



Running Jobs on WestGrid

Martin Siegert, SFU
Roman Baranowski, UBC
Stephen Cartwright, UofC
Masao Fujinaga, UofA

<http://www.westgrid.ca/support/>



Overview

- Which is the right system for my program?
- How do I submit a program?
- How do I write a submission script?
- What should I know about scheduling policies so that I can adjust my jobs for optimum efficiency?
- How do I monitor submitted jobs?



WestGrid

Which System for which Job?

Cortex et al.: Parallel jobs using shared memory or MPI, large memory jobs, short run time

Nexus et al.: Parallel jobs using shared memory or MPI, large memory jobs, short run time

Matrix: Parallel jobs using MPI

Lattice: Parallel jobs using MPI, shared memory jobs up to 4 proc., Gaussian jobs

Glacier: Serial jobs, naturally parallel jobs using MPI, not more than 2GB of memory per process

Robson: Serial jobs, naturally parallel jobs using MPI, long run times



Submitting a Job

All WestGrid systems use a queuing and scheduling system Torque/Moab in order to

- maximize the use of the resources
- distribute resources fairly between users

running a job:

- ◆ write a submission script (text editor)
- ◆ submit script using the **qsub** command
- ◆ results in `<jobname>.o<jobid>`
errors in `<jobname>.e<jobid>`

Example

```
Glacier
File Edit Settings Help
siegert@nunatak2:~/c-progs/example> ls
hello hello.c wg-serial.pbs
siegert@nunatak2:~/c-progs/example> cat wg-serial.pbs
#!/bin/bash
#PBS -N hello-job
#PBS -l walltime=00:00:01
#PBS -l nodes=1

cd $PBS_O_WORKDIR
./hello
siegert@nunatak2:~/c-progs/example>
```

submission script

```
Glacier
File Edit Settings Help
siegert@nunatak2:~/c-progs/example> qsub wg-serial.pbs
2837522.teva.westgrid.ubc
siegert@nunatak2:~/c-progs/example> ls -l
total 32
-rwxr-xr-x  1 siegert  siegert   4670 Jan  3 12:42 hello
-rw-r--r--  1 siegert  siegert   237  Jan  3 12:41 hello.c
-rw-----  1 siegert  siegert     0  Jan  3 13:52 hello-job_e2837522
-rw-----  1 siegert  siegert    13  Jan  3 13:52 hello-job.o2837522
-rw-r--r--  1 siegert  siegert    99  Jan  3 13:46 wg-serial.pbs
siegert@nunatak2:~/c-progs/example>
```

job submission:

jobid

errors

output



Typical Job Submission Script

```
#!/bin/bash
```

```
#PBS -N wg-serial
```

```
#PBS -l walltime=48:00:00
```

```
#PBS -M siegert@sfu.ca
```

```
#PBS -m ae
```

```
#PBS -r n
```

```
#PBS -l nodes=1
```

```
cd $PBS_O_WORKDIR
```

```
./myprogram
```

shell

Name

Runtime

email

email at abort/end

restart?

of cpus

directory

program

Save script in file, e.g., wg-serial.pbs

Submit job with: qsub wg-serial.pbs



Parallel Job Scripts

Very system dependent!

(see system dependent section later)

Details on the web site:

www.westgrid.ca/support/programming/#parallel



Priority: Fairshare

Fairshare algorithm:

- every WestGrid project has an assigned fairshare target: usage percentage of the system
- priority depends on the difference between the target and the actual usage
- the actual usage is calculated within several fairshare windows with exponentially decreasing weights, i.e., historic usage is taken into account, but with decaying weights.

