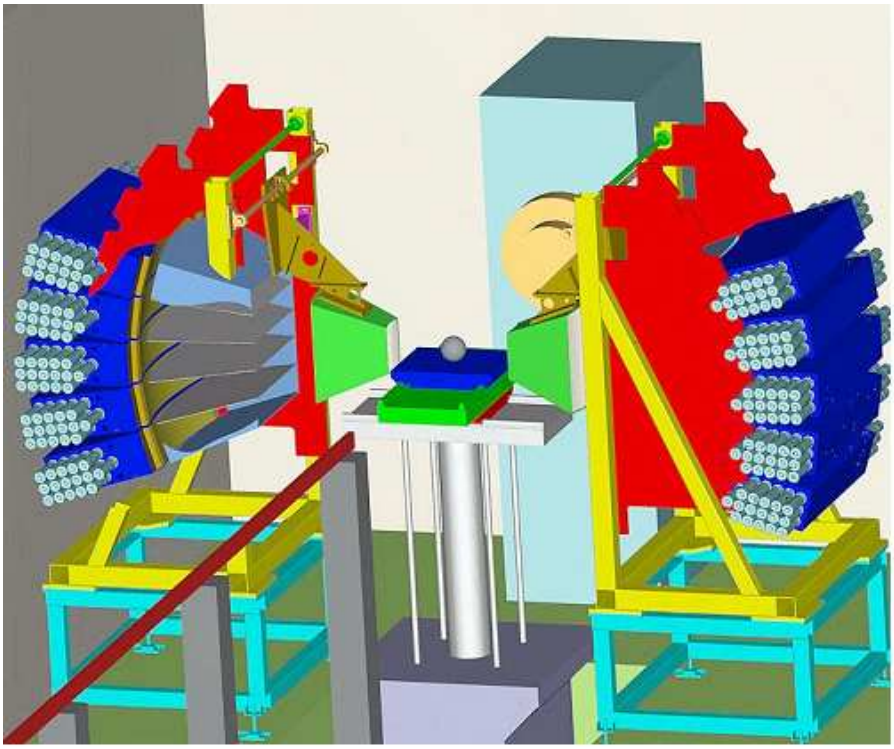
ENGIN-X User Manual



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1 Introduction

The purpose of this document is to help you gain the maximum benefit from the use of ENGIN-X. In conjunction with the information provided on the ENGIN-X website (www.isis.rl.ac.uk/engineering), it will help you to successfully plan and safely run your experiment, and to analyse your results.

You should not need to read the entire manual, but it would be helpful if you familiarise yourself with the sections which are relevant to your experiment before arriving at ISIS. This will save time once you are here and help to prevent simple mistakes. If you are a new user, it would be particularly useful for you to read Chapter 4: Getting Started, Chapter 13: Pitfalls, and to familiarise yourself with the data analysis software, EX-SBA, by downloading it (see Section 9.9) and following the examples in Chapter 9.

If you have any queries, please get in touch with your local contact. Also, please let us know if you spot something in the manual which you do not believe to be accurate: ENGIN-X is an evolving instrument, and details of its operation are liable to change over time! Some useful contact details are listed below.

Name	**Phone Extension** *	**Mobile (internal)**	**Mobile (external)**	**e-mail**
Javier Santisteban	5434			j.r.santisteban@rl.ac.uk
Ed Oliver	5792	1242	07765 852892	e.c.oliver@rl.ac.uk

*From outside RAL, dial +44 (0)1235 44 and then the extension. Please only ring mobiles during office hours, or to contact your local contact during an experiment.

Table 1: Contact details.

2 Preparing for your experiment

2.1 Before you arrive

This section details the things you should do before arriving at ISIS.

2.1.1 Contact the Instrument Scientist

Well in advance of your experiment, you should contact the Instrument Scientist to inform them of your plans and discuss your requirements. In particular, if your experiment involves the use of non-standard procedures or equipment, please make these known as early as possible so that preparations can be made. If you are intending to bring your own equipment, this must be brought to ISIS at least two days before the start of your experiment to allow safety checks to be carried out.

2.1.2 Arrange your experimental team

You should arrange for colleagues to assist you on the experiment. Generally, two or three people are required to ensure full use of the beamtime 24 hours a day. Please remember that your local contact is there to help you, but not to run your experiment!

2.1.3 Contact the ISIS User Office

Register with the User Office (isisuo@rl.ac.uk, tel +44 (0)1235 445592) using the form sent to the original contact applicant for the experiment. They will book accommodation for you as required. The earlier you do this, the better your chances of securing the best accommodation – the on-site guesthouse (R70) is very convenient if you will need to perform sample changes in the middle of the night!

2.1.4 Plan your experimental schedule

Before arriving for your experiment, you should have thought in some detail about the schedule of measurements you intend to make. This means thinking about the following parameters, which your local contact can help you decide upon:

- **Incoming beam size** (0.2 – 10 mm wide, 0.2 – 30 mm high).
- **Outgoing beam size** (0.5, 1, 2, and 4 mm available). For stress rig experiments, space restrictions mean that only the 4mm option is possible.
- **Wavelength range required**. This will determine the settings for the disc choppers and data acquisition electronics (DAE). The choppers are most commonly operated at 25Hz, giving a 40000μs time-of-flight window, which corresponds to a wavelength window of about 3.1Å. However, by altering the chopper opening times, this window can be placed anywhere in wavelength space, e.g. from 0.5 to 3.6Å, or 2 to 5.1Å. For a greater wavelength window, the choppers must be operated at lower frequency (e.g. 16.67Hz or 12.5Hz), with a corresponding reduction in intensity. Some examples of chopper and DAE settings are given in Appendix A – Chopper and DAE Settings.
- **Count times**. Ultimately, the count time required to obtain a diffraction spectrum of sufficient accuracy will determine how many measurements you can make. The count time depends on all of the above parameters (gauge volume, chopper frequency, etc.), as well as the sample properties and the path length of material through which the beam must travel.

2.2 When you arrive

Experiments generally begin at 10am. Please arrange to arrive before this time or on the previous day, to give you time to complete the following tasks before the beginning of your beamtime:

- Report to the MCR (main control room) for the issue of your access pass and film badge. These must be carried with you at all times during your visit.
- Go to the User Office (building R3, lower ground floor) to collect your meal vouchers (ISIS will no longer pay for meals eaten outside the site restaurant).
- Watch the safety video and read the safety pack with which you will be provided.
- Meet up with your local contact.
- Collect your sample record sheet(s) (ask your local contact where to collect them).

3 Description of ENGIN-X

This section summarises the main components of the ENGIN-X instrumentation. Specific operating instructions are given in later sections.

3.1 Design principles

ENGIN–X has been designed with the primary aim of making engineering elastic strain measurements: essentially the accurate measurement of polycrystalline material lattice parameters, at a precisely determined location in an object. The instrument is a time-of-flight neutron diffractometer which is optimised for this purpose in terms of intensity, resolution, sample environment, ease of use, and capacity for both large and small samples.

3.2 Incident beam

The instrument receives neutrons from a 100K liquid methane moderator. The moderator-sample distance (primary path length) is 50m and the sample-detector distance (secondary path length) is 1.5m. The beam travels to the sample along a curved **supermirror guide**, with m=3. There are two sets of counter-rotating **disc choppers** located along the beam path at distances of 6.4m and 9.6m from the moderator, allowing the frequency of neutron pulses to be set to various values between 5Hz and 50Hz, and enabling the wavelength range to be chosen according to the experiment. The lowest achievable wavelength is defined by the curvature of the incident neutron guide, and is approximately 0.5Å. Two pairs of motorised slits (named ***Jaws 1*** and ***Jaws 2***) are located along the incident beam path at distances of 4m and 1.5m respectively from the sample position, and allow the incident horizontal and vertical angular divergence to be modified.

3.3 Definition of scattering volume

The user is usually mainly concerned with the instrumentation which lies downstream of ***Jaws 2.*** A third set of motorised slits (named ***Jaws 3***) defines the gauge cross-section of the incident beam. This can be varied between 0.2 – 10 mm wide, and 0.2 – 30 mm high. ***Jaws 3*** sits on a motorised arm and can be moved towards and away from the sample position.

The outgoing beam dimension is defined by the use of ***radial collimators***. There are four sizes of collimator, defining gauge lengths of 0.5, 1, 2 and 4mm. The collimators are kinematically mounted for accurate positioning. You should decide which size of collimator is most appropriate for your experiment, taking account of the trade-off between spatial resolution and intensity.

3.4 Sample positioning

Beyond ***Jaws 3*** lies the ENGIN-X ***positioner***. This is a motorised positioning table with 3 orthogonal translation axes and a vertical rotation axis. It is capable of holding loads of up to 1.5T. Samples are accurately aligned using the positioner and ***theodolites*** which sit at nominal angles of $\pm 45^{o}$ to the incident beam. Use of the positioner is described in Chapter 6.

A robotic arm for rotary sample positioning is in the process of being commissioned. A goniometer can also be borrowed from the ROTAX beamline if agreed in advance.

Automated positioning can be achieved using SSCANSS (Strain SCANning Simulation Software). Details of the use of this software are given in Chapter 10.

3.5 Detectors

The diffraction ***detector banks*** sit behind the radial collimators. There are currently two diffraction detector banks, which are centred on horizontal diffraction angles of $\pm 90^{o}$ to the incident beam, and span angular ranges of 30^{o} in both horizontal and vertical directions. The North bank (also called bank 1) lies furthest from the entrance to the experimental hutch, while the South bank (bank 2), sits just in front of the entrance. Each bank consists of 1200 ZnS/^{6}Li scintillator detector elements, arranged in 5 units stacked vertically above one another, each comprising 240 horizontally stacked elements. The spatial resolution of the detector elements is 3mm (horizontally) x 150mm (vertically). The scintillator detector elements are monitored via fibre optics using photomultiplier tubes. The horizontal dimension provides an angular contribution to resolution which matches the flight path, and thus defines the highest resolution mode that the instrument is anticipated to run in.

There is also a pixellated ***transmission detector***. This lies in front of the beam stop (i.e. along the direction of the incident beam, behind the sample position), and can be manually slid forward towards the sample. This detector comprises a 10x10 array of 2x2mm detector elements, on a vertical and horizontal pitch of 2.5mm.

3.6 Sample environment

A 50kN hydraulic ***stress rig*** with a horizontal loading axis can be mounted on the positioning table for in situ testing of materials. Testing can be performed at temperatures up to 1200°C and within inert atmosphere using a ***radiant furnace***. Temperatures from -30°C to +150°C can also be achieved using grips cooled or heated by a refrigerated/heated oil bath. All this temperature control equipment can also be used independently of the stress rig.

3.7 Auxiliary equipment

A ***Coordinate Measurement Machine*** (***CMM***) is located outside the experimental hutch. This equipment can be used to accurately measure the relief of a component's surface, using a combination of a Metris laser scanning head and touch probes. The coordinates can be stored in a format which can be read by SSCANSS, allowing automated positioning and data analysis.

A second hydraulic stress rig for offline use in the process of being commissioned.

A **2T radio-controlled crane** is used to move heavy equipment. Only holders of CCLRC crane operator licences are permitted to use the crane. Anyone can take the training course to gain a licence - this might be useful for frequent users. Ask your local contact for details, or send an email to Dennis Abbley (D.D.Abbley@rl.ac.uk).

3.8 Computing

An important part of the development of ENGIN-X has been in the production of software tools for the control of the instrument and analysis of data. The major components of the software suite are the *Ray of Light* instrument control program, the ENGIN-X Script Based Analysis software (EX-SBA), and SSCANSS. The details of these packages are given in separate chapters below. Instrument control and data analysis are performed in the ENGIN-X cabin.

4 Getting Started

The purpose of this section is to provide the basic information required to obtain a diffraction profile using ENGIN-X. The subsequent manual chapters will give you more detailed information on individual components of the ENGIN-X hardware and software.

4.1 Interlock system

As with other instruments at ISIS, ENGIN-X makes use of an interlock system to ensure that no one remains in the experimental hutch while the beam is open. Your local contact will show you the procedure to open and close the hutch, but it is also written here for your reference.

4.1.1 Closing up the hutch

- After ensuring no one else is in the hutch, press the white search button (on the far wall, diagonally left from the hutch entrance). A warning bell will ring to inform people that the hutch is about to be closed. Note: if you have opened the door to the tunnel (far left from the hutch entrance), you will need to press the search button at the far end of the tunnel and close the tunnel door before hitting the main search button.
- Close the hutch entrance. If the latch prevents the door from closing, this is because you have either forgotten to press the search button(s), or allowed too much time to pass. In either case, press the button(s) again.
- Insert the spring-loaded bolt into the Fortress Interlocks lock, and turn upwards. This will enable you to remove the slave key from the door by turning **anticlockwise**. Note: the bolt and key can be a bit stiff: shake the bolt a little if you have trouble turning it.
- Put the slave key in the available slot on the blue key housing box, to the right of the door (push in and turn **clockwise**).
- Remove the MASTER KEY (labelled with a tag) from the blue box (turn **anticlockwise**), and insert in the slot in the green box sitting directly below the blue box (turn **clockwise**).
- The location of the master key in the green box ensures that all of the slave keys are housed in the blue box, and thus that access to the hutch is not possible. Therefore at this point it is safe to press the OPEN button on the orange box sitting directly above the blue key house. This opens the shutter and lights the "BEAM ON" indicator light.

Key tip: *Always make sure you have opened the shutter before beginning data acquisition, or you will not count any neutrons!!*

4.1.2 Opening the hutch

Press the CLOSE button on the orange box, and then follow the rest of the procedure for closing the hutch, but in reverse order (except for pressing the search button).

4.2 Instrument Control Computer

A brief introduction to the software used to control ENGIN-X is given here, because you will need to use the Instrument Control PC right from the outset of your experiment.

The Instrument Control PC is known as ***NDXENGINX***, and is located directly in front of you as you enter the ENGIN-X cabin. Communication with the various components of the ENGIN-X hardware is all conducted via this PC. There are two methods of communication:

1. Via the ***Ray of Light*** graphical interface.
2. Via the ***Open Genie*** command line.

Ray of Light is useful for performing operations a step at a time, while the ***Open Genie*** command line is required in order to issue lengthy sequences of operations as control scripts.

