

MX BAG training: software session programme

Time	Presenter	Description
13:00	James Parkhurst	Introduction and machine setup
13:15	Graeme Winter	MX pipelines and XIA2 at Diamond
13:30		
13:45	Richard Gildea	DIALS overview and graphical tools
14:00		
14:15	James Parkhurst	CCP4 I2 Scaling with Aimless
14:30		
14:45		Coffee break
15:00		Tutorial: Data processing with DIALS
15:15		
15:30		
15:45		
16:00		Tutorial: CCP4 I2
16:15		
16:30		
16:45		
17:00		Questions and general problem solving
17:15		
17:30		Coach to Wantage

General Information

Logging into Diamond Computers

You will all have been issued a FED ID – an alpha-numeric string consisting of 8 characters. This is the username which you use to log into the Diamond computers. **Anyone unable to use their FED ID to login, let us know as soon as possible!**

Where to work

Do not work in your home directory: /home/\${MY_FEDID} !!!

Disk space quotas on the home area are too small for large data files. You can work only in the processing directory of your visit. Each attendee will create and work in his/her directory by opening a terminal and doing the following. **(N.B. replace \${MY_FEDID} by your own FED ID).**

```
$ cd /dls/i03/data/2016/mx14586-2/processing/ # Go to the visit directory
$ mkdir ${MY_FEDID} # Make a directory for yourself
$ cd ${MY_FEDID} # Go to your new directory
```

This will give you the following working directory:

```
/dls/i03/data/2016/mx14586-2/processing/${MY_FEDID}
```

It can be convenient to add a symbolic link in your home directory to make it easier to navigate to. This can be done as follows:

```
$ cd ~
$ ln -s /dls/i03/data/2016/mx14586-2/processing/${MY_FEDID} bag_training
```

Some software may save data in your home directory. To check your disk quota type the following command:

```
$ quota -s
```

How to load software

At Diamond, software is loaded using the “module” system. In order to use DIALS or CCP4 I2, you need to load the module on your computer. A list of useful module commands is given below.

Task	Command
To check which modules are available	<code>\$ module avail</code>
To list which modules you have loaded	<code>\$ module list</code>
To unload a module	<code>\$ module unload \${MODULE_NAME}</code>
To load the CCP4 7.0 module	<code>\$ module load ccp4/7.0.4</code>
To load the DIALS latest module	<code>\$ module load dials/latest</code>