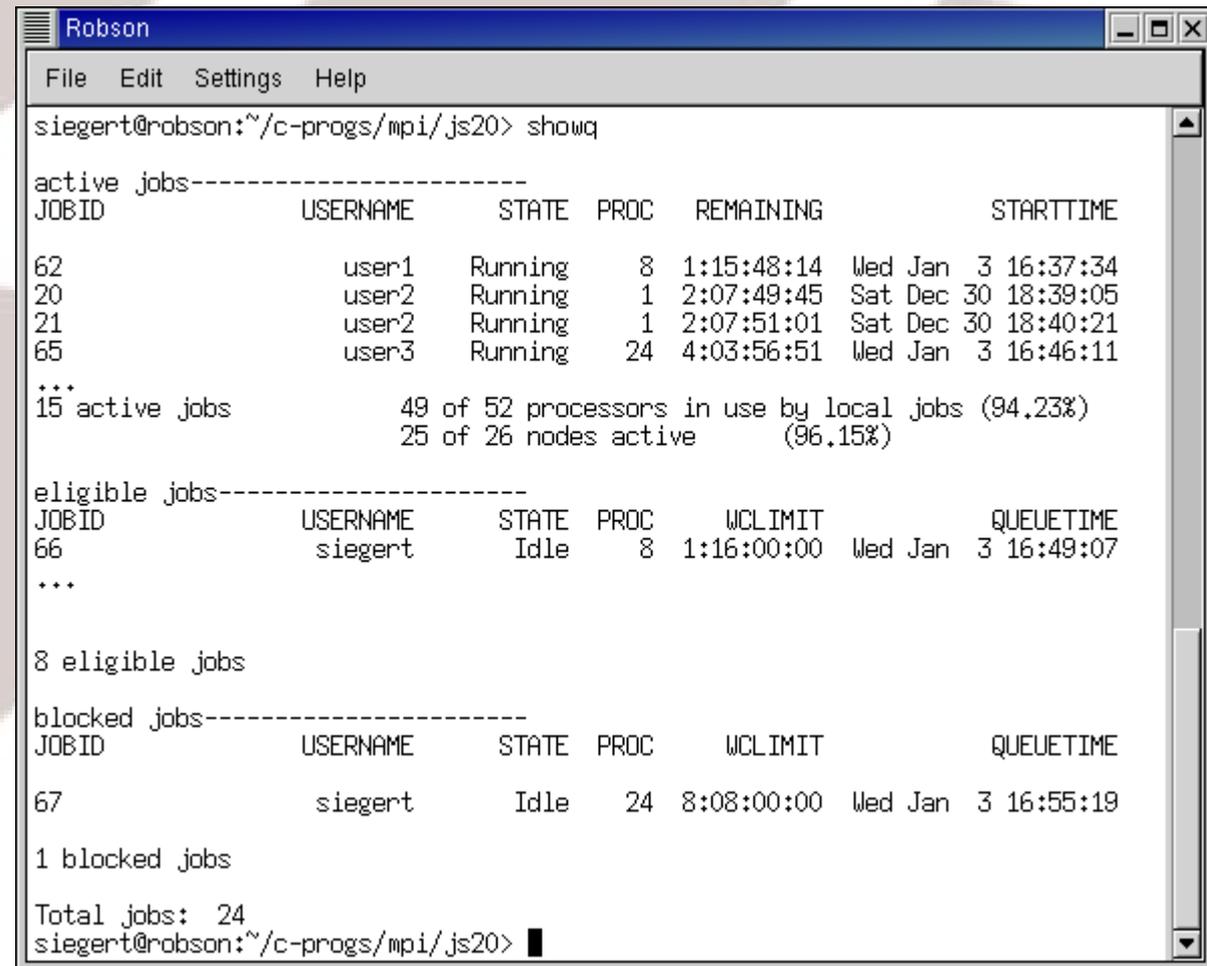
Monitoring

- List of jobs:

```

qstat -a
qstat -u <username>
showq
showq -r running
showq -i idle
showq -b blocked