4.2.1 Introduction to the *Ray of Light* Instrument Control Program

Ray of Light is based on the LabView programming language, and consists of a number of graphically-based programs known as "**Virtual Instruments**" or "**VI**s", which control various parts of the ENGIN-X instrumentation. Some of these VIs are launched automatically when the computer is booted; others are started as and when they are needed. A typical view of the *Ray of Light* screen is shown in Figure 1. Various components of the screen are indicated on the right hand side and are described below.

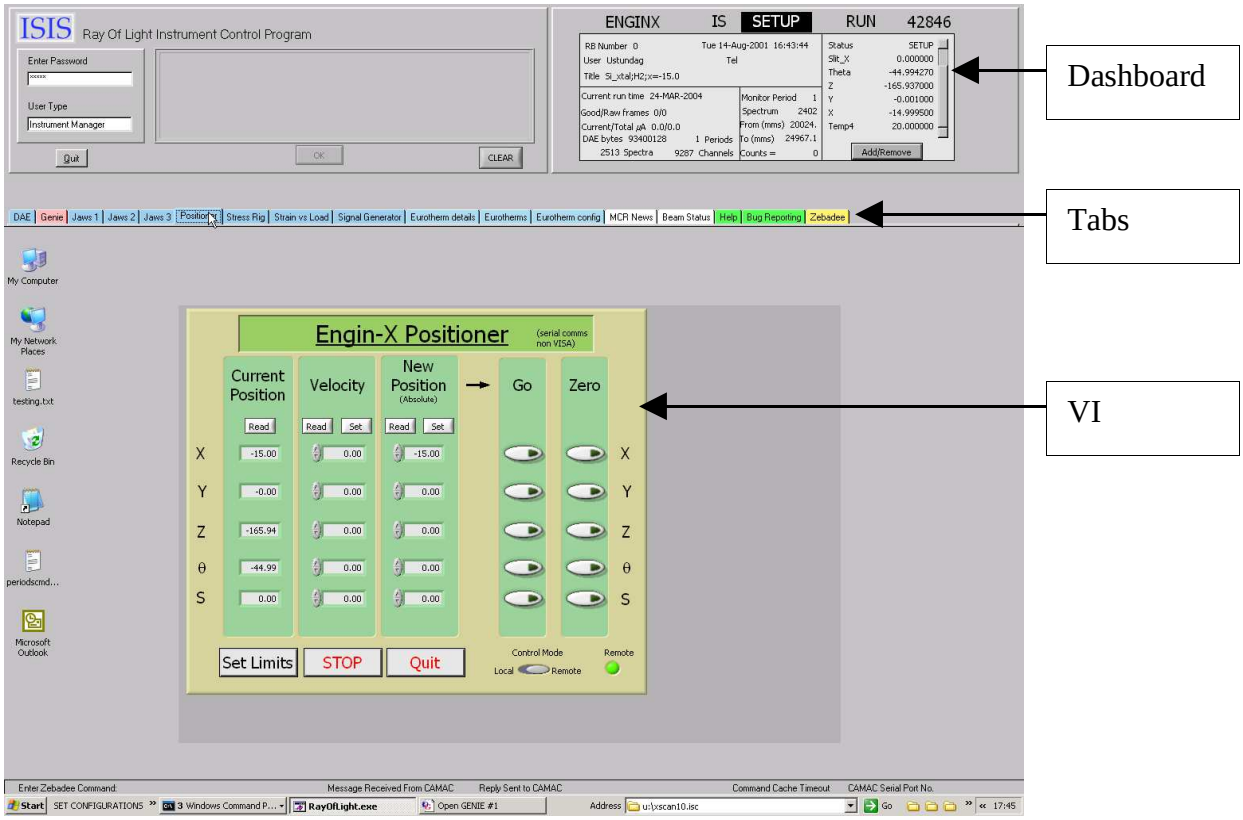

Figure 1: View of Ray of Light Instrument Control Program.

i) **Dashboard**: The dashboard gives information about the present neutron data acquisition. More detail will be described in section 4.4: Acquiring a diffraction spectrum.

ii) **Tabs**: Click on one of the tabs to display the graphical interface for the corresponding VI. This is then shown below (labelled VI in Figure 1).

4.2.2 Introduction to the *Open Genie* command line

Clicking on the "Genie" tab in *Ray of Light* should bring up an *Open Genie* command window. If it does not, you may need to click on the *Open Genie* icon in the Task Bar. Note that there may be two *Open Genie* windows open. If so, only the most recently opened will accept data acquisition commands. Use the window labelled *Open Genie* #2. If in doubt, you can open a new *Open Genie* window from the Start Menu.

In the *Open Genie* window, you can issue commands to perform the same operations as via the graphical interface. However, you can also issue scripts containing a series of commands. To find out how to do this see section 5.4: Using scripts.

4.3 Checking sample alignment

In order to align a sample, you will need to use the ENGIN-X positioner. Use of this is described in Chapter 6. However, for this Getting Started guide, it is assumed that you want to get a single diffraction profile from a sample which can simply be placed

on a suitable mount upon the positioner table. Nevertheless, you will still need to check that the gauge volume – as defined by the incident slits and the radial collimators – lies within the sample. In order to do this, look through the **theodolite** which sits on the left as you enter the hutch, and through the telescope which sits on the other side of the incident beam (climb under the beam guide). These should both be centred on the gauge volume – so move your sample until it is centred in the sights of both the theodolite and telescope.

Tip: The theodolite can be adjusted to point at any angle. Before you look through it, check the display to ensure that it is looking in the horizontal plane (Hz) at 0° and in the vertical plane (V) at 90°. Only then will it be aligned to look at the gauge volume. The angle can be adjusted by using the small knobs on the theodolite – DON'T move the large handles on its stand, or it will need to be re-aligned.

4.4 Acquiring a diffraction spectrum

Before acquiring a diffraction spectrum, the instrument should be in SETUP mode. This is indicated on the dashboard, an example of which is shown in Figure 2.

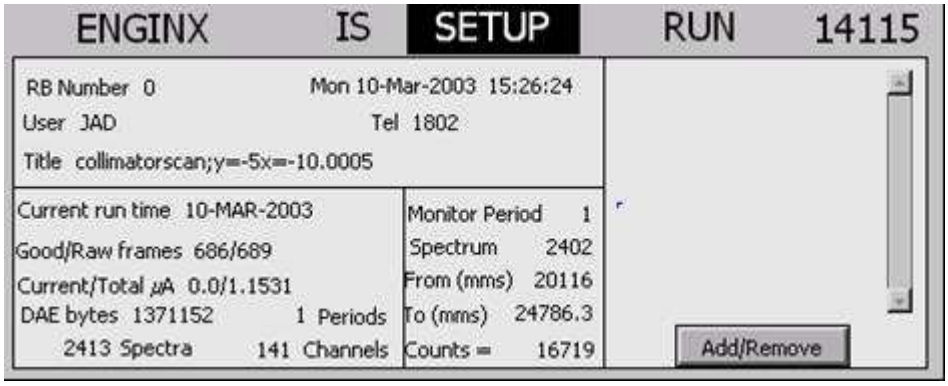

Figure 2: Dashboard.

You can **begin** data acquisition in two ways:

i) Type **begin** at the *Open Genie* command prompt.

ii) Use the **DAE** (Data Acquisition Electronics) VI in *Ray of Light*. This is accessed by clicking on the DAE tab. The DAE VI is illustrated in Figure 3. Data acquisition is started by clicking the "Begin Run" button at the top right of the VI.

Tip: *Ray of Light* is not very sensitive to mouse clicks. When clicking on a button, it should appear to depress slightly. If you do not see this happen, be aware that the click may not have registered. Get into the habit of checking whether your intended action is actually being executed, and be prepared to click again if nothing has happened. This will not usually cause any problems.

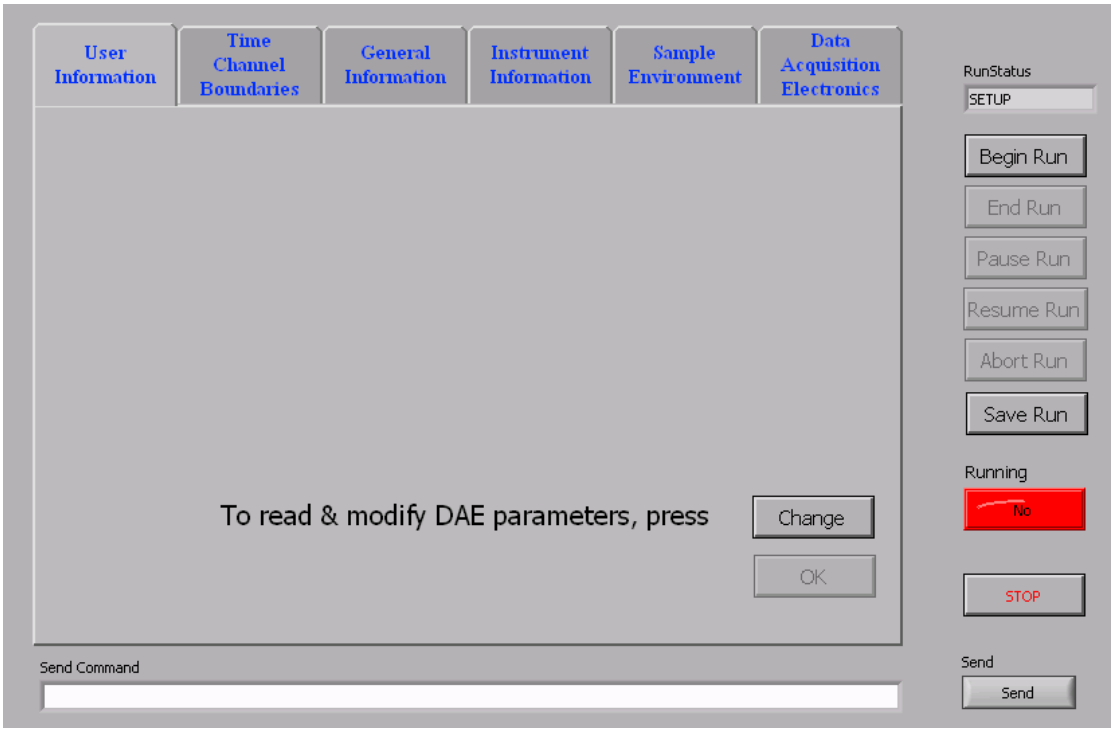

Figure 3: DAE VI

After beginning in one of these ways, the display at the top of the dashboard should read **ENGINX IS RUNNING**. This indicates that the data acquisition electronics are counting the number of neutrons arriving at the detectors.

A data acquisition interval is known as a run. The number of the current run is shown at the top right of the dashboard (i.e. 14115 in Figure 2). This number will automatically increment every time you finish a run and begin a new one.

After beginning a run, you should give it a title. The easiest way to do this is from the *Open Genie* command line, using the command **cha title="my title"** (including the quote marks). The new title will be displayed on the dashboard.

Tip: Keep titles to less than 24 characters. Although longer titles will be happily displayed on the dashboard, they will be truncated in the datafiles.

To **end** data acquisition, you can either type **end** at the *Open Genie* command line, or hit the "End Run" button in the DAE VI. This will return the display at the top of the dashboard to **ENGINX IS SETUP**. Upon ending a run, a binary datafile is created, called ENGXXXXX.RAW (where XXXXX is the run number), containing all the information on the data acquired during that run.

Tip: The dashboard contains other useful information. For example, the **Current/Total µA** line displays the present beam current, and the integrated current over the duration of the present run. You can also log experimental variables using the dashboard, such as the ***Jaws 3*** settings, or the current positioner positions. Click "Add/Remove" to bring up a list of variables. Select those you wish to log using shift+click, and click OK. The variables which are being logged will be displayed above the Add/Remove button on the dashboard (give it a minute to update).

4.5 Viewing your spectrum

ENGIN-X is equipped with a custom-written software suite for the full analysis of diffraction spectra, known as EX-SBA. Chapter 9 gives a complete description of this software, including showing you how to fit diffraction profiles in order to extract elastic strains. In order to get started, however, this section tells you how to view the diffraction spectrum you have acquired.

4.5.1 The ENGIN-X Data Analysis Computer

Data analysis is performed on the PC in the far right corner as you enter the cabin. This computer is known simply as ***ENGINX***. Your raw datafile and log files will be automatically copied to this computer a few seconds after the run is ended.

On the desktop, click on the 

icon, to launch EX-SBA. This will bring up two windows – an Open Genie command window, and a graphics window, labelled PGOLEDriver. In the command window, you will be asked for a one-word directory name. Your working directory will be given that name, and will reside on the G:\ drive. To view a spectrum, the data from all of the detector elements has to be summed, taking account the differences in flight path. This process is known as focussing. You can separately focus bank 1 (the North detector bank), and bank 2 (the South bank). To focus a run and view the resulting spectrum, type

xfocus *run bank* (arguments separated by spaces: e.g. **xfocus 14115 1** for run number 14115, bank 1).

This will display your spectrum in the graphics window.

Tip: You may wish to perform some or all of the analysis on your laptop. There should be no difficulty in setting this up, and it offers the advantages that you will not need to transfer your data at the end of your experiment, and can easily continue your analysis after you have left. See Section 9.9 to find out how to install the data analysis software, EX-SBA, and Section 12.1 for details of connecting your laptop to the network.

5 Instrument Control

This Chapter gives more information on using the *Ray of Light* interface and *Open Genie* command line for the purpose of controlling the instrument. However, separate chapters are devoted to the control of some of the more important or complex pieces of equipment.

5.1 Launching and halting VIs

As noted previously, some of the VIs begin running directly after boot-up of the control computer, whereas others are started as and when you need them. A VI which is not running will have a panel at the top consisting of several buttons, including one which shows a small arrow:  . This is the run button. To start the VI, click on the run button.

Most VIs have a QUIT button. Press this to halt the VI. Alternatively, click somewhere on the VI such that the pointer becomes a small hand:  . You can then halt the VI by simultaneously hitting CTRL and the full stop key (.).

