MSc in High Performance Computing
Notes for first practical to set up machine accounts

Session 1: Informatics DICE desktop accounts

An Informatics DICE account is required to log in to desktop machines in the Informatics training rooms.

- You can set your initial DICE password at https://pp.inf.ed.ac.uk/.
- If you do not have access to a DICE desktop, you can test your account by logging in to student.ssh.inf.ed.ac.uk
- This is only a gateway system with minimal software – for serious work you should then log in to student.compute.ed.ac.uk

For documentation, see http://computing.help.inf.ed.ac.uk/.

Session 2: Applying for a Cirrus account

Cirrus is a national tier-2 HPC machine, hosted and managed by EPCC, which we will be using throughout the MSc. You need to apply for an account on Cirrus and this is a two-step process:

1. Sign up for a SAFE account at https://www.archer.ac.uk/tier2
    - Email address: **MUST** be your sms email e.g. s1234567@sms.ed.ac.uk
    - Nationality: **MUST** be your actual nationality – don't just use default (United Kingdom)
    - Institution: University of Edinburgh
    - Department: EPCC
    - Phone number/address: UK address/number
    - Opt out of user Emails: Don't check this box
2. Once you have received your SAFE password by email you need to request a machine account:
    - Log into SAFE (https://www.archer.ac.uk/tier2)
    - Under the "Login accounts" drop down, click "Request login account"
    - Select the project d167 from the drop down list.
    - Machine name is Cirrus
    - Your username **MUST** be your UUN e.g. s1234567

You will then receive an email informing you that your Cirrus account has been created and details about how to log in to the machine.

Session 2: Applying for a ARCHER account

Although you should be able to do all your semester-1 practical work on Cirrus, we encourage you to obtain an account on ARCHER as well.

To apply for an account on the UK national supercomputer, ARCHER, is very similar to Cirrus, again this is a two-step process (note the different URLs):

3. Sign up for a SAFE account at https://www.archer.ac.uk/safe/signup.jsp
    - Email address: **MUST** be your sms email e.g. s1234567@sms.ed.ac.uk
    - Nationality: **MUST** be your actual nationality – don't just use the default (UK)
    - Institute for RAE reporting: University of Edinburgh (scroll down drop-down menu)
    - Institution: University of Edinburgh
    - Department: EPCC
    - Phone number/address: UK address/number
    - Opt out of user Emails: Don't check this box

4. Once you have received your SAFE password by email you need to request a machine account
    - Log into SAFE (https://www.archer.ac.uk/safe/login.jsp)
    - On the Main page, click the "Request New Account" button
    - Select the project d167 from the drop down list.
    - Machine name is archer
    - Your username **must** be your UUN e.g. s1234567

You will later receive an email informing you when your ARCHER account has been created which will include details of how to log on to the machine. Whilst Cirrus accounts are created almost instantaneously, ARCHER accounts can take up to a few hours to create.

More details at http://www.archer.ac.uk/documentation/safe-guide/safe-guide-users.php
Detailed ARCHER documentation at http://www.archer.ac.uk/documentation/user-guide

Session 3: Logging into Cirrus and running a job

Logging in to Cirrus

Once you have received the email with your new account details then follow the instructions to retrieve your password.

You will need to use the Secure Shell, ssh, to connect to Cirrus.

- Linux: open a terminal and use the command `ssh`.
- Mac: as for Linux, but you also have to install “Xquartz” from https://www.xquartz.org/.
- Windows: install MobaXterm from https://mobaxterm.mobatek.net/.

Next, type: `ssh -XY cirrus-msc.epcc.ed.ac.uk` *(the –XY flags forward any UNIX X window graphics to your local machine.)* You can change your password with the `passwd` command

If you are very unfamiliar with UNIX then it is worth jumping to section 5 and working through the shell and editors documents before coming back to this section.

Open a terminal window and start a text editor e.g. `emacs`:

```
[cirrus-login2]$ emacs &
```

Emacs is a very sophisticated edirto but can be quite daunting for new users – you may find gedit easier to use:

```
[cirrus-login2]$ gedit &
```

Write a simple program (e.g. one that just prints “hello world”) in C, C++ or Fortran.

There are links Unix and editors guides on the Learn MSc Programme Information hub, see section 6 of this worksheet for more information.

