Cheese Cluster Training

The Biostatistics Computer Committee (BCC)
Anjishnu Banerjee
Dan Eastwood
Chris Edwards
Michael Martens
Rodney Sparapani
Sergey Tarima
and The Research Computing Center (RCC)
Matthew Flister
Greg McQuestion

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Review of Cluster Management Software

- Portable Batch System (PBS): early job scheduler started at NASA in 1991
- OpenPBS: open source version of PBS released in 1998 with the OpenPBS license
- Terascale Open-source Resource and QUEue manager (TORQUE): a cross-platform fork of OpenPBS originally released in 2003 with the OpenPBS license
- TORQUE: a distributed resource manager for the cluster providing control over queued jobs and distributed computers
- Maui: an open source scheduler which integrates with PBS/OpenPBS/TORQUE to improve overall utilization, scheduling and administration of the cluster (started mid-90s)
- Moab: a commercial scheduler originally based on Maui
- Adaptive Computing of Provo, UT: develops, maintains and supports TORQUE, Maui and Moab
- LANL Roadrunner runs TORQUE/Moab: ranked as the world's fastest supercomputer in 2008

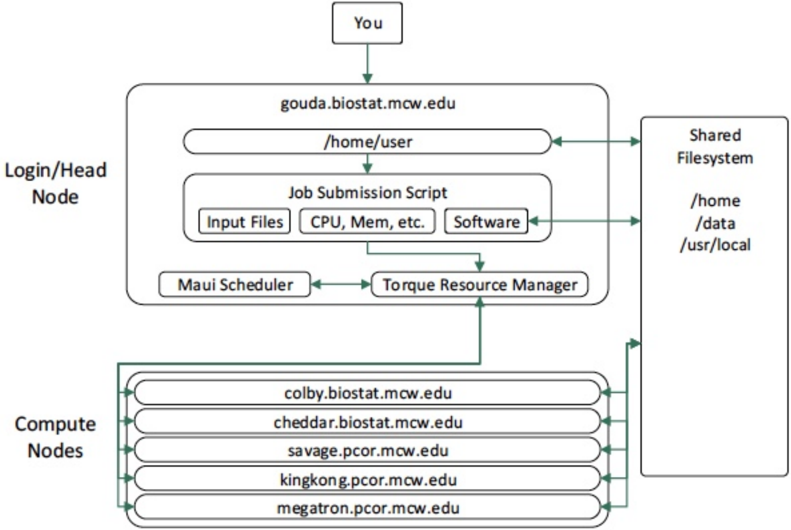
TORQUE Enhancements to OpenPBS

- More fault tolerant
- Better scheduling
- More user friendly
- More scalable

Cheese Cluster Timeline

- 2010, Jan: Oracle buys Sun Microsystems
- 2010, Mar: AMD releases AMD64 Opteron CPU with 12 cores
- 2010, Dec: PCOR switches to Linux with Dell 4 CPU servers
- 2014, Nov: BCC “discovers” TORQUE/Maui
- 2014, Nov: RCC forms and adopts TORQUE/Moab
- 2015, Mar: BCC adopts TORQUE/Maui
- 2015, May: PCOR acquires, godzilla, a large storage array
- 2015, Jun 4: Biostat moves to Linux with Dell
- 2015, Jul: Biostat and PCOR unite to create Cheese Cluster
- 2017, Jan-May: /home, /data, /usr/local moved to godzilla
- 2017, May 4: Cheese Cluster moves into Test phase
- 2017, Jun: Production phase

The Biostatistics/PCOR Cheese Cluster and You



Cheese Cluster Nodes: AMD64 Architecture

Node	Role	CPU	Core	Thread	Total
gouda	head/master	2 Intel Xeon	8	16	32
cheddar	compute/slave	4 Intel Xeon	8	16	64
colby	compute/slave	4 Intel Xeon	8	16	64
kingkong	compute/slave	4 AMD Opteron	12	12	48
megatron	compute/slave	4 AMD Opteron	12	12	48
savage	compute/slave	4 AMD Opteron	12	12	48

TORQUE/PBS Commands Batch: gouda$ qsub dm20

```
#!/bin/sh
####################################################
#this is the contents of script file dm20
#PBS -N dm20                # Set the job name
#PBS -l nodes=1:ppn=31      # N nodes with M threads
#PBS -l mem=2gb             # Xb/kb/mb/gb RAM (integer)
#PBS -l walltime=5:00:00    # H:00:00hrs elapsed time
cd $PBS_O_WORKDIR          # move to your current dir
time R --no-save < dm20.R >& dm20.Rout
#this is the end of script file dm20
####################################################
```

Take care with `-l mem` and `-l walltime`!

In R, use liberally: `object.size()`, `saveRDS()`, `rm()`, `gc()`

Each job generates 1 file for stderr: `NAME.eNNN` , e.g., `dm20.e97`

And 1 file for stdout: `NAME.oNNN` , e.g., `dm20.o97`

The output of `time` ends up in stderr

Notice that we don't need `nohup` nor `nice`

TORQUE/Maui Commands

TORQUE	submit a batch job	`gouda$ qsub` *script_file*
	submit an interactive job	`gouda$ qsub -I` *script_file*
		`gouda$ qsub -I`
	with X windows	`gouda$ qsub -I -X`
	check job status	`gouda$ qstat`
		`gouda$ qstat -u` *user_id*
	delete a job	`gouda$ qdel` *job_id*
	debug a job	`gouda$ tracejob` *job_id*
Maui	show queue	`gouda$ showq`
	show usage stats	`gouda$ showstats -u` *user_id*

TORQUE/Maui and PBS Documentation

- TORQUE/Maui: `man` *command_name*
- PBS environment variables and options: `man qsub`
- `#PBS -l` *resource_list*: `man pbs_resources_sunos4`

Cheese Cluster Queues

Name	Walltime Limit	Threads Limit	Jobs/User Limit	Description
small	72:00:00	8	3	Single node only
medium	96:00:00	32	2	Multiple nodes allowed
large	168:00:00	128	1	Multiple nodes allowed

- Multiple node jobs: the Message Passing Interface (MPI) for multiple nodes, i.e., suppose you need to run your job on 2 or more nodes simultaneously with TORQUE

Cheese Cluster Etiquette

- Do not start CPU intensive work on head/master gouda
  if gouda becomes unresponsive: all queued jobs may crash
  (GPU computing on gouda is OK, but please be careful)
- All CPU intensive jobs must be run through TORQUE
- Please refrain from logins to the compute/slave nodes unless you are debugging a failed job
  N.B. you can only login to a compute/slave node from gouda

Cheese Cluster Training Wrap-up

- This presentation and the final documentation will be put on our web page ASAP
- Keep in mind that we are sharing this precious resource
- Don't unnecessarily inflate `-l mem` or `-l walltime`
  your job may be repeatedly placed at the end of the queue
- Please look over the documentation
- If you have any problems, then contact Chris
  and thank him for all of his hard work!
- CRAN R packages: 8951 installed out of 10629
  Also, working on Bioconductor 1383 packages
- To "turn on" all of the nodes, we need to schedule a system shutdown. What is a good time for everyone?
- TORQUE demo
- Any questions?