5.2 The DAE VI

The DAE VI has already been introduced in Section 4.4. Look again at Figure 3. The buttons down the right hand side relate to simple data acquisition commands which can also be issued via the *Open Genie* command line. Those which were not introduced in Section 4.4 were:

- **Pause Run** – use this to pause the run if, for example, you wish to enter the hutch for some reason in the middle of a run. The display at the top of the dashboard will change to ENGINX IS PAUSED. The same action can be achieved by typing **pause** at the command line.
- **Resume Run** – use this to resume after having paused a run. Alternatively, type **resume** at the command line.
- **Abort Run** – you can abort the present run by hitting this button, but beware – the data will be lost forever! Alternatively, type **abort** at the command line.
- **Save Run** – use this if you wish to view a spectrum from the present run without actually ending the run. This will create a file of exactly the same format as the datafile created at the end of a run, but with the name ENGXXXXX.S01 instead of ENGXXXXX.RAW. If you hit **Save Run** again, it will create ENGXXXXX.S02, and so on - you can save as many times as you like. The same action is achieved at the command line by the command **updatestore**. To view the spectrum on the data analysis computer, you have to change the default extension, by issuing the command **set/ext "s01"** (or **set/ext "s02"** , etc.). Then you can issue the **xfocus *run bank*** command to view the spectrum, as explained in Section 4.5.1.
- **STOP** – this button stops the VI. It *does not* stop the current run. There should be no need for you to press it.

Tip: Although the shutter can be closed while ENGIN-X is running, always remember to pause if you wish to enter the hutch during a run. Otherwise, the normalisation of

your spectrum will be incorrect. Also, remember to resume once you come out of the hutch again – it is easily forgotten!

To access the tabs at the top of the VI, you need to press the **Change** button. You can then click on the tabs to bring up different sets of information about the DAE settings. However, these settings are mainly for the Instrument Scientist, and you should not need to change anything other than perhaps the information contained under the **User Information** tab. Here, you can enter information such as your name and institution. The other tab which is commonly used is the **Time Channel Boundaries** tab, where the time-of-flight window for data acquisition is set (start time and end time). This window depends upon the chopper settings, and you should not attempt to alter it unless you have been instructed by your local contact. The time-of-flight (TOF) width over which data is binned can also be set under the **Steps** heading. The default value is 0.0002 (in units of $\Delta T/T$, where ΔT is the width of the time window, and T the TOF). The wider the bins, the lower the resolution of your spectrum, but the smaller the size of the .RAW files. This reduces the down time between runs, so using wide time bins (e.g. setting to 0.01) can be useful if you wish to acquire a number of spectra quickly, and are interested only in the total intensity, rather than accurate peak positions – for instance, if you are scanning through the wall of a sample to accurately locate its position.

Tip: Instead of making the time bins wider in the DAE VI, you can issue the command **wallscan/on** from the command line. This sets the bin setting as 0.01, which is appropriate for wall scans. However, *remember to revert to high resolution afterwards*, by issuing the command **wallscan/off**. Otherwise your diffraction spectra will be blocky, and probably useless!

5.3 The Jaws VIs

The three pairs of incident slits - *Jaws 1*, *Jaws 2* and *Jaws 3* – are each controlled by a separate VI. You should not need to change the settings of *Jaws 1* or *Jaws 2* without first consulting your local contact. However, the VIs operate in exactly the same way as the *Jaws 3* VI, which is described here.

The *Jaws 3* VI is only activated when the slit dimensions need to be changed. The rest of the time, it is switched off to avoid unwanted oscillations of the slits due to feedback in the motor system. To alter the slit dimensions:

1. On *Ray of Light*, click on the Jaws 3 tab (see Figure 4 below).
2. Run the VI by clicking the play button:  .
3. Wait for the Status (Figure 4, top right) to change from “Initialising” to “OK”).
4. In the “Symmetrical Gap Setpoints” box (Figure 4, centre), enter the required vertical and horizontal gaps (in mm) in the corresponding boxes.
5. Hit the MOVE button (Figure 4, centre).
6. Wait until the Status changes from “Moving” to “OK”.
7. Hit the Quit button (Figure 4, bottom right).
8. Check that the reported slit dimensions, (Figure 4, top left) are sufficiently close to the required setpoints. If not, wait for the VI to stop running, and repeat the procedure.

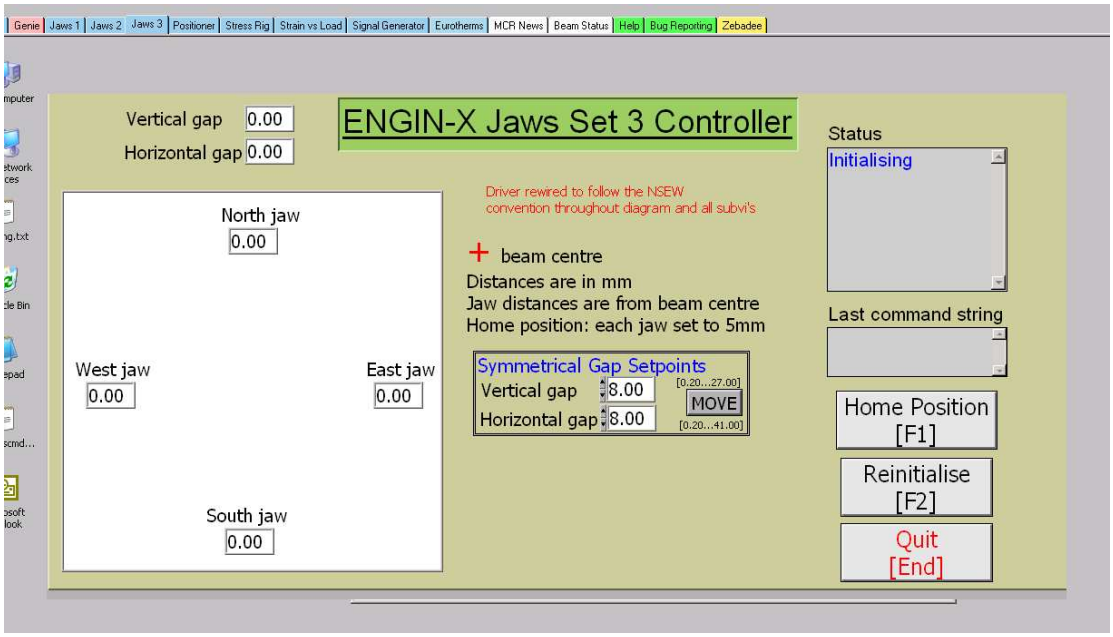

Figure 4: Jaws 3 VI.

5.4 Using scripts

You will quickly find that manually starting and stopping runs using the DAE VI or the Open Genie command line is not only tedious, but impractical. Therefore, most experiments make use of scripts to perform sequences of runs, changing parameters such as position or sample environment factors (stress, temperature, etc.) between runs. Scripts are text files containing commands which you could otherwise issue directly at the command line (e.g. to change position, or begin a run). However, you can also make use of Open Genie structures such as loops, if statements and arrays to give your scripts extra functionality and to make them smaller and more readable. You can also use blank lines and indentations to improve legibility. Scripts should be written in a text editor (such as Notepad) and saved with the extension .isc (e.g. **myscript.isc**).

5.4.1 A simple example of a script

A short example script appropriate for a strain scanning experiment is given below. The script moves the positioner's x motor to 2 values (5mm and 10mm), acquiring a diffraction spectrum at each position (see Chapter 6 for more information about using the positioner). The script is annotated by comments which come after the # sign. This tells Open Genie to ignore the rest of the line. The example highlights some of the important aspects of script writing.

```
LOCAL xpt          # always declare variables at the start
                   # using the LOCAL command
xpt=5.             # set the value of your variable
motor/x xpt        # send the positioner x motor to position xpt (see
                   # Chapter 6.
```

```
waitfor seconds=10          # give the motor time to move

BEGIN                       # start data acquisition
  waitfor seconds=1         # always allow 11 seconds after beginning a run
  change title="First run"  # change the title
  waitfor uamps=20.         # count neutrons for 20μA-hrs
 END                        # end data acquisition

xpt=10.                     #
motor/x xpt                 # change the x motor position and repeat
                            #
waitfor seconds=10
BEGIN
  waitfor seconds=11
  change title="Second run"
  waitfor uamps=20.
 END
                            # ALWAYS end scripts with a carriage return!!
```

5.4.2 Script-writing pitfalls – *read this section before running scripts!!*

There are some less than user friendly aspects of Open Genie which should be noted before attempting to issue scripts. Take note of the points below in order to avoid Open Genie objecting to your syntax, or worse – issuing wrong commands!

- All variables which you use in the script should be declared using the LOCAL command, as shown above.
- Open Genie is very fussy about variable types. It expects a decimal point for real variables, and is unhappy if it sees one in an integer variable. Note the waitfor commands in the above script – uamps is assigned a real variable, with a decimal point (20.) but, rather illogically, seconds is assigned an integer value (e.g. 12). You simply have to learn which variables should be real and which integer – and then make sure you assign them with or without a decimal point!!
- It is necessary to end all scripts with a carriage return.
- Open Genie is rather unpredictable as to whether or not it is concerned about upper or lower case. Generally, it is important to write the basic programming keywords (e.g. IF, LOOP, ENDIF) in upper case, but the higher level instrument control commands (e.g. motor, begin) can be written in either upper or lower case.

5.4.3 Running scripts

You should save scripts on the u:\\ drive on *NDXENGINX***.** To run the script you first issue the following commands at the Open Genie command line (given here for a script called myscript.isc):

loadscript "u:\\myscript.isc" ← this command loads the script into memory. You will be informed (in red text) if errors were detected in the script. If the script is loaded successfully, it is run by issuing:

myscript (without the .isc extension).

5.4.4 Script-writing tips

There are various programming structures which you can use to improve the functionality and legibility of your scripts. In general, it helps to have short scripts which can be easily read through to check for errors with potentially damaging consequences!

Titles and string variables

You can incorporate the present values of variables (such as position, stress, etc.) into titles. For example, the following statements read the current values of stress and strain reported from the stress rig (see Chapter 7), and incorporate them into the title:

```
cur_sts=stressrig:query("load")          # read current stress
cur_stn=stressrig:query("strain")        # read current strain

sts_str=as_string(cur_sts, "%.2f")       # convert stress to a string variable
stn_str=as_string(cur_stn, "%.2f")       # convert strain to a string variable

mytitle="myrun; stress=" + sts_str + "; strain=" + stn_str
                                         # concatenating strings to make a new
                                         # string variable

change title=mytitle                     # update the title
```

Note the use of the **as_string** command for converting a real variable to a string variable, so that it can form part of the title. The "%.2f" qualifier specifies the format – in this case the stress and strain variables are rounded to 2 significant figures after the decimal point.

Loops

Loops are one of the primary tools for writing succinct scripts. The relevant Open GENIE keywords are LOOP, FROM, TO and ENDLOOP. For example, the script below performs an 11-step x-scan, from an x motor position of –5mm to +5mm (i.e. in steps of 1mm):

```
LOCAL i xcen xrange nsteps xstep xpos mytitle

xcen=0.                                  # centre position
xrange=10.                               # scan range
nsteps=11                                # number of steps

xstep=xrange/(nsteps-1)                  # step size

LOOP i FROM 1 TO nsteps                  # start the loop
  xpos=xcen-xrange/2.+xstep*(i-1)        # define the new position
  motor/x xpos                           # start the motor
  waitfor seconds=10                     # give the motor some time to move
```

```
  BEGIN
    waitfor seconds=11
    change title="xscan;x="+as_string(yloc)
    waitfor uamps=20.
  END
ENDLOOP
```

Conditional loops

Infinite loops can also be set up by not using a counting variable. A conditional statement can be used to exit the loop, using the EXITIF command. For example, the following script, which is appropriate for a stress rig experiment, increments the stress in 5MPa intervals using a loop, and stops if the strain increases by more than 5%:

```
LOCAL start_stn cur_sts cur_stn

start_stn=stressrig:query("strain")      # read initial strain (see section 7.4.4)
cur_sts=0.                               # centre position

LOOP                                     # start the loop
  cur_sts=cur_sts+5.                     # increment stress variable by 5MPa
  stressrig/setpoint stress cur_sts      # change stress (see section 7.4.4)
  waitfor seconds=21                             # give stress rig time to ramp
stress
  BEGIN                                  # start data acquisition
    waitfor seconds=11
    change title="stress="+as_string(cur_sts)
    waitfor uamps=20.
  END
  cur_stn=stressrig:query("strain")      # read current strain
  EXITIF cur_stn>start_stn+5.            # exit loop if strain has increased by 5%
ENDLOOP
```

Arrays

Arrays are another useful tool for writing succinct scripts, if you wish to increment a variable but not in constant sized steps. For example, the following script – which is appropriate for strain scanning – fills an array with a number of x positions, and then uses a loop to run through these positions:

```
LOCAL nsteps xarr i

nsteps=5
xarr=dimensions(nsteps)                  # define the array
xarr[1]=0.1                              # fill the array with x values
xarr[2]=0.2
xarr[3]=0.5
xarr[4]=1.0
xarr[5]=2.0
```

```
LOOP i FROM 1 TO nsteps                 # start the loop

motor/x xarr[i]                         # drive x to the i-th position
waitfor seconds=10
BEGIN                                   # start data acquisition
  waitfor seconds=11
  change title="x scan"+as_string(xarr[i],"%.1f")
  waitfor uamps=45.
END

ENDLOOP
```

6 The ENGIN-X Positioner

Almost all ENGIN-X experiments use the positioner to a greater or lesser extent, so it is worthwhile familiarising yourself with its operating procedures.

6.1.1 Description of the Positioner

The positioner system consists of the following components:

- The positioner itself.
- An operator panel, mounted in the hutch on a wheeled station.
- A handheld control pad.
- The main controller, which is the first beige cabinet on the right hand side as you enter the tunnel.
- Control software on the Instrument Control PC.

The positioner has three orthogonal linear motor drives: X and Y (horizontal), and Z (vertical). In addition, a rotary drive supplies rotation about the vertical axis – this drive is interchangeably called θ, ω or W! The motorised travel of the ***Jaws 3*** slits towards and away from the sample is controlled in exactly the same way as the positioner drives. It will therefore be treated as an additional drive, denoted S, or "Shutter". Table 2 summarises the characteristics of each of the drives.