```



```

Robson
File Edit Settings Help
siegert@robson:~/c-progs/mpi/js20> showq

active jobs-----
JOBID          USERNAME      STATE  PROC  REMAINING      STARTTIME
62             user1         Running  8  1:15:48:14  Wed Jan  3 16:37:34
20             user2         Running  1  2:07:49:45  Sat Dec 30 18:39:05
21             user2         Running  1  2:07:51:01  Sat Dec 30 18:40:21
65             user3         Running 24  4:03:56:51  Wed Jan  3 16:46:11
...
15 active jobs          49 of 52 processors in use by local jobs (94.23%)
                        25 of 26 nodes active      (96.15%)

eligible jobs-----
JOBID          USERNAME      STATE  PROC  WCLIMIT      QUEUETIME
66             siegert       Idle   8    1:16:00:00  Wed Jan  3 16:49:07
...

8 eligible jobs

blocked jobs-----
JOBID          USERNAME      STATE  PROC  WCLIMIT      QUEUETIME
67             siegert       Idle  24   8:08:00:00  Wed Jan  3 16:55:19

1 blocked jobs

Total jobs: 24
siegert@robson:~/c-progs/mpi/js20>

```

- WG Portal <https://portal.westgrid.ca/login.php>



Monitoring

(cont'd)

- estimated start time:

showstart <jobid>

```
Robson
File Edit Settings Help
siegert@robson:~/c-progs/mpi/js20> showstart 66
job 66 requires 8 procs for 6:06:00:00

Estimated Rsv based start in           00:44:08 on Wed Jan  3 17:58:44
Estimated Rsv based completion in      6:06:44:08 on Tue Jan  9 23:58:44

Best Partition: base

siegert@robson:~/c-progs/mpi/js20>
siegert@robson:~/c-progs/mpi/js20>
```



Monitoring (cont'd)

● problems?

checkjob <jobid>

```
Robson
File Edit Settings Help
siegert@robson:~/c-progs/mpi/js20> checkjob 67
job 67

AName: ac
State: Idle
Creds: user:siegert group:siegert class:q24 qos:qos24
WallTime: 00:00:00 of 8:08:00:00
SubmitTime: Wed Jan 3 16:55:19
      (Time Queued Total: 00:01:29 Eligible: 00:00:00)

Total Requested Tasks: 24

Req[0] TaskCount: 24 Partition: ALL
Network: --- Memory >= 0 Disk >= 0 Swap >= 0
Opsys: --- Arch: --- Features: ---

Flags:      PREEMPTOR
Attr:      checkpoint
StartPriority: 5028
EstimatedStart: H: 6935 R: -89 B: 62519
NOTE: cannot select job for partition base (job 67 violates active HARD MAXPS 1
limit of 9676800 for class q24 user (Req: 17280000 InUse: 0)
)
siegert@robson:~/c-progs/mpi/js20>
```

● disappeared?

tracejob <jobid>

tracejob -n 4 <jobid>



Cortex

- Mainly parallel or large memory jobs
- Serial jobs allowed on headnode
- Short runtimes (24 hours)
- IBM Power5 processors (plus one machine with Power4 processors)
- 4, 32, or 64 processor machines with 16, 156, or 256 GB memory, respectively
- <http://www.ualberta.ca/AICT/RESEARCH/WestGrid>



Cortex Policies

- **Jobs for the Power5 machines are submitted to a single queue and job sent to a machine that satisfies the resource requirement requested**
- **Jobs for the Power4 machine are submitted to a different queue (pwr4)**
- **Priorities according to fairshare**

MPI job on cortex

```
#!/usr/bin/bash
```

```
#PBS -S /usr/bin/bash
```

```
#PBS -l ncpus=2
```

```
cd $PBS_O_WORKDIR
```

```
# Note: MP_PROCS should be set to the number of  
processors required.
```

```
export MP_PROCS=2
```

```
export MP_HOSTFILE=/usr/local/etc/mpihosts/host.list
```

```
export MP_SHARED_MEMORY=yes
```

```
./pn
```

Machine limits

Machine name	Duration (hours)	Min. ncpus	Max. ncpus	Max. memory Gbytes
cortex	24	1	2	16
dendrite	24	3	64	256
synapse	24	32	62	256
bigfoot	24	1	32	16



