Gridengine Basics

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TL;DR: To use James or Charles servers as if you were sshing into them as before, just ssh renown then qlogin.

1 Who is this for

People who use the James or Charles servers. Until now we have ssh'd into the servers but now ssh access has been removed from all but a few. Now in place is Son of a Grid Engine (SGE) to control access to servers. This guide shows you how to continue much like before and how to use basic SGE commands.

Son of a Grid Engine is an open source version of Univa Grid Engine (née Oracle Grid Engine (née Sun Grid Engine))

1.1 Useful references

- Informatics Documentation
- SGE project site
- SGE documentation
- man qsub from within renown

- MIT SGE introduction
- Informatics guide to connecting from outside the university

2 Getting started

Log in to the gridengine machine renown. If you're outside the forum you will need to set up AFS and Kerberos first. See the informatics guide to connecting from outside the University and external login via ssh

```
## If not on a dice machine
kinit s0816700
aklog
ssh -K s0816700@staff.ssh.inf.ed.ac.uk
# ssh -K s0816700@student.ssh.inf.ed.ac.uk
ssh renown
```

You will be in your home directory, in my case, /home/s0816700. We can see that lots of space has been added to the /home/ directory (/mnt/cdt_gridengine_home)

```
df -h
```

Filesystem	Size	Used	Avail	Use% Mounted on
/dev/vda1	24G	5.1G	18G	23% /
devtmpfs	2.0G	0	2.0G	0% /dev
tmpfs	2.0G	0	2.0G	0% /dev/shm
tmpfs	2.0G	9.4M	2.0G	1% /run
tmpfs	2.0G	0	2.0G	0% /sys/fs/cgroup
/etc/glusterfs/gv0.vol	147G	84G	57G	60% /disk/glusterfs/gv0
<pre>charles11.inf.ed.ac.uk:/cdt-gridengine-common</pre>	385G	264M	365G	1% /mnt/cdt_gridengine_common
anne.inf.ed.ac.uk:/cdt-gridengine-home	2.7T	432G	2.2T	17% /mnt/cdt_gridengine_home
/dev/vda4	7.6G	65M	7.1G	1% /var/cache/afs
AFS	2.0T	0	2.0T	0% /afs
tmpfs	396M	0	396M	0% /run/user/656624
tmpfs	396M	0	396M	0% /run/user/28328
tmpfs	396M	0	396M	0% /run/user/1559549
tmpfs	396M	0	396M	0% /run/user/1421660

Not covered here: how to run parallel jobs and writing to the distributed file system 'Gluster'. For information on running parallel jobs using SGE, see the latter half of the MIT SGE introduction.

3 Basic SGE commands

3.1 Interactive session on a node (just like sshing)

```
qlogin
```

Useful options:

• specify a specific node

```
qlogin -l h=charles14
```

• specify resource must have a GPU

```
# qlogin -l gpu=1 # old command
qlogin -q gpuinteractive
```

3.2 Submit a script to the queue

```
qsub myscript.sh
```

OUTPUT two files containing the stdout and sterr [script-name].o[jobnr] and [script-name].e[jobnr], and whatever files or directories your script creates

3.3 View status of your subitted jobs

```
qstat
```

OUTPUT

job-ID	prior	name	user	state	submit/start at	queue	slots
15	0.55500	long_sleep	s0816700	r	06/03/2016 22:54:38	all.q@charles11.inf.ed.ac.uk	1

 $\mathtt{state} \ = \ *qw*/**r** \ \texttt{for} \ *\texttt{queued} \ \texttt{and} \ \texttt{waiting*/**running**}$

3.4 Deleting Jobs

qdel

3.5 Viewing Node Status

qhost

OUTPUT

HOSTNAME	ARCH	NCPU	NSOC	NCOR	NTHR	LOAD	MEMTOT	MEMUSE	SWAPTO	SWAPUS
global	-	-	-				-			
anne	lx-amd64	64	4	64	64	0.02	995.6G	8.5G	31.2G	0.0
charles01	lx-amd64	32	2	16	32	1.01	62.7G	8.3G	31.3G	0.0
charles02	lx-amd64	32	2	16	32	0.27	62.7G	3.7G	31.3G	0.0
charles03	lx-amd64	32	2	16	32	0.01	62.7G	3.2G	31.3G	0.0
charles04	lx-amd64	32	2	16	32	0.04	62.7G	2.5G	31.3G	0.0
charles05	lx-amd64	32	2	16	32	13.61	62.7G	6.0G	31.3G	0.0
charles06	_	_	_	_	_	_	_	_	_	_