Drive	Amount of travel	Nominal accuracy
X	500mm	0.005mm
Y	500mm	0.005mm
Z	500mm	0.005mm
θ	370°	0.002°
S (Shutter)	500mm	0.01mm

Table 2: Positioner drive specifications.

The positioner has two modes of operation: "local control", when you control its motion using the handheld controller within the experimental hutch, and "remote control", when you issue commands via the Instrument Control PC.

6.1.2 Safety

The positioner drives are extremely powerful and could easily crush body parts which got in their way! For this reason, an interlock is fitted so that the positioner cannot be moved in remote control when the door to the hutch is open. This ensures that noone can issue commands remotely when there is a chance that someone in the hutch might get trapped by one of the drives. Switching between local and remote control modes is achieved on the instrument control PC (see section 6.3.2), and *can only be done when the MASTER KEY is stowed in the green interlock box* (see section 4.1 above).

When using the positioner in local control, ensure your own safety by following these simple common sense rules:

- Ensure you know how to use the positioner - if in doubt, ask.

- Exercise caution whenever any part of the body is within the movement range of the positioner, especially when changing samples.
- Be aware of the locations of the emergency stop buttons.
- Two people should be present whenever samples are being changed.
- NO ONE should enter the area under the decking while power is applied to the positioner.

6.2 Local Control of the Positioner

Note: if the display on the operator panel reads "REMOTE PC IS IN CONTROL", you will have to use the Instrument Control PC to transfer back to local control. Read section 6.3 for details.

To operate the positioner locally, you need to use the operator panel, and the handheld control pad. The operator panel consists of an LCD display, a keypad and an Emergency Stop button. The handheld control pad has five buttons: Start, Stop, Jog +ve, Jog –ve, and Emergency Stop.

Key Tip: If you think a collision is about to take place, hit the Stop button or, if more urgent, hit one of the Emergency Stop buttons. To re-start after hitting an Emergency Stop button, twist the button clockwise to release it, and hit the green Control On button on the main controller (in the tunnel).

6.2.1 Jogging a motor

If you want to change the position gradually as you observe the movement, follow these instructions for jogging a motor:

- Press the relevant axis key (X / Y / Z / W / S) on the operator panel. If, for example, you pressed X, the panel will read "X AXIS IS SELECTED".
- Press the Jog +ve or Jog –ve button on the handheld control pad. Hold down until the position has changed by the required amount. The motor will stop driving as soon as you remove your finger from the button.

6.2.2 Moving to a setpoint

If you wish to drive a motor to a specific position, follow the instructions below.

- Press the relevant axis key (X / Y / Z / W / S) on the operator panel. The LCD display will show which axis you have selected, the current setpoint (Pos. Cmd.), and the current actual position (Act. Pos.).
- To change the setpoint, select Edit, using the selection keys under the LCD display. You can then type in the required setpoint. There is no decimal point key on the keypad. Therefore, the value is entered by typing in the correct digits, followed by zeros to push the decimal point to the correct position. To input a negative value, select +/- (shown on the LCD) using the selection key. After inputting the number, hit Enter on the keypad.
- Hit Start on the handheld control pad to start the motor. It is a good idea to keep your eye on the positioner while it is moving, and be ready to hit the stop or emergency button if it looks like a collision might take place.

- When the movement is complete, check on the LCD that Act. Pos. is equal to Pos. Cmd. (i.e. that the positioner has correctly moved to the specified setpoint).

6.2.3 Setting the zero position

At any stage, you can set the current motor position as the zero point. For example, you may wish to set the zero point when a sample edge is lined up with the cross hairs in the theodolite. To set the zero, press the SET DATUM key on the operator panel. The display will read:

This will store the current (N) AXIS position as datum. Continue? YES NO

Select YES using the appropriate selection key.

6.2.4 Homing an axis

The true zero position of an axis is found by a procedure which moves the motor to a particular encoder reference point. The procedure is started by pressing the HOME key on the keypad, and may take a couple of minutes to complete. You should not need to home an axis unless the positioner has to be powered off and on again for some reason. This usually results in the current θ position being set as zero, in which case you will need to home the θ axis to find the true zero position. After homing θ, you should move to –0.16˚, and SET DATUM. This ensures that the x-axis is aligned parallel to the neutron beam when θ=0˚.

6.2.5 Limits

If you drive an axis too far, it will trigger an end-of-travel microswitch, and move slightly back away from the switch. An alarm will sound. Press the ACCEPT selection key on the operator panel to resume operation.

6.3 The *Ray of Light* Positioner VI

The Positioner VI is accessed by clicking on the Positioner tab on the *Ray of Light* display on the Instrument Control PC. The VI display is shown in Figure 5. If the VI is not running, you will see various icons along the top, including the play button:  . Hit this to start the VI.

Key Tip: Remember that in order to use the VI, the hutch Master Key must be stowed in the green interlock box (see Section 4.1).

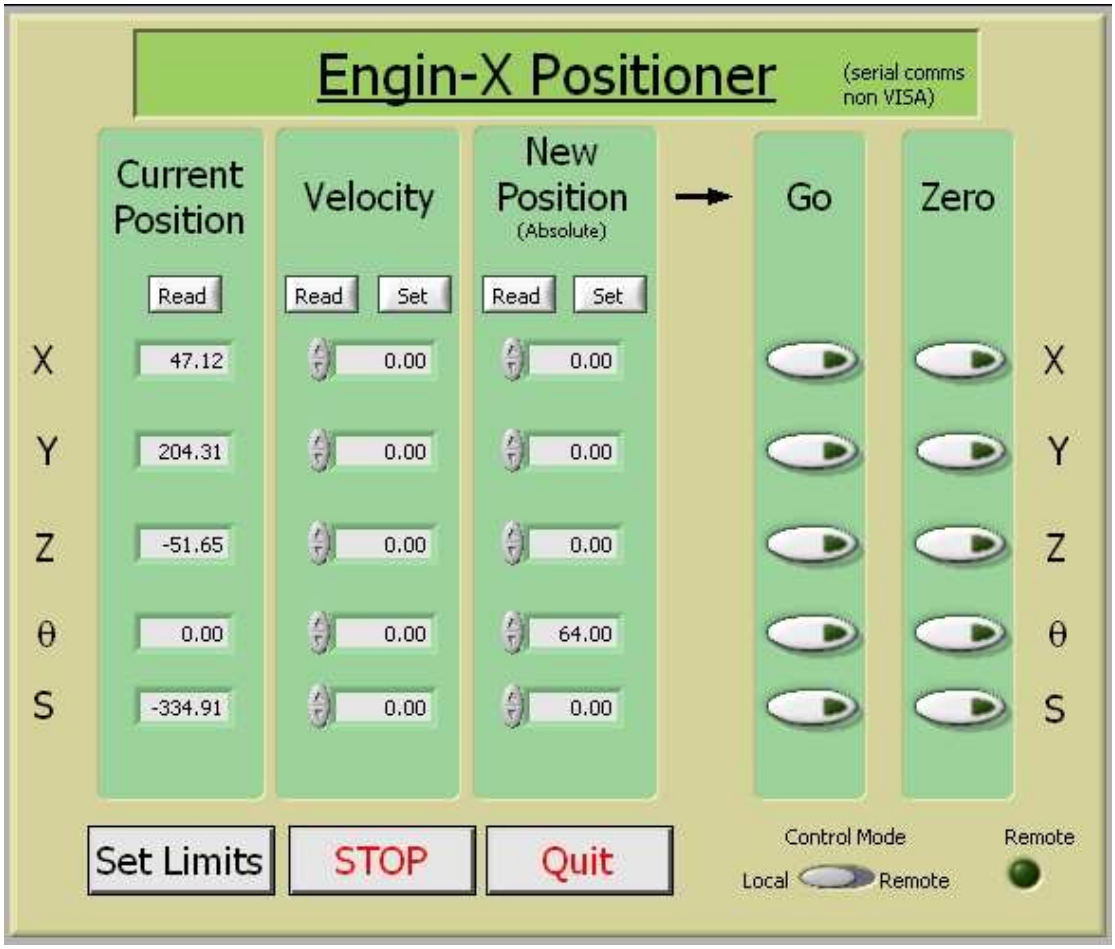

Figure 5: The Positioner VI.

6.3.1 Switching between local and remote control

Click the "Control Mode" switch at the bottom right of the VI to toggle between local and remote control. When in remote mode, the "Remote indicator light" on the right of the switch should be lit (i.e. bright green – it is unlit in Figure 5). If it fails to light, check that the hutch is closed up.

6.3.2 Remote control using the VI

Caution: When operating the positioner remotely, take special care to ensure that you do not issue commands which may cause a collision.

To issue motor commands via the VI, follow this procedure:

- In the New Position column, type the motor position you wish to move to in the box corresponding to the relevant axis.
- In the New Position column, hit the Set button.
- In the Go column, hit the button corresponding to the relevant axis. This will start the motor moving.

- After allowing sufficient time for the motor to move, hit the Read button in the Current Position column. This will update the current positions for all axes, allowing you to verify that the movement took place successfully.

If you think you have issued an incorrect value and then pressed the Go button, hit the Stop button as soon as possible to prevent a collision.

6.4 Remote Control using Open Genie commands

In addition to remote control of the positioner using the VI, you can also issue Open Genie commands. The main purpose of this is for incorporating a large number of movements into a script for strain scanning. The basic command is

motor/A pos

where **A** should be replaced by either **x**, **y**, **z**, **t**, **s**, depending on the axis (where t stands for theta – i.e. the rotation axis), and **pos** is the value you wish to move to. For example, if you wished to move x to 20.5mm, you would issue the command

motor/x 20.5

either from the Open Genie command line, or from within a script.

To read the current motor positions into a variable, issue the command

curpos=pt()

The variable **curpos** then contains all the current positions. If, for example, you wish to output the current x position to the screen, issue the command

printn curpos.x

6.5 Aligning your sample

Given below is a procedure which uses one theodolite and the positioner to align the centre of a cuboidal sample with the centre of the neutron beam. For more complex sample geometries, it may be beneficial to make use of the SSCANSS software: see Chapter 10 for details.

- Use the theodolite on the left-hand-side as you enter the hutch. Ensure from the display that line of sight is set correctly, i.e. with the vertical angle (V) set to 90.00°, and the horizontal angle (Hz) set to 0.00°. If the angles are not correct, they can be adjusted using the knobs on the left and right of the theodolite.
- Mount your sample on the positioning table so that one edge is parallel to the x-axis.
- Rotate θ to +45°, so that the x axis is perpendicular to the line of sight of the theodolite.

- Jog z so that the top edge of the sample is aligned with the crosshairs. Record the value of z.
- Jog z so that the bottom edge is aligned with the crosshairs, and again record the value.
- Move z to the average of the two recorded values, to ensure that the sample is vertically centred on the beam. If you wish, you can SET DATUM for the z axis at this point.
- Repeat this procedure for the x-axis, by jogging x so that the left and right sample edges are aligned with the cross hairs, and then moving to the average position.
- Rotate θ to -45°, so that the y-axis is perpendicular to the line of sight of the theodolite.
- Repeat the jogging procedure to centre on the y-axis.
- Rotate θ back to 0°.

7 The INSTRON stress rig

A 50kN Instron hydraulic stress rig is available on ENGIN-X for in situ mechanical loading. Please **do not attempt to use the rig unless you have received proper training from your local contact** - even if you have had experience using hydraulic loading systems elsewhere. The stress rig can be used on the ENGIN-X positioner within the hutch, or outside the hutch. It is moved in and out of the hutch using the crane – only the Instrument Scientists are permitted to do this. The rig can be operated in two ways:

- Locally, using the front panel.
- From the control computer (***NDXENGINX***), using the Stress Rig VI.

Full (but not necessarily user friendly!) operating instructions for the stress rig are available in the set of grey Instron folders which sit on the windowsill in the ENGIN-X cabin. Among these, the folder labelled "Operator's guide (dynamic testing)" provides basic operating instructions for the stress rig. However, this chapter gives a basic description of the equipment and summarises the operating procedures most commonly used.

7.1 Physical components

The stress rig system consists of the following components:

- **Hydraulic pump:** This is positioned outside the ENGIN-X building, in the kennel. It can only be run with the cooling system running (the cooler is a large box located outside the kennel). The power supply is 3 phase, switched on via a large red switch on the wall above and to the right of the pump. The stress
- **Intermediate hydraulic stage:** This sits on a portable frame close to the stress rig.
- **Load frame**.
- **Control tower**.
- **National instruments GPIB interface box:** This controls the communication between the stress rig control tower and ***NDXENGINX***, the ENGIN-X control computer.
- **Front panel:** The front panel allows full local control of the stress rig (including cyclic loading, alteration of limits, etc.). **Please use only the features which you have been shown by the Instrument Scientist**.

7.2 Safety

The stress rig can exert large forces very rapidly. For ductile samples (metals), there is little chance of shards being produced during failure, but it is possible that compression samples could be squeezed out from the grips at high speed. There is also the possibility of getting fingers or other body parts trapped. Caution should be exercised at all times when using the stress rig. Ensure that no one can operate the rig remotely while someone else is inserting/removing a specimen. This can be achieved by locking the control computer, ***NDXENGINX***. Tests should not be run when

people can interfere or be close to the rig. Therefore the rig should be surrounded by barriers when used outside the hutch. In the hutch, tests should only be carried out when the entrance is shut.

Hydraulic re/dis-connections should only be made under supervision of an Instrument Scientist, and never while power is supplied to the hydraulic pump. ***Emergency stops*** are located on the pump, the control tower and the load frame – these will turn off the pump, and terminate any programs which are running.

7.3 Local operation of the stress rig

For in situ testing during neutron data acquisition, you will probably control the stress rig remotely from the ENGIN-X cabin. However, to mount samples, you will need to use the front panel to control the stress rig locally. You do not need to switch between local and remote control – this is done automatically.

7.3.1 The front panel

Local operation is controlled using the front panel. A schematic of the front panel is shown in Figure 6. There are 2 LCD displays: the upper display provides information such as the present stress or actuator position. The lower display supplies options for you to select. You choose an option by pressing one of the selection keys below the display.