Nexus

- Mainly parallel or large memory jobs
- Serial jobs allowed on two of the machines
- Short runtimes (24 hours)
- SGI MIPS processors of varying speeds
- 8 to 256 processor machines with 8 to 256 GB memory
- <http://www.ualberta.ca/AICT/RESEARCH/WestGrid>



Nexus Policies

- **Jobs are submitted to different queues corresponding to each machine**
- **Each queue has minimum and maximum limits on the number of CPUs as well as the amount of memory**
- **Priorities according to fairshare**
- **Job priority increases with time in queue**
- **Job priority decreases with recently run jobs**

MPI job on nexus

```
#!/usr/bin/bash
```

```
#PBS -S /usr/bin/bash
```

```
#PBS -q nexus
```

```
#PBS -l ncpus=2
```

```
# Script for running MPI sample program pn on nexus
```

```
cd $PBS_O_WORKDIR
```

```
# Note: NCPUS is a variable set by TORQUE to match the  
ncpus request above.
```

```
mpirun -np $NCPUS ./pn
```

Queue limits

queue name	duration (hours)	min ncpus	max available ncpus	max available memory (GBytes)
nexus	24	1	6	8
arcturus	24	64	256	256
borealis	24	8	64	16
australis	24	16	64	32
corona	n/a	n/a	n/a	n/a
helios	24	1	32	16



Lattice Resources

- 4 CPU Alpha machines (667 MHz – 1250 Mhz)
- Tru64 Unix operating system
- 17 DEC ES40s and 37 ES45s
- ES45s have Quadrics interconnect
- ES45s for parallel jobs, ideally 4-16 CPUs
- ES40s only good for 1-4 CPU jobs
- Memory available on a single machine ranges from 2GB to 8 GB
 - Most machines have 4 GB
 - Can be long wait times for 8 GB nodes



Lattice Resources

- 10GB quota for home
- /scratch and /scratch2 available for running jobs
 - 1.5 TB and 1.6 TB respectively
 - Not for long term storage!
- Most machines have local scratch (/local_scratch) with 100-136 GB capacity
 - This local disk has been found to be six times faster in a Gaussian test vs. non-local disk
- No quota on scratch filesystems, so please be reasonable with usage
 - Clean up old files!



Lattice Running Jobs

- Parallel jobs are preferred, however serial jobs are allowed to run
- G03 queue can be accessed using qsub's "-q" flag: i.e. "**qsub -q g03**"
- Jobs submitted to this queue have access to local scratch and three weeks (503 hours) run time
- G03 queue sends jobs to ES40s and ES45s, default queue jobs only go to ES45s
- No jobs > 4 CPUS submitted to g03 queue



Lattice

Running Jobs Continued

- Run time for default queue is restricted to one week (168 hours)
- There are also two nodes that only allow short (3 hour) jobs and ten nodes that only allow 24 hour jobs
- One interactive node (wg1) which is accessed using the interactive queue "**qsub -q interactive**" and limited to 1 hour run time



Matrix Overview

- 128 nodes
- Dual AMD 2.4 GHz Operton processors
- 2 GB of memory per node
- Fast Infiniband interconnect, good for parallel jobs
- 832 GB space for home (all users)
- 3.1 TB /scratch
- No quota so please be reasonable
- Linux operating system



Matrix

Running Jobs

- Very homogeneous environment
- No serial jobs except for debugging and benchmarking
- Great for larger (i.e. 16-64) CPU jobs that can make use of the fast interconnect
- Max walltime is 3 days (72 hours)
- Two nodes (m1 and m2) reserved for 3 hour jobs
 - Allows for testing
- “tracejob” command is not available for users on Matrix



Glacier

- serial jobs, naturally parallel MPI jobs (GigE)
- 3 head-nodes - nunatak{1,2,3}.westgrid.ca
glacier.westgrid.ca
- 840 nodes x 2 Intel Xeon CPU 3.06GHz (32bit)
- 90% nodes 2GB; 1 rack ice55_1,...,ice60_14 4GB
- <http://guide.westgrid.ca/>