Preparation to compile your code

Cirrus uses the module environment for selecting the appropriate compiler and libraries. We need to load the `mpt` and `intel-compilers` modules in order to have available the SGI parallel libraries and Intel compiler.

```
[cirrus-login2]$ module load mpt
[cirrus-login2]$ module load intel-compilers-17
```

To automate this, these two commands can be added into your `.bash_profile`

Compiling your code

To compile your code

- Fortran: use `mpif90`
  - `mpif90 -o hello hello.f90`
- C: use `mpicc`
  - `mpicc -cc=icc -o hello hello.c`
- C++: use `mpicxx`
  - `mpicxx -cc=icpc -o hello hello.cpp`

Both GNU and Intel compilers are available, we will use the Intel compilers here and in future practicals you will explore switching between compilers and the differences that this results in.

Running on the login node

Now you have compiled your code you can run it on the login node like any other program:

```
[cirrus-login2]$ ./hello
```

If you have followed the instructions above then you have compiled your code to use MPI, this is one of the key parallel libraries which you will be learning about in great detail during the MSc. We will now run four copies of your program in parallel on the login node:

```
[cirrus-login2]$ mpirun -np 4 ./hello
```

Running on the backend compute nodes

To run your executable on the backend compute nodes, you need to package it up into a submission script and submit this to the queue. There is an example you can copy and use:

```
[cirrus-login2]$ cp /lustre/home/shared/subhello.pbs subhello.pbs
```

(Note this script assumes your executable is called `hello`, if it is something different then you will need to edit the script.)

A queuing system called PBS is used, you can submit a job to it via the `qsub` command

```
[cirrus-login2]$ qsub -q R348954 subhello.pbs
```

You can use `qstat -u $USER` to list your queued or running jobs, or `qstat` to list all jobs.

Important: Once this has run you will find the output in a file named helloworld.oxxx (where xxx is a unique number). There will also be a helloworld.exxx containing any error messages.
Important: We are submitting with ***-q R348954*** which tells the queue system to use pre-reserved compute nodes for your job. This is known as a reservation and we will often use this during practicals in order to avoid having to wait in the machine's main queue. The exact reservation code will change from practical to practical.

You can always submit a job to the general Cirrus queue using:

```
[cirrus-login2]$ qsub subhello.pbs
```

Without a reservation, your job will be in the same queue as all other users and could take a long time to run depending on the overall usage of Cirrus.

Charging code

All jobs on Cirrus (and on ARCHER) are charged to an account or budget of CPU time. The default is the general d167 budget, specified by the following line in subhello.pbs:

```
#PBS -A d167
```

All students have access to their own budget indicated by your UUN, e.g. d167-s1234567.
Edit the script to charge to your own personal budget and check that you can still run your program using qsub. When running jobs on the MSc you should always use your own budget. Note that, if we provide you with a script, it will probably be set up to charge to the default d167 budget so you will need to edit the PBS scripts before running.

Session 5: Using ARCHER

The general principals are the same as Cirrus but with some minor differences. There are different compiler commands such as `cc` for C, `CC` for C++ and `ftn` for Fortran. After creating the executable `hello`, write a script called `hello.pbs` containing the following:

```
#!/bin/bash --login
cd $PBS_O_WORKDIR
./hello
```

You can submit this to the backend via

```
-bash-4.1$  qsub -Vl select=1,walltime=0:01:0 -A d167 hello.pbs
```

On ARCHER you may also use `qstat -u $USER` to list your jobs, or `qstat` to list all jobs.

Section 6: Shell and editors guide

There are guides for working with the UNIX shell and common editors on the MSc *Programmes Information Hub* Learn course. These can be found under the *induction* page (*Introduction to machine accounts* pane) and are prerequisite information for many of the labs. It is therefore worth working through this material to ensure you are fully familiar with it.

- The shell PDF is an introduction to the Unix Shell
- The introduction to Unix editors PDF provides an overview of the most common ways of editing files on Unix.

Section 7: Other Useful information

Register for EASE
http://www.ed.ac.uk/schools-departments/information-services/services/help-consultancy/help-services/online-help-guidance/students/it-help/guides/ease-guide

Register for Wireless
http://www.ed.ac.uk/schools-departments/information-services/computing/connecting/registering