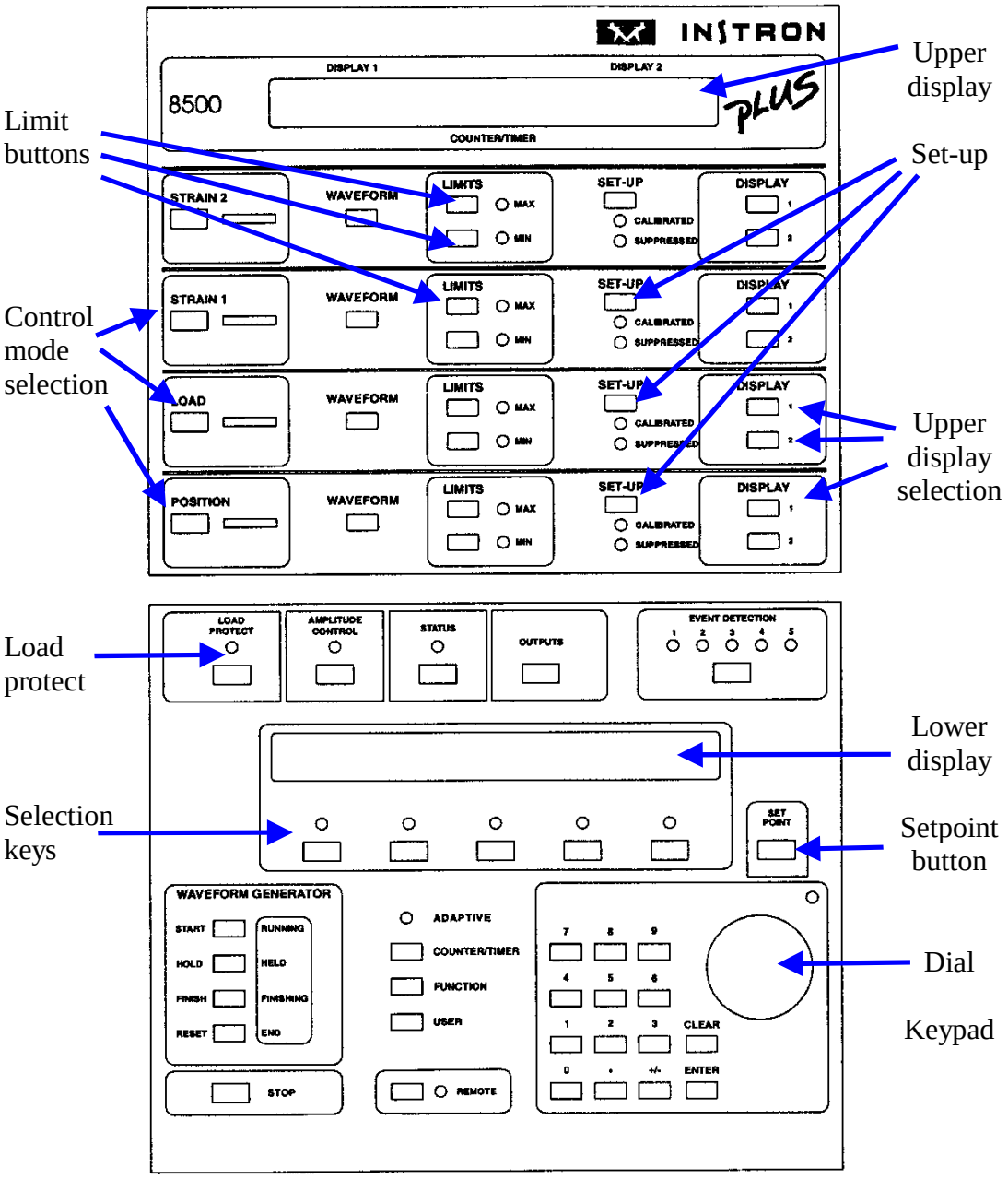

Figure 6: Schematic of the stress rig front panel.

7.3.2 Starting up the stress rig

The Instrument Scientist will ensure that the stress rig is set up correctly (hydraulic hoses attached, electrical connections made, etc.). However, at some stage it may be necessary for you to turn the rig on. The procedure for this is as follows:

- Flick the white on/off switch on the back of the controller. You should see the lights on the front panel flicker, and the display will indicate that several tests are being performed. These take a couple of minutes to complete.
- Press and hold the yellow “hydraulics on” button on the front on the controller. After a few seconds you should hear a sound as oil flow is initiated. You can then

take your finger off the button. If the button does not remain lit, try holding for longer.

- Hit the "actuator off", "low", "high" buttons on the front of the controller, in that order.
- The load cell will need to be automatically calibrated. Ensure the cell is not under any load, then press the set-up button (see Figure 6) corresponding to the load channel. Various menu options will be shown on the lower display. Navigate through the menus by selecting Cal→ Cal→Auto→Go. The auto calibration will be performed, and the green LED below the set-up button will stop flashing.

Hint: After starting up the rig, a red LED labelled STATUS may flash on the front panel. If you press the button below it and select "Frame status" from the lower display, this will indicate that the oil filter is blocked. However, this error message usually disappears once the hydraulic oil has had time to heat up. If it does not go away after about half an hour, ask the Instrument Scientist to replace the oil filter.

7.3.3 Choosing the control mode

The stress rig operates in either stress, strain or position control. This means that depending on the selected mode, it will try to maintain either constant stress, strain or actuator position. To change mode:

- Hit the corresponding control mode selection button (indicated on Figure 6).
- From the options shown on the lower display, choose IMMED (for immediate transfer of control).

7.3.4 Moving the actuator arm

The actuator arm has a travel of 100mm (from –50mm to +50mm). Before you insert a specimen, you will need to move it to roughly the right position:

- Select position control, as explained in section 7.3.2.
- Press 'Set Point' button above the dial.
- Either: tap in the value you require on the key pad and press ENTER – *this will change the position instantaneously, and so should be done with CAUTION!!*
- Or: rotate the dial to change the position gradually.

7.3.5 Inserting / removing a specimen

Depending on your sample type, there are a range of different grips for holding specimens (screw thread / Hounsfield type / compression, etc.). In most cases, the sample is located within the grips, and then the actuator arm is slowly moved towards the grip, and located by inserting a pin. Move the actuator arm using the dial, as explained in the previous section.

Tip: it is a good idea to turn on "load protect" when inserting a specimen. This ensures that only very small loads may be applied. Firstly, ensure that position control is selected. Then press the load protect button, as shown on Figure 6, and select On/Off from the lower display, to toggle on and off. When on, a red LED is lit next to the load protect button.

A typical sequence of actions for inserting a specimen are given below:

- Measure the cross-sectional area of your sample.
- Input this value (in mm^2) into the front panel by pressing the setup button for the load channel (see Figure 6) and navigating through the menus, selecting cal → cal → mm2 → mm2, and then inputting your value via the keypad.
- Insert your specimen by moving the actuator arm, as described above.
- Turn off load protect, and gradually dial up the position until a load of approximately 5MPa is applied.
- Transfer to stress control.
- Attach an extensometer, if required. Two extensometers are available – for room temperature and high temperature use, respectively. Your local contact will show you how to attach them.
- If using the room temperature extensometer, remove the zero point pin.
- Balance (not calibrate) the extensometer, by pressing the setup button for the strain 1 channel, and navigating through the menus, selecting cal → cal → balance.
- If possible, press the setpoint button and use the dial to gradually dial up the applied stress, up to a value which will not alter the state of your sample (e.g. 50MPa for stainless steel). This helps to ensure that the extensometer is properly seated. Then dial the stress back down to 5MPa.

When you wish to remove your specimen, transfer to position control, and turn load protect on. This should remove the load and slacken off the grips. You should then be able to remove the pin / unscrew the screw threads, or whatever is required for your particular grip system.

Tip: For some grip designs, load protect can cause problems, and not allow you to move the actuator arm. If you have this problem, turn load protect off. However, **before doing this**, ensure that the position setpoint is set to the current position. Otherwise the actuator arm may move suddenly when you turn load protect off, and possibly wreck your sample.

Caution: Make sure you are not in strain control before you attempt to remove an extensometer. The extensometer strain will change when you touch it, and this will confuse the controller if it is trying to maintain constant strain, with potentially sample-wrecking results!!

7.3.6 Setting limits

It is good practice to set limits to the maximum and minimum stresses, strains or positions which you expect to work within. For instance if you expect to work within 5MPa to 250MPa, set limits of e.g. –5MPa and 300MPa. Usually you should choose the effect of tripping a limit as transfer to position control and hold at present position. This allows easy recovery if limit trip is accidental, but is effective in stopping specimen failure.

To set a limit:

- press the appropriate limit button (see Figure 6), e.g. max load or min position.
- From the menu, select the present value – this will then enable you to input a new value via the keypad.
- Select the action you wish to be taken should the limit be tripped (e.g. transfer to position control / turn actuator off).
- Select On/Off to turn the limit on – this is indicated by a red light next to the limit button.

7.4 Remote control of the stress rig

The stress rig is controlled from the Instrument Control PC using the Stress Rig VI. This is accessed by clicking the tab labelled Stress Rig on *Ray of Light*. A typical view of the VI is shown in Figure 7. On the left, the current values of position, stress and strain are shown numerically. In the centre, updating plots of these variables are shown versus time. Control of the VI is done using the panels on the right hand side.

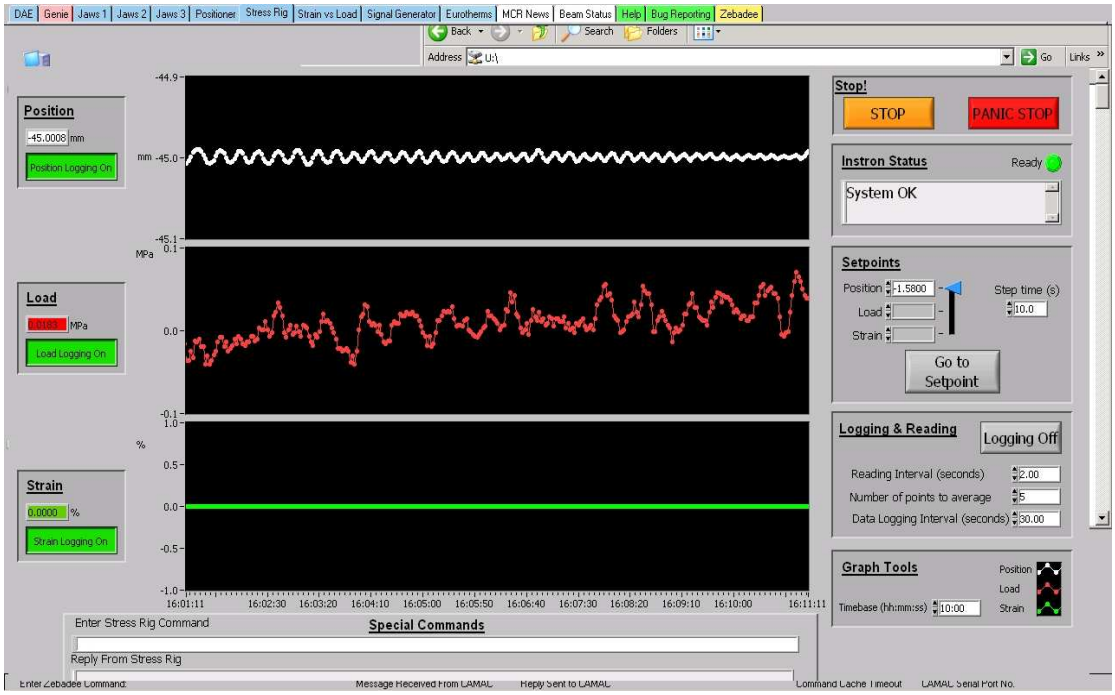

Figure 7: The Stress Rig VI.

7.4.1 Starting and stopping the Stress Rig VI

You should stop and re-start the Stress Rig VI every time you replace your sample. Otherwise, the correct cross-sectional area for the new sample will not be read, and the stresses which are logged will be incorrectly scaled.

To stop the VI: click near to a scale, until the mouse pointer becomes a small hand:  . Then press Ctrl + . (full stop).

To re-start the VI, press the play button:  . This will bring up the Strain vs Load screen (which plots strain versus stress during the test). Click on the Stress Rig tab to bring up the view of the Stress Rig VI once more.

7.4.2 Data logging

The values of stress, strain and position can be logged every few seconds to a text file. Logging is controlled by the panel labelled **Logging and Reading**, to the bottom right of the VI (see Figure 7). To start logging:

- Change the reading interval, data logging interval and number of points to average to your desired values. Recommended values are 1sec, 5 points and 5sec: this will write the instantaneous values of position, stress and strain to a file every 5sec, together with the values averaged over the last 5sec.
- Press the button labelled "Logging off". The button will turn yellow and the label will change to "Logging on".
- Click on the Strain vs Load tab on the Ray of Light display. You should see a plot of strain against stress with the frequency specified by your data logging interval. The plot is only updated if logging is switched on.

The log files are written to the directory **d:\logs\Stress Rig** on the Instrument Control PC. A new file is created each time you run the VI. The filenames contain the date and time of the file creation, e.g:
Stress Rig-2004 04 07, April Wednesday14,11,25.dat
The files are in ascii format, and contain labelled columns of data – open a file in Notepad to have a look at it.

7.4.3 Changing stress / strain /position

To change stress, strain or position using the VI, use the panel labelled **Setpoints**:

- Alter the step time if required – this is the ramp time over which the variable will be changed. 20secs is a reasonable time for lots of increments.
- Slide the blue arrow to the channel (stress / strain / position) you wish to choose as the control mode. This will instantaneously change control to that channel.
- Input the value you wish to ramp to, in the text box on the right of the blue arrow. Don't worry – the stress rig won't start ramping yet! ***Note:*** you should specify the absolute value, not the value relative to the current value. ***Also note:*** strains should be given in %.
- When you are ready, press the "Go to Setpoint" button. This will turn yellow, and remain yellow for the step time, indicating that ramping is under way.
- *If the response is not what you expect, hit the orange STOP button. This should stop ramping. If it does not, you can hit the red PANIC STOP button, but note that this will turn the actuator off and thus remove all stress from the sample.*

Caution: When you change control mode by moving the blue arrow, don't assume that the value which appears in the setpoint box is the current value of the channel. It is easy to assume this, and then attempt to apply an increment by adding some value to that shown. In fact the value shown is the last setpoint applied to this channel, which may be substantially different to the current value. This could cause you to apply a somewhat larger increment than you had intended!

