Using the Computer Science Cluster

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Computer Science (CS) High-Performance Computing (HPC) Cluster

- CS cluster has over 5200 nodes.
- Designed to run large scale computing jobs in batch mode (non-interactive mode).
 - Limited graphics-based interactive computing services.
- Users should set up their code to run in batch mode.
- Users who primarily need graphics-based interactive computing should use Economics Department cluster, ISD services, or desktop computers.

More information

- CS cluster webpage: http://hpc.cs.ucl.ac.uk/how_to_login/.
 - Get username and password from IT support,
- Econ GitHub page: https://github.com/UCL/ECON-CLUSTER
 - Contact Fatima or Andrew to be added to the UCL user group.
- If you need help,
 - CS support: cluster-support@cs.ucl.ac.uk
 - ECON IT support: economics.it@ucl.ac.uk

Obtain account

- Fill out and submit application form (see Fatima or Andrew).
- Wait 5-7 days and go to CS Cluster office: (4.20 Malet Place Engineering Building).
- They will set up two accounts
 - OS departmental account (for remote access).
 - OS Cluster account (to use cluster).
- By default, both accounts have same username and password.

Connect to cluster

There are three ways to connect to the cluster:

- Onnect using ThinLinc (graphical interface).
- Connect using ssh (command line interface).
- Onnect using ftp (data transfer).

Connect using ThinLinc

Connecting using ThinLinc is a two-step process:

- Connect to a CSRW (Computer Science Remote Worker) using your CS Department Account username and password.
 - Instructions to dowload Thinling.
- Then connect to one of the cluster login nodes ("vic" or "wise") using your CS Cluster Account username and password.
 - Open terminal inside CSRW window.
 - Then type one of the following
 - ssh vic
 - ssh uctpXXX@vic
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Connect using ssh

- For remote access (i.e. when not connected to UCL network), connecting is a two step process:
 - Connect to "tails", "storm" or "jet" using your CS Department Account username and password.
 - Connect to the cluster using your CS Cluster Account username and password.
- For access from within the UCL network (e.g. a desktop in Drayon House or the Econ HPC), skip step 1.

Step 1: connect to "tails", "jet" or "storm"

- Open an ssh client (e.g. putty) or a terminal.
- Type
 - ssh -X uctpXXX@tails.cs.ucl.ac.uk
- Enter your CS dept. password.
- Note:
 - The option '-X' allows graphics to be forwarded from the CS cluster to your computer.
 - The username "uctpXXX" is that given when you are assigned your CS department account.
 - The text after the '@' is the address of the server.

Step 2: connect to cluster

- Logon to the CS cluster using ssh.
- Type
 - ssh -X uctpXXX@vic
- Enter your CS cluster password.

Connect to the CS disk storage using sftp

- To transfer files to cluster storage use sftp instead of ssh.
 - Open a terminal or an FTP client.
 - 2 Type
 - sftp uctpXXX@tails.cs.ucl.ac.uk
 - Senter your CS department password.
- From tails, you can directly access the CS data storage.
- For example, if you have previously requested CS to create a storage directory named "Nesheim-IO", you can access this by typing:
 - cd /slash/economics/research/Nesheim-IO
- See below requesting CS data storage.

Typical workflow

- Logon to cluster.
- Transfer data and/or files to cluster (using ftp or email).
- Edit files or code.
- Write a script to submit your job to SGE (Sun Grid Engine).
 - SGE is the scheduler that manages allocation of jobs to nodes on the cluster.
- Submit your job.
- Monitor job progress if necessary.
- Download results to your local computer (using ftp or email).

SGE sessions: two types

- There are two types of SGE sessions
 - Interactive sessions
 - Start session with "qrsh".
 - Interact with compute node directly on command line.
 - Good for developing code and testing things.
 - Non-interactive sessions
 - Start session with "qsub".
 - Job runs in background.
 - Good for running large scale, long running, or multiple jobs.
 - Cluster is optimised for this type of job.
- SGE jobs are command line only jobs.
- If you need to do GUI based interactive work, it is best to use an alternative cluster.

Interactive SGE sessions

- Use the "qrsh" command and specify running time and memory.
- For example, at the command line, type:
 - qrsh -l h_vmem=1.9G,tmem=1.9G,h_rt=8:0:0
- This command starts the session and requests 1.9 GB memory and 8 hours running time.
 - 'qrsh' is the login command for an interactive session.
 - '-I' is a flag for resource requests for the interactive session.
- Resource options listed after the '-I' flag are:
 - 'h_vmem=XG,tmem=XG' requests X Gb of memory
 - 'h_rt= H:M:S' requests that the session run for 'H' hours, 'M' minutes,
 'S' seconds
- For further command line options for 'qrsh' type: 'man qrsh'

User tips

- After starting SGE session, you need to load and open the software you require. See below for details.
- It may take a short while (1 5 minutes) to be allocated a node.
- To increase chances for quick allocation, request as little memory as necessary,
- For a small job, 2G is likely to be sufficient. For Matlab, request at least 4G.
- If you need a lot of memory (i.e. X > 2G), omit the 'h_rt' option from your 'qrsh' command.
- For example, to request a 14G session type:
 - qrsh -l h_vmem=14G,tmem=14G

Submitting batch jobs

To run a batch job:

- First, write a script (e.g. a text file names 'job1.sh') detailing what resources to request from SGE and what commands/programs to run.
- Then, submit the script using the command 'qsub'.
- For example, first create the file 'job1.sh' and then type the command
 qsub job1.sh
- Instructions for writing a script: job script instructions.

Some example command options to include in script

• Request memory and running time:

```
#$ -1 h_rt=1:10:35
#$ -1 tmem=1.9G,h_vmem=1.9G
```

Each line containing SGE flags starts with '#\$'.

Submit batch job to compute node: non-interactive session

Job status

Disk storage

Software available

Memory management

Graphics on jake or elwood

Cluster rules

- Never run jobs on head nodes (wise, vic, tails)
- Store important data and/or large data on /SAN/economics/...
- Avoid high frequency reading/writing of large datafiles to/from disk
- If you need support, send email to cluster support, go visit them in person.
- Update wiki page with tips for colleagues about how to solve common problems.
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