Using compute nodes interactively

Tutorial 2:
HPC at NYU

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Using compute nodes interactively
Some things require user interaction - debugging, and many uses of Matlab for example. And sometimes when preparing a job script it is helpful to work through it interactively first. However, the login nodes are not suitable for work requiring large amount of memory or computation. To support interactive use in a batch environment, Torque allows for interactive batch jobs.

**Options for running interactively on the compute nodes:**

- `-I`
  - Don’t just submit the job, but also wait for it to start and connect `stdout`, `stderr` and `stdin` to the current terminal.
- `-X`
  - Enable X forwarding, so programs using a GUI can be used during the session (provided you have X forwarding to your workstation set up)
- `-V`
  - Pass the current environment to the interactive batch job
To leave an interactive batch session, type `exit` at the command prompt.

Certain tasks need user interaction - such as debugging and some GUI-based applications. However the HPC clusters rely on batch job scheduling to efficiently allocate resources. Interactive batch jobs allow these apparently conflicting requirements to be met.

When you start an interactive batch job the command prompt is not immediately returned. Instead, you wait until the resource is available when the prompt is returned and you are on a compute node and in a batch job - much like the process of logging in to a host with `ssh`. To end the session, type `exit`, again just like the process of logging in and out with `ssh`.

```bash
$ qsub -I -X
qsub: waiting for job 3707318.soho.es.its.nyu.edu to start
qsub: job 3707318.soho.es.its.nyu.edu ready
$ hostname
compute-12-3
```

To use any GUI-based program within the interactive batch session you will need to extend X forwarding with the `-X` option or directive. This of course still relies on you having X forwarding at your login session - try running `xterm` before starting the interactive to verify that this is working correctly.

You can request resources for an interactive batch session just as you would for any other job, for example to request 4 processors with 4GB memory for 2 hours:

```bash
$ qsub -I -X -l nodes=1:ppn=4 -l mem=4GB -l walltime=2:00:00
```

If you do not request resources you will get 1 CPU and 2GB of memory, for 1 hour.

**Your interactive session will start in your home directory**, you can jump to the directory you submitted from with:

```bash
$ cd $PBS_O_WORKDIR
```

**Exercise**

Start an interactive batch session with the `-X` option for X forwarding. NYU has a site license for Matlab, so find and load the Matlab module, and start the GUI. Tinker with it, if you wish.

(Don't forget to quit Matlab and exit the interactive batch session after you're done)

**Advanced queuing options**

Torque also supports scheduling jobs depending on the outcomes of other jobs, treating large sets of similar jobs as a single unit, and other advanced usage. We won't cover them here, but the NYU HPC Wiki has further information.