7.4.4 Stress rig script commands

Most of the time, you will control the stress rig not directly via the VI, but using Open Genie commands contained in scripts. An example of a script suitable for a stress rig experiment has been given in section 5.4.4. Table 3 summarises the available stress rig commands.

General form of command, plus example	Function and notes
Stressrig/help	brings up a summary of all stress rig commands
stressrig/time value *Example*: **stressrig/time 10.0**	sets the step time to the specified **value**. This command has the same effect as typing a value into the step time box on the VI.
stressrig/control channel *Example*: **stressrig/control strain**	transfers control to the specified **channel** (which can be one of **stress**, **strain** or **position**).
stressrig/setpoint channel value *Example*: **stressrig/setpoint stress 150.**	changes the setpoint of the specified **channel** (**stress**, **strain** or **position**). Then ramps to the specified value, ***if and only if*** the stress rig is in the appropriate control mode.
stressrig/query channel *Example:* **stressrig/query position**	returns the current value of the channel to the screen.
var=stressrig:query("channel") *Example:* **cur_stn=stressrig:query("strain")**	alternative Open Genie syntax for the query command, allowing the returned value to be assigned to a variable. This is useful for scripts where, for example, you may wish to exit a loop depending on the value of a certain variable (see the example script given in section 5.4.4).

Table 3: Stress rig script commands.

Caution: Before issuing a setpoint command, make sure that the stress rig is in the correct control mode. Otherwise, the command will effectively be ignored.

8 The Coordinate Measurement Machine

The Coordinate Measurement Machine (CMM) is used to probe the locations of many points on the surfaces of components. It produces datasets of many hundreds or thousands of point coordinates. These datasets are known as point clouds. The point cloud data can be imported, either in its original form or after "meshing", into the SSCANSS package, which can then be used as a virtual laboratory, for experimental planning, execution and analysis. This chapter provides "getting started" operating instructions for the CMM – for more detail, ask an Instrument Scientist, or consult the manuals, which are stored under "CMM" in the filing cabinet in the ENGIN-X cabin.

Figure 8: The CMM.

8.1 Physical components

The CMM system is comprised of the following components:

- The LK HC-90 CMM itself (shown in Figure 8), operated by a handheld control pad.
- The control cabinet and PC, which sit to the left of the CMM.
- The Hydrovane air compressor, located at the top of the stairs (a large blue box).
- The Metris Laser head, touch probes, reference spheres and other accessories, stored in the drawer labelled "CMM" in the desk on your right as you enter the ENGIN-X cabin.

8.2 Basic operating instructions

These instructions provide a basic guide to measuring point cloud data using the Metris laser head. For information on other procedures (meshing, using touch probes, etc.), consult the Instrument Scientist.

8.2.1 Start up

- Turn on the air compressor by pressing the yellow button. If there is no response, check that the emergency stop button is released by twisting it, the try pressing the yellow button again.
- With the CMM turned off, ensure that the CMM arm is towards the right hand side of the machine and not at the bottom of its travel – if not, push it there manually. This is to ensure that the machine can find its home position correctly.
- Turn on the CMM, by twisting clockwise the large red power switch on the right hand side of the control cabinet.
- Flick the black power switch on the control PC, which is housed at the bottom of the control cabinet (access from the left hand side).
- Log on as administrator – no password.

8.2.2 Homing the CMM

- Start LK Studio-Inspect, by double clicking the icon on the desktop.
- Mount the laser head by inserting the T-bar key and turning it clockwise – you should hear a bleep, indicating that the head has located correctly (mounting the head is very simple, but ask your local contact to show you the first time).
- Select the CMM drop-down menu, and choose On-line.
- At the prompt, press the MASTER START button on the control pad, firstly ensuring that the emergency stop button (also on the pad) is released. Then click OK on the computer.
- Ensure that the CMM arm can movely freely up and down and towards the left, without danger of collision. Then accept the computer prompt by clicking OK. The arm will then move to its home position – click OK to accept the end of the initialisation.
- Close Studio-Inspect.

8.2.3 Starting Metris Scan (laser scanning software)

Laser scanning is done using the Metris software. Icons for this software are located in a box on the PC's desktop, labelled Metris Software.

- Double click the Stop Communication icon.
- Double click the Restart Communication icon.
- Double click Metris Scan 3.1. If an error message appears, click Retry. If the same message appears again, start the process again, stopping and restarting communication several times.
- Switch on the laser. This is done by depressing the  button in the Camera Preview window (Figure 9) (check that a laser spot appears). If the Camera Preview window is not showing, bring it up by clicking the  icon, located towards the right of the second row of icons at the top of the Metris Scan window.

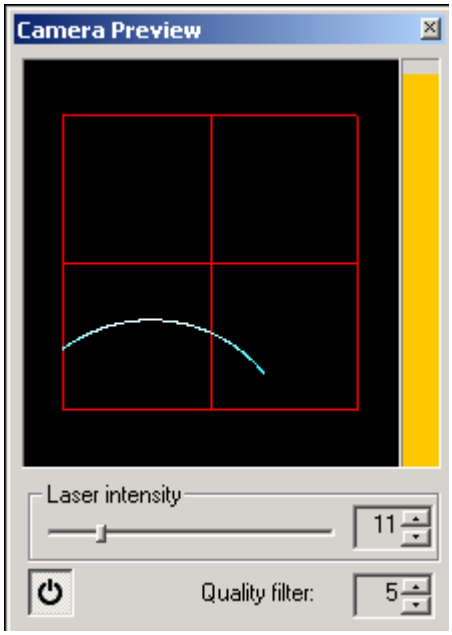

Figure 9: Camera Preview in Metris Scan.

8.2.4 Moving the laser head

The CMM probe arm can be moved using the handheld control pad, as follows:

- Operate the control pad whilst facing towards the ENGIN-X cabin. Then the X and Y arrows on the pad correspond to the real movement directions.
- Ensure that the emergency stop button is released (by twisting) and press the MASTER START button if it is lit.
- Use the left hand knob for horizontal movements (X and Y), and the right hand knob for vertical movements (Z).

The laser head has a field of view of 15mm. For successful scanning, you need to position the head at the correct distance from the object so that a trace is seen in the Camera Preview (as in Figure 9). This may take a little practice, so apply the following tips:

- Use the alignment laser spot to roughly position the head over the object.
- Look closely to see a thin line of laser light. It is this which actually performs the scanning. If you cannot see it on the object, adjust the position of the head until you can.
- Move the head towards or away from the object until the laser line roughly intersects the spot. This occurs when the head is approximately the correct distance away from the object (about 10cm from the tip of the head to the object's surface).
- Keep an eye on the Camera Preview, adjusting the head position until the trace appears. Centre it in the window as well as possible.
- You may need to adjust the laser intensity using the sliding scale on the Camera Preview. If having trouble finding the trace, set the intensity to maximum.
- The colour bar on the right of the Camera Preview indicates the intensity of reflected light. Adjust the intensity until this fluctuates between green and yellow/red.

- If you still cannot find a trace, it may be because your surface is too shiny. White developer powder is available for spraying on such surfaces.

8.2.5 Calibrating the laser head

The laser head can point in a range of directions over a hemisphere, to allow the operator to select the most appropriate orientation(s) for their scan. A calibration must be performed for each head orientation.

The orientation is defined by 2 angles: angle A which defines the rotation of the probe away from the arm of the CMM (0º to 105º), and angle B which defines the rotation about the axis of the arm (-180º to 180º). For example, A=90º, B=180º points the probe straight downwards.

For convenience, the calibrations for a set of commonly used orientations are stored in a file. These are labelled according to the angles A and B (e.g. A=90.0 B=180.0). The calibrations are set to automatically expire after a 1 month period, so you may have to re-calibrate, as described here. The head calibrations are known in Metris as qualifications, and calibrations are performed by scanning a reference sphere.

- If unseen, bring up the Qualification Manager window (Figure 10) by clicking the  icon on the 2nd row of icons at the top of the Metris Scan screen.

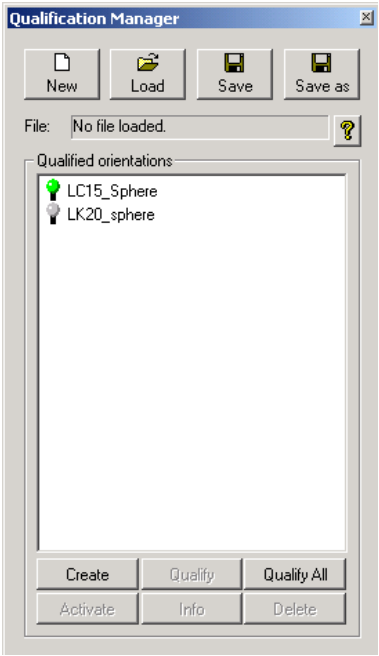

Figure 10:Qualification Manager in Metris Scan.

- Click the Load button and check that the browser window is open at the folder E:\Qualifications. The calibrations are stored in .qlf files named by the calibration month. For example, March04.qlf contains the calibrations for March 2004. Open the most recent of these files.

- If the message “Expired qualifications have been added to the list. These are no longer valid” is displayed, you will need to re-calibrate (click OK to close the message). Otherwise you should be OK.
- To re-calibrate, mount the white, 15mm diameter reference sphere in an accessible position on the CMM table (the sphere screws into a mounting rod, an extension rod is available to mount it at the correct height).
- On the Qualification Manager, check to see whether the symbol next to LC15_Sphere is green or grey (calibrated or uncalibrated). If it is green, right click on LC15_Sphere and select “Sphere has moved”. This informs the CMM that the sphere has been newly positioned on the table, and not to assume it is located at a previous position. Accept the warning which is issued.
- On the Qualification Manager, click Qualify All. In the dialogue box which is brought up, check that LC15_Sphere is selected under the Sphere dropdown menu.
- Click Start.
- Using the handheld control pad, move the head to a position where it can freely rotate without risk of collision.
- Click Next.
- Move the head over the sphere so that a trace appears in the middle of the Camera Preview window (see Section 8.2.4).
- Click Next.
- The CMM should now automatically scan the sphere for all head orientations. If this is your 1st attempt at calibrating, it may be worth hovering over the emergency stop button until you are confident that the procedure is working properly!
- At the end, click Accept. The Qualification Manager should now show green symbols, indicating that all head orientations have been calibrated.
- Click the Save As button, and save the calibrations, using the filename convention date_yourname.qlf, e.g. july04_oliver.qlf.

8.2.6 Scanning

- Turn the laser on, as explained in section 8.2.3, and bring up the Qualification Manager window, as explained in section 8.2.5.
- Click the load button on the Qualification Manager, and open the most recent .qlf file (named by month of creation).
- If a window appears warning you that the qualifications have expired, follow the instructions given in section 8.2.5 for re-calibrating.
- Otherwise, selection the probe orientation you wish to use (e.g. A=90.0 B=180.0) and click Activate.
- Make sure the head can rotate freely without obstruction, then click Yes to rotate the head.
- Move the head over the object you wish to scan, until you see a trace in the Camera Preview window (see section 8.2.4 for details).
- If unseen, bring up the Scan window by clicking the 

icon towards the top right of the Metris Scan screen. The Scan window is shown in Figure 11.
- Keeping an eye on the trace, move the head to the position you wish to start scanning at.
- Click Mark on the Scan window. The coordinates of the current head position will be shown on the line labelled Start.

- Scans can be single line scans, or an area or volume scan. The dimensions of the line/area/volume are defined in the rows labelled Length, Width and Height in the Scan window (see Figure 11). The choice of line, area or volume scan is made by selecting or de-selecting these rows, by toggling the lights on the right between red and green.

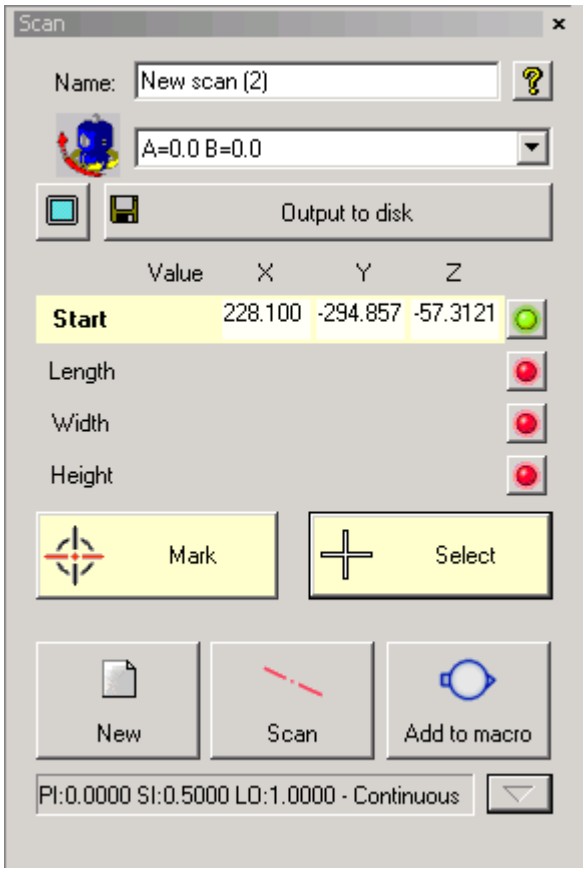

Figure 11: The Scan window in Metris Scan.

Performing a line scan

- Move the head to the end of the line along which you wish to scan, and click Mark again. The new head coordinates will be shown on the Length row, and the light at the end of the row will go green to indicate that the line scan is activated.
- Click the Scan button – your line scan will then be run, and the point cloud data displayed on screen.

Performing an area scan

- After defining the length coordinates, click the Length light, to turn it back to red. Then click Scan – the head will move back to the start position, but not perform the line scan.
- Click the Length light to turn it green once again – this will then highlight the Width line, to enable you to define the width of the area scan.

