Using the Computer Science Cluster

Alan Crawford
Lars Nesheim

June 27, 2018

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
  1. CS departmental account (for remote access).
  2. CS 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:

1. Connect using ThinLinc (graphical interface).
2. Connect using ssh (command line interface).
3. Connect using ftp (data transfer).

Connect using ThinLinc

Connecting using ThinLinc is a two-step process:

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

Connect using ssh

- For remote access (i.e. when not connected to UCL network), connecting is a two step process:
  1. Connect to "tails", "storm" or "jet" using your **CS Department Account** username and password.
  2. 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

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

Connect to the CS disk storage using sftp

- To transfer files to cluster storage use sftp instead of ssh.
  1. Open a terminal or an FTP client.
  2. Type
     - sftp uctpXXX@tails.cs.ucl.ac.uk
  3. Enter 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

1. Logon to cluster.
2. Transfer data and/or files to cluster (using ftp or email).
3. Edit files or code.
4. 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.
5. Submit your job.
6. Monitor job progress if necessary.
7. Download results to your local computer (using ftp or email).

SGE sessions: two types

- There are two types of SGE sessions
  1. Interactive sessions
     - Start session with "qrsh".
     - Interact with compute node directly on command line.
     - Good for developing code and testing things.
  2. 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.
  - '-l' is a flag for resource requests for the interactive session.
- Resource options listed after the '-l' flag are:
  1. 'h_vmem=XG,tmem=XG' requests X Gb of memory
  2. '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:

  ```
  #$ -l h_rt=1:10:35
  ```

  ```
  #$ -l 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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