Glacier Policies

- Maximum run time 10 days
#PBS -l walltime=240:00:00
job needs more time – **send e-mail** in advance
default runtime = 3h
- Nodes are shared ==> specify memory for job
#PBS -l mem=1024mb
default memory = 768mb (memory violation policy in effect)
- Parallel job (more than 4 cpus) **ask** for “parallel”
Quality of Service (qos)
#PBS -l qos=parallel



Glacier Policies

- Short debugging job (max 4 cpus, 10 min run time) **ask** for “debug” Quality of Service (qos)
#PBS -l qos=debug
ice1_1+ice1_2
- For a serial job maximum available memory
2007MB on 2GB node
4005MB on 4GB node
- Combine all “-l” options
#PBS -l nodes=10,mem=10gb,qos=parallel



Glacier Policies

- MATLAB users:

```
#PBS -W x=GRES:MATLAB,Image_Toolbox
```

- If your job requires multiple software licenses

```
#PBS -W x=GRES:MATLAB+2
```

```
#PBS -W x=GRES:MATLAB+2,Image_Toolbox+2
```



Glacier job monitoring and statistics

- qsort

```
nunatak1|2> qsort -c
```

Chassis	Load	Jobs	B L A D E S			C P U S		
			Down	Busy	Free	Down	Busy	Free
iceflow1	18.96	24	0	12	2	0	24	4
.....								
iceflow10	20.9	28	0	14	0	0	28	0
iceflow50	14.54	28	0	14	0	0	28	0
iceflow51	17.97	28	0	14	0	0	28	0
iceflow52	15.54	28	0	14	0	0	28	0
iceflow53	17.74	28	0	14	0	0	28	0
iceflow54	18.79	28	0	14	0	0	28	0
iceflow55	26.7	28	0	14	0	0	28	0
iceflow56	25.14	28	0	14	0	0	28	0
iceflow57	21.62	28	0	14	0	0	28	0
iceflow58	25.64	28	0	14	0	0	28	0
iceflow59	25.51	28	0	14	0	0	28	0
iceflow60	21.11	26	1	13	0	2	26	0

```
=====  
Total: Unique jobs running = 558; Load = 1195.11  
CPUs: Down = 2 ; Busy = 1671 ; Free = 7  
Cluster utilization ~= 99.4%  
nunatak1|3>
```

- glacier: /global/system/common/FS-Jan08
/global/system/common/Stats/stats-Jan08



Robson

- serial jobs, naturally parallel MPI jobs (GigE)
- long runtimes (no limit for serial jobs)
- 54 PowerPC 970 processors (1.6 GHz , 64 bit)
- 2 proc./node, 4GB/node, 24GB swap/node
- <http://www.westgrid.ca/support/robson>



Robson Policies

- max. 8 processors/user or 1 job using 8 to 24 processors
- max. run time: $112 \text{ days}/(\# \text{ of processors})$
e.g., 2 weeks for 8 processor job
- no limit for serial jobs (must specify walltime in submission script)
- no limits for preemptible jobs
- no increase of job priority due to waiting time in queue



Robson Parallel Job Script

```
#!/bin/bash
# torque script for MPI job on robson
#PBS -N robson-par
#PBS -l walltime=168:00:00
#PBS -r n
#PBS -l nodes=16

cd $PBS_0_WORKDIR
mpiexec -machinefile $PBS_NODEFILE -n $PBS_NCPUS ./mpi-program
```

● **Do not use** nodes=8:ppn=2

● details at www.westgrid.ca/support/robson



Robson Preemption

- Preemptible Jobs: the system is allowed to kill job when job with a higher priority gets submitted
- Checkpoint periodically: program has to write data to file that then can be used to restart job.
- resubmit automatically: add to submission script
`#PBS -r y`
- you decide:
 - submit with: `qsub -q pre script.pbs`
 - or add line to script file:
`#PBS -q pre`
- high throughput



Questions?