- Move the head in a direction perpendicular to the line scan, to define the width of the area, and then click Mark. Now both the Length and Width lights should be green.
- Click Scan to perform the area scan.

Performing a volume scan

- The depth of field of the laser head is 15mm. Therefore, if the relief on your surface varies by more than this depth, you will have to scan at different approach distances, by doing a volume scan, as described here. The procedure is simply an extension of that described above for an area scan.
- Follow the procedure for defining an area scan, but do not click Scan at the end.
- Instead, deactivate the Length and Width lines (by turning the lights red), and then click Scan, to return the head to the start position.
- Reactivate the Length and Width lines (turn the lights green), to highlight the Height line.
- Move the head in a direction perpendicular to the Length and Width dimensions, to define the 3rd dimension of the volume scan.
- Click Scan to start.

8.2.7 Using your point cloud

As the scan is completed, the point cloud will gradually be displayed on the screen. You can manipulate the display (zoom, rotate, etc.) using the icons on the left of the Metris screen (see Figure 12). Generally, the number of points contained in the cloud will be far greater than you require, and this will cause processing to be very slow. It is therefore a good idea to reduce the number of points by filtering. To do this, select your point cloud by making sure that the  icon is depressed, and then clicking on the point cloud – this should surround it by a red box outline, as illustrated in Figure 12. You can then select FilterMeshrandom from the Point Cloud drop-down menu (also illustrated illustrated in Figure 12). This will give you various options to filter points and then mesh them together, if required. For details, see the Metris Scan manual, which is clearly written and kept in the ENGIN-X filing cabinet in the "CMM-Metris" file. Please put it back afterwards.

After processing your point cloud, you will need to save it. Do this by selecting the cloud and then selecting File→ Export. For an unmeshed point cloud, you can then choose either option: Selection to File (export as a .mbf file), or Pointcloud(s)/ Polyline(s) (export as an ascii text file).

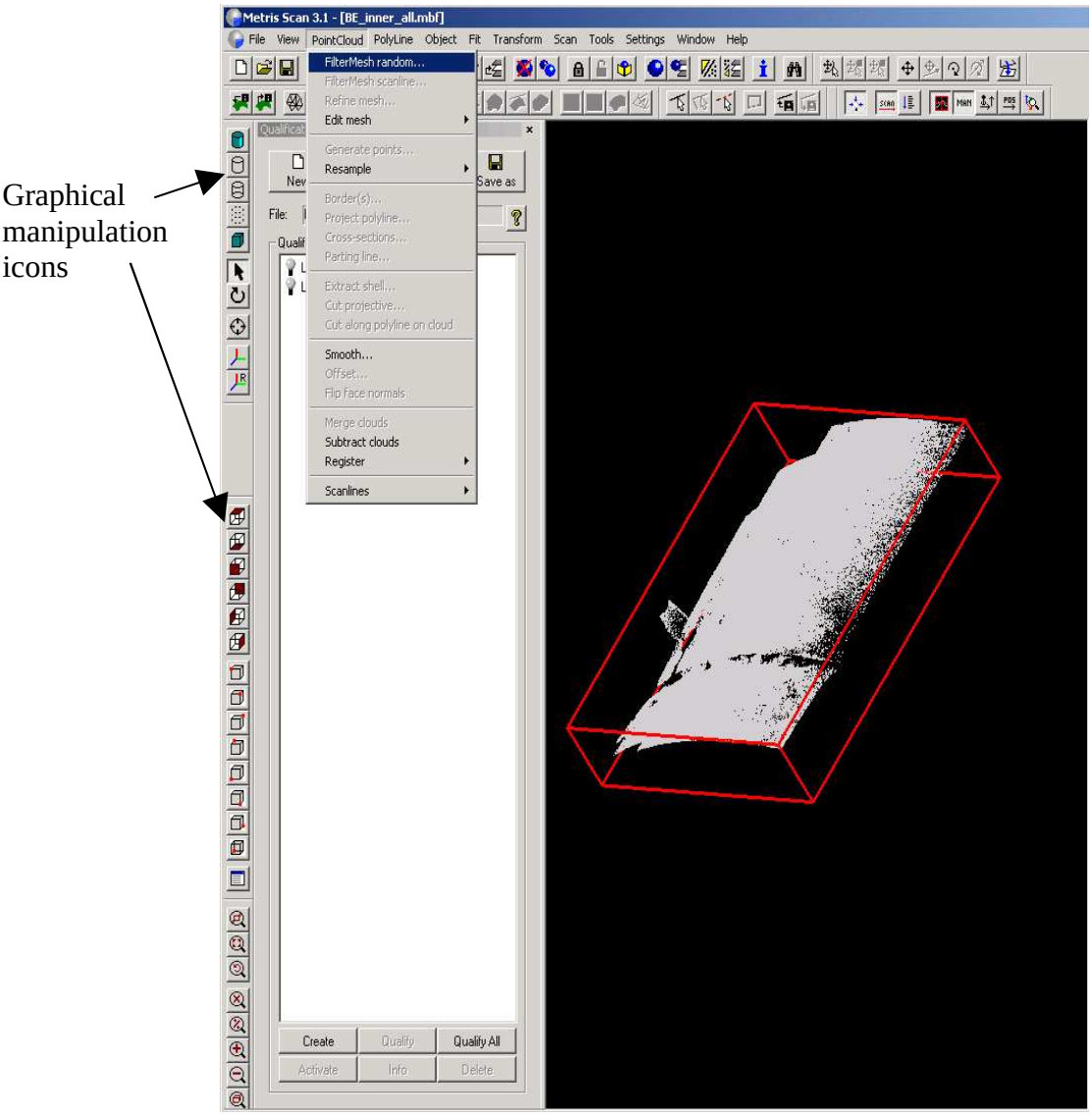

Figure 12:Metris Scan screen, showing graphical manipulation icons and Filtermeshrandom option.

8.2.8 Shutting down the CMM

- Move the CMM arm to the right, upwards and outwards, to ensure successful homing next time it is turned on.
- Before removing the laser head, make sure you turn the laser off by clicking the  button in the Camera Preview window.
- Remove the head using the T-bar key.
- Close Metris Scan.
- Shut down the computer.
- Turn the CMM power off by twisting the red power switch anti-clockwise.
- Turn off the air compressor by pressing the red emergency stop button.

8.3 Further information

This chapter has highlighted only the basics of the use of the CMM. Additional topics which you may like to learn about include filtering and meshing point clouds, and combining point clouds from scans of the same object in different orientations. These topics are well described in the Metris Scan manual, which is kept in the filing cabinet in the ENGIN-X cabin, in the “CMM-Metris” file. You may also wish to use touch probes to gain coordinate information about holes and bores, etc. If so, ask one of the Instrument Scientists.

9 Data analysis using EX-SBA

9.1 Introduction to EX-SBA

EX-SBA, the ENGIN-X Script Based Analysis software, is a system to explore and analyse the neutron diffraction spectra measured at ENGIN-X. EX-SBA is a powerful system to manipulate, plot and analyse diffraction data from polycrystalline specimens. The most common operations have been made accessible through simple menu-driven programs. EX-SBA is written using the Open Genie programming language, developed at ISIS (see http://www.isis.rl.ac.uk/OpenGENIE). EX-SBA uses the computer package GSAS (see http://www.ncnr.nist.gov/programs/crystallography/software/gsas.html) for automatic Rietveld refinement of the diffraction spectra.

You can use EX-SBA either on the data analysis PC, or on your own laptop. The latter has the advantage that you will not need to transfer all your data at the end of the experiment, and you can easily carry on data analysis once you have left. For details of installing EX-SBA, see section 9.9.

9.2 File types and locations

The following table summarises the files used by EX-SBA, and where they are stored.

File type	Description	Location
ENG*nnnnn*.RAW where: *nnnnn* is the run no.	The raw datafile containing the individual TOF spectra recorded by the data acquisition electronics for every single detector element.	On ***ndxenginx*** at: D:\data and also on ***enginx*** at: G:\data
ENG*nnnnn*_myvar.txt where: "myvar" is an instrument variable, e.g. "X", "Y", "Z", "load", "strain", "temp4".	Ascii log files, containing the values of a particular variable as a function of time through the run. The variables to be logged are chosen from the dashboard – see section 4.4.	On ***enginx*** at: G:\data
ENG*nnnnn_b*.his where: *b* is the bank number (1 or 2).	To create a single diffraction spectrum from all the elements in a bank, the individual spectra are summed together, taking account of the differences in time-of-flight, by a process called "time focussing". The focussed spectra are stored in the .his files.	On ***enginx***at: G:\enginx_focus

Table 4: EX-SBA file types and locations.

Tip: In order to perform data analysis using your own computer, you will need to copy across either the .RAW or the .his files. *It is strongly recommended that you copy*

the .his files rather than the .RAW files, which are very large and in most cases are unnecessary. The .his files should be copied into the my_drive:\enginx\focus directory on your computer.

9.3 How to use this chapter

If you have installed EX-SBA on your own computer (see section 9.9) then the datafiles required for the examples used in this chapter are included in the installation. You can therefore follow the chapter through as a tutorial, typing the commands as written and observing the output. The commands to be typed are shown in green. Italics are used for generic descriptions of arguments – do not type these as shown, but instead put in the specific arguments (e.g. `rfocus 23131 1` rather than `rfocus` *`run bank`*).

If you are a first-time user of ENGIN-X, it is highly recommended that you complete this exercise before arriving. It should not take more than an hour or so and will make data analysis much more straightforward for you during your experiment.

9.4 Starting EX-SBA

If you are using the ENGIN-X data analysis computer, ***enginx***, click on the 

icon on the desktop to launch EX-SBA. If you are using your own computer, click on enginx.bat, in the directory my_drive:\ENGINX\ (where my_drive is the name of the drive you installed EX-SBA on).

Upon starting EX-SBA, you will be asked for an experiment name. You should type a single word (e.g., my_name), which will be used to create a directory (g:\my_name) where all the results of your analysis will be stored. Two windows will be shown: a text console for input and output of text, and a graphics window, where all the plots will be shown (see Figure 13). You can print any graph from this window using the colour printer located in the ENGIN-X cabin. Alternatively, you can copy the graphs and paste them onto any other Windows program.

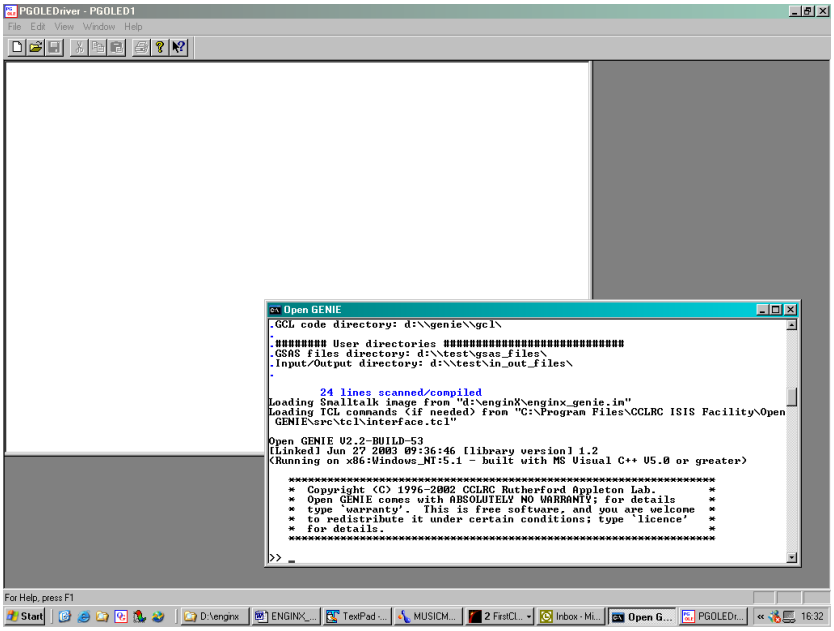

Figure 13: EX-SBA start up screen.

9.5 Viewing a spectrum

After you have created a run (i.e., a file ENG*nnnnn*.RAW) you can look at the TOF spectra stored in it. Each ENGIN-X detection bank consists of 1200 small detectors that need to be added together in order to produce a spectrum having the statistical quality required for strain determination. You do that by typing

`rfocus` *`run bank`*

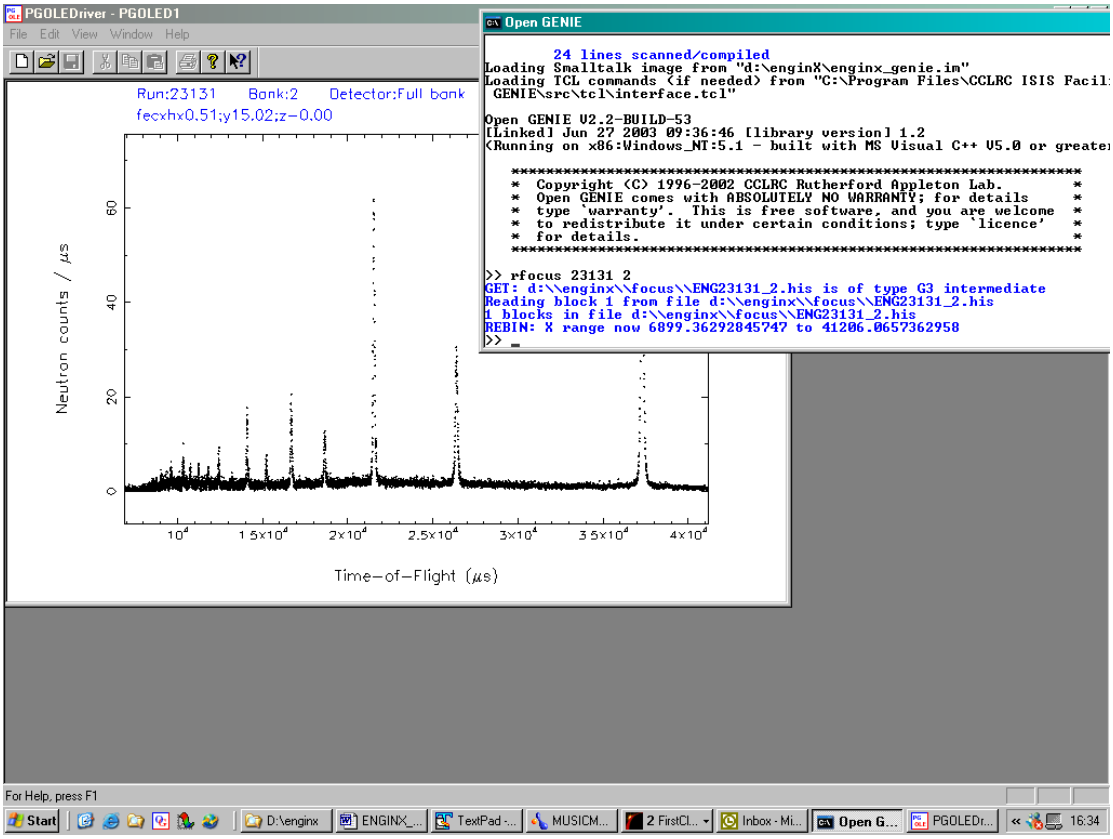

Figure 14:Displaying a spectrum using EX-SBA.