charles07	-	_	-	-	_	-	-	-	_	-
charles08	_	-	-	-	_	-	_	-	_	_
charles09	_	-	-	-	_	-	_	-	_	_
charles10	_	-	-	-	_	-	_	-	_	_
charles11	lx-amd64	24	2	12	24	0.01	62.8G	2.6G	31.4G	0.0
charles12	lx-amd64	24	2	12	24	0.01	62.8G	2.4G	31.4G	0.0
charles13	lx-amd64	24	2	12	24	0.01	62.8G	2.6G	31.4G	0.0
charles14	lx-amd64	24	2	12	24	0.01	62.8G	2.6G	31.4G	0.0

4 Example 1: Running an IPython Notebook and accessing it from outside DICE

- 1. Setup python virtual environment with IPython Notebook installed
 - Tip: install it in your home directory on DICE
- 2. qlogin to your server of choice
- 3. Check GPU use with nvidia-smi
- 4. activate your python virtual environment (you'll need to kinit & aklog if this is located on your DICE home as recommended)

```
source /afs/inf.ed.ac.uk/user/s08/s0816700/venv/nolearn/bin/activate
```

• Alternatively, if you have logged into your cdtcluster home repository, you can use:

```
id_number=s0000000
source /home/${id_number}/anaconda2/envs/deeplearning/bin/activate
```

keep in mind that anaconda2/envs/deeplearning refers to a conda environment that I set up, you will need to change that to yours.

5. create a password hash using python

```
from IPython.lib import passwd
passwd()
exit
```

6. start the IPython Notebook

```
longjob -28day -c 'ipython notebook --ip="*" --NotebookApp.password=sha1:0880f873e98f:9ddab2358586
```

- 7. access the notebook
 - From within forum simply browse to http://charles13:1337 (replacing charles13 with where you were)
 - Outside the forum either:
 - first kinit & aklog then, ssh port forward charles13:1337 back to your computer: ssh -K -L 8889:charles13:1337 s0816700@staff.ss.inf.ed.ac.uk then go to http://localhost:8889

 or connect to infromatics-via-forum using OpenVPN, find the address of the server to connect to (e.g. by sshing into informatics and ping charles12, and navigate to this IP on your computer

WARNING: If anyone finds/hacks your password...they have access to your filesystem

AWESOME WIN: this longjob process allows continual access to your filesystem after the original afs ticket expires

5 Example 2: Running GPU Jobs

Running jobs on the cluster requires setting all environment variables correctl in a bash script before executing it. Here we have a template of such a script:

```
#!/bin/bash
id_number=s1473470
export CUDA_HOME=/opt/cuda-7.5.18
export CUDNN_HOME=/opt/cuDNN-7.0
export LD_LIBRARY_PATH=${CUDNN_HOME}:${CUDA_HOME}/lib64:$LD_LIBRARY_PATH
export PATH=${CUDA_HOME}/bin:${PATH}
#export PATH="/home/s1473470/stuff" # use this for any local packacode you write
export PYTHON_PATH=$PATH
source /home/${id_number}/anaconda2/envs/deeplearning/bin/activate
#export theano_flags=THEANO_FLAGS=mode=FAST_RUN,device=gpu,floatX=float32
#you need to put this in front of any gpu theano processes
python tensorflow_example.py
THEANO_FLAGS=mode=FAST_RUN,device=gpu,floatX=float32 python keras/examples/cifar10_cnn.py
```

NOTE: This is a script that loads cuda and then tests tensorflow and runs a keras script that trains a CNN on the CIFAR10 dataset. To be able to run this you need to have installed theano, tensorflow and keras in your conda environme you could change the commands to your liking, but do include the libraries at t beginning.

6 Current issues

- Automatic resource allocation doesn't appear to take into account GPU use...
- ... working with Charles and Iain Rae on that
- IPython Notebook solution isn't very secure
- If you are running a script containing longjob using qsub, how is your kerberos ticket handled

7 Tips

- when logged in to renown type q then double tap tab to get a list of the commands for use!
- nvidia-smi lets you check the GPU use on a server if the command doesn't work then the server
 you are on doesn't have a GPU; try to login to another server; you can specify a specific server with
 qlogin -1 h=charles14