples

```
# ask for 12 nodes
qsub -l nodes=12

# ask for 2 servers and 14 other nodes
qsub -l nodes=2:server+14

# ask for  2 processors on each of 4 nodes
qsub -l nodes=4:ppn=2

# task requires 200 MB of available RAM
qsub -l mem=200mb /home/torque/torque_demo

# wait until node01 will have 200MB of free RAM
qsub -l nodes=node01,mem=200mb /home/torque/torque_demo

# run on a node with gaussian resource
qsub -l other=gaussian /home/torque/torque_demo
```

Environment variables

Variable	Description
PBS_JOBNAME	Job name supplied by the user
PBS_O_WORKDIR	Working directory
PBS_ENVIRONMENT	N/A
PBS_TASKNUM	Number of tasks
PBS_O_HOME	Home directory of the submitting user
PBS_MOMPORT	mom active port
PBS_O_LOGNAME	user name
PBS_O_LANG	lang variable for the job
PBS_JOBCOOKIE	Job cookie

Environment variables

Variable	Description
PBS_NODENUM	id of the node executing the task
PBS_O_SHELL	shell script
PBS_O_JOBID	job id
PBS_O_HOST	node executing the task
PBS_QUEUE	name of the queue from which the task is executed
PBS_NODEFILE	file with list of nodes assigned to the job
PBS_O_PATH	Execution path

PBS batch script

```
#!/bin/sh

# example.pbs
# An example batch script for Torque.
# Lines beginning with #PBS are PBS directives, i.e.
# they contain arguments of the  qsub command.

# Name of the job:
#PBS -N ExampleJob

# Number of nodes, estimated execution time
#PBS -l nodes=1,walltime=00:01:00

# Which queue?
#PBS -q short

# Email address of the user  (for notification purposes)
#PBS -M username@hostname.domain

# Notification modes (a - stopped, b - started ,e - finished)
#PBS -m abe

# go to working directory
cd $PBS_O_WORKDIR

#execute task
date
```

Jobs in Torque

- submit a job

```
qsub example.pbs
```

- check status of jobs run by a user:

```
qstat [-u <username>]
```

- delete a job:

```
qdel <jobid>
```

- delete all jobs of a user:

```
qdelmine
```

What about Windows?

LIST STATISTICS

R_{max} and R_{peak} values are in GFlops. For more details about other fields, check the TOP500 description.

TOP500 Release

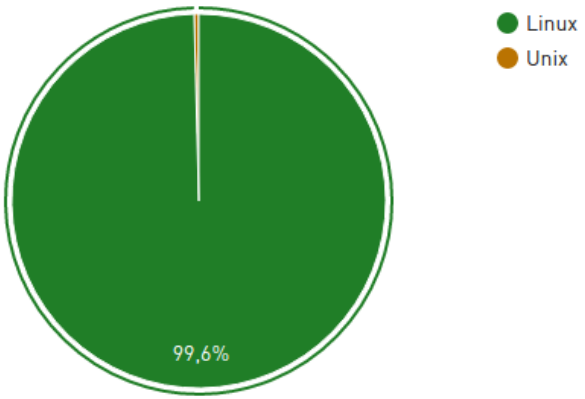
November 2016

Category

Operating system Family

Submit

Operating system Family System Share



Still not convinced?

- Microsoft HPC Pack
- PBS Pro