For instance,

```
rfocus 23131 2
```

will focus the data recorded by bank number 2 (South) during the run number 23131 and will display the spectrum on the screen, together with some information from the run, in this case a ferritic steel specimen with a cold expanded hole in it (see Figure 14). You can assign a name to this spectrum if you would like to see it later on, or if you want to perform some algebraic operation on it. You do that by typing

`my_spectrum=rfocus(`*run*`,`*bank*`)` (e.g. `my_spectrum=rfocus(23131,1)`)

You can display the spectrum at any time by typing

```
display my_spectrum
```

or

```
d my_spectrum
```

You can set the X limits of the graph (Figure 15) by typing

```
d my_spectrum xmin xmax
```

For instance

```
d my_spectrum 20000  28000
```

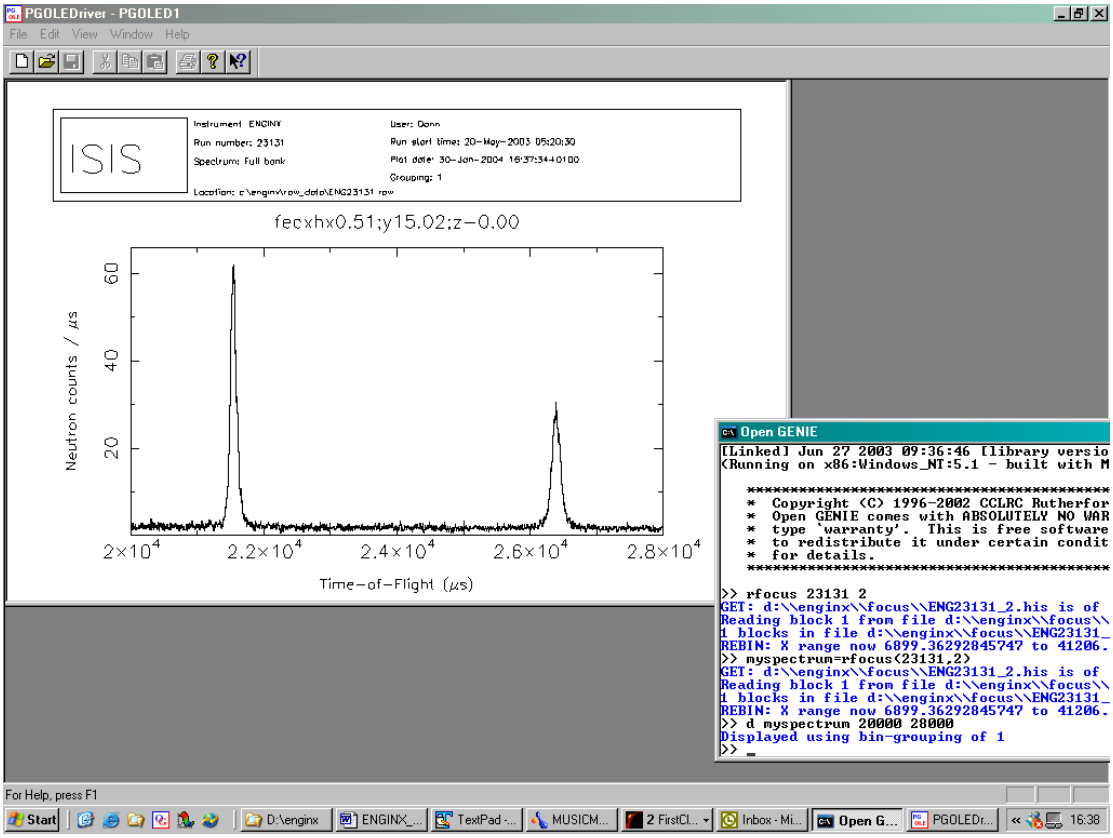

Figure 15: Setting x-limits on a plot in EX-SBA.

You can compare different spectra by plotting them on the same graph (Figure 16). Suppose that you have defined spectrum1 and spectrum2 by

```
spectrum1=rfocus(23132,1)
spectrum2=rfocus(23140,1)
```

To compare them you first plot one:

```
d spectrum1 20000 28000
```

and then add the second spectrum into the graph by typing

```
add spectrum2 $red
```

where the last word indicates the colour to be used ($blue, $red, $green, $yellow, $orange, $cyan, $purple). There is a list of all possible colours in the Open Genie Reference Manual.

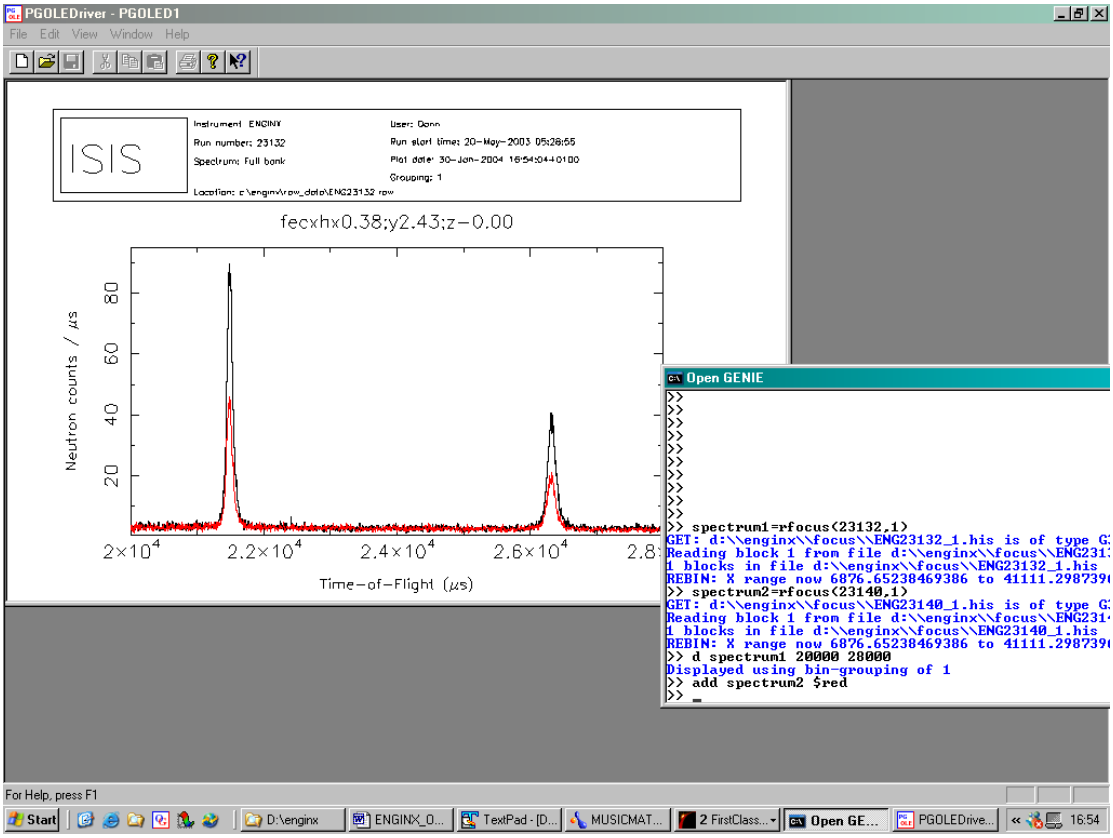

Figure 16: Displaying two spectra on the same plot in EX-SBA.

By default, all the spectra are displayed in TOF, but you can change the units of a spectrum to be shown on a d-spacing scale by typing

```
units/d my_spectrum
```

and the next `display` command will then plot the spectrum on a d-spacing scale.

The `rfocus` command only actually performs focussing if it does not detect a focussed spectrum datafile (i.e. a .his file) in the appropriate directory (my_drive:\enginx\focus on your own computer, or G:\enginx_focus on ***enginx***). If no .his file exists, it invokes the `xfocus` command, which actually carries out the focussing. You can force focussing to be carried out (over-writing the .his file, if it exists) by typing

```
xfocus run bank
```

For instance:

```
xfocus 23430 1
```

If this does not work, check that the corresponding raw file (in this case ENG23430.RAW) is present in the raw file directory (my_drive:\enginx\raw_data on your own computer, or G:\data on ***enginx***).

One reason that you may wish to re-focus and overwrite the .his file is that the TOF range is too small, so that some of the spectrum is truncated. This can occur if you

change samples and alter the DAE settings (i.e. extend the TOF range). To re-set the range, use the commands

```
enginx.bank[1].t_min=1000      (set bank 1 minimum TOF to 1000μs)
enginx.bank[1].t_max=99000     (set bank 1 maximum TOF to 99000μs)
```

and similarly for bank 2. The TOF range you require will most likely be within these extremes. When you next issue a focus command, the TOF range will then be reset to that contained within the RAW file.

Occasionally, electronic "spikes" appear on a focussed spectrum, which result in a spectrum having a very large number of counts, restricted to only one or two TOF channels. If that happens, you can use a more advanced (and slower) focussing routine by typing

```
xfocus/spikes
```

This will prompt you for the run number and bank to be focussed, and will also ask for a maximum number of counts to be allowed on an individual TOF channel. A value of 5000 counts will work for most cases, but if it doesn't, you can play with this value until you get a spectrum with no spikes in it.

9.6 Analyzing a single run

9.6.1 Rietveld refinement of a single run

For neutron strain scanning we need to know the precise value of the lattice parameter for each of the runs we have measured. For a single run, this can be done by typing

```
analyze
```

The system will then ask you a series of questions including the run and banks to be analyzed, the TOF range to be used, and the material composing the sample. The program will perform a Pawley-type full spectrum refinement using the GSAS code, and it will show the experimental, calculated and difference spectra on the screen. For those who have experience with GSAS, all the files used during the GSAS refinement are stored in the directory my_drive:\my_directory\gsas_files (or in G:\my_directory\gsas_files on ***enginx***). As an example, you can try the `analyze` command with run 23131, consisting of ferritic steel (Fe_alpha), following the steps below:

```
>> analyze
Run number: 23131
Bank: 1
```

The system will focus the run and will show you the resulting spectrum. Then, after a lot of output to the screen it will ask you the TOF range that you want to use for the Rietveld analysis.

Tip: For strain scanning experiments, it is sensible to use a minimum TOF which is not too short, as peaks at small d-spacings tend to very overlapped and will not contribute greatly to the refinement, but will cause it to proceed much more slowly.

```
O/PREPARE/Please look at the plot and decide.


Minimum TOF to use in the refinements?: 13000
Maximum TOF to use in the refinements?: 40000
```

And, after a lot of output to the screen, you will be asked to define the material composing the sample, from a list of possibilities. You can give any name to your sample (fecxh in this case) but it must be a single word. If your material is not in the list, please contact the Instrument Scientist. You will also be asked for the sample temperature.

```
O/PREPARE/Sample not defined!
O/PREPARE/Please define the sample
New sample name (a single word, please ?)(q=CANCEL): fecxh
Number of phases?(n<3, please): 1

 Template Materials

 Aluminium                    (Al)
 Alpha alumina              (Al2O3)
 Beryllium                    (Be)
 Calcium fluoride           (CaF2)
 Cerium oxide               (CeO2)
 Chromium                     (Cr)
 Copper                       (Cu)
 Alpha Iron              (Fe_alpha)
 Gamma Iron              (Fe_gamma)
 Molybdenum                   (Mo)
 Nickel                       (Ni)
 Lead                         (Pb)
 Silicon                      (Si)
 Alpha Silicon carbide (SiC_alpha)
 Beta Silicon carbide   (SiC_beta)
 Grey Tin                (Sn_alpha)
 Grey Tin                 (Sn_beta)
 Alpha Titanium          (Ti_alpha)
 Beta Titanium            (Ti_beta)
 Alpha Uranium            (U_alpha)
 Tungsten                     (W)
 Tungsten Carbide            (WC)
 Alpha Zirconium         (Zr_alpha)

Name of phase 1 (e.g: Zr_alpha)?: fe_alpha
Sample temperature (K): 293
```

After a lot of output you will be told that the sample has been defined, and a simulated spectrum corresponding to this material will be displayed. You will be asked whether you wish to proceed with this sample, just in case you've made a mistake:

```
O/PREPARE/
O/PREPARE/Current material is fecxh
O/PREPARE/


Do you want to define a new material (y/n)?: n
```

And, after more output to the screen the system will show you a first approximation to the measured spectrum, inform you about the number of peaks found within the specified TOF range, and ask whether you wish to proceed:

```
################################################
 The current sample is fecxh
```

```
 The shorter TOF to be used in the analysis is 13000.0
 The longer TOF to be used in the analysis is 40000.0
 There are 8 reflections within this range
 The lower reflection in this range is (1,1,0)  at  37190.0
 The higher reflection in this range is (4,0,0)  at  13150.0
 The peak with maximum intensity is (1,1,0)  at  37190.0
##################################################

Do you want to use these settings?: y
Do you want to fit the data (y/n)?: y
```

After yet more intermediate output, the system will show you a plot of the experimental and GSAS-refined spectra (Figure 17), and output the fitted lattice parameters and errors:

```
#################################################################L
attice parameter a=2.865597+/-0.000022999999999
Lattice parameter b=2.865597+/-0.000022999999999
Lattice parameter c=2.865597+/-0.000022999999999
#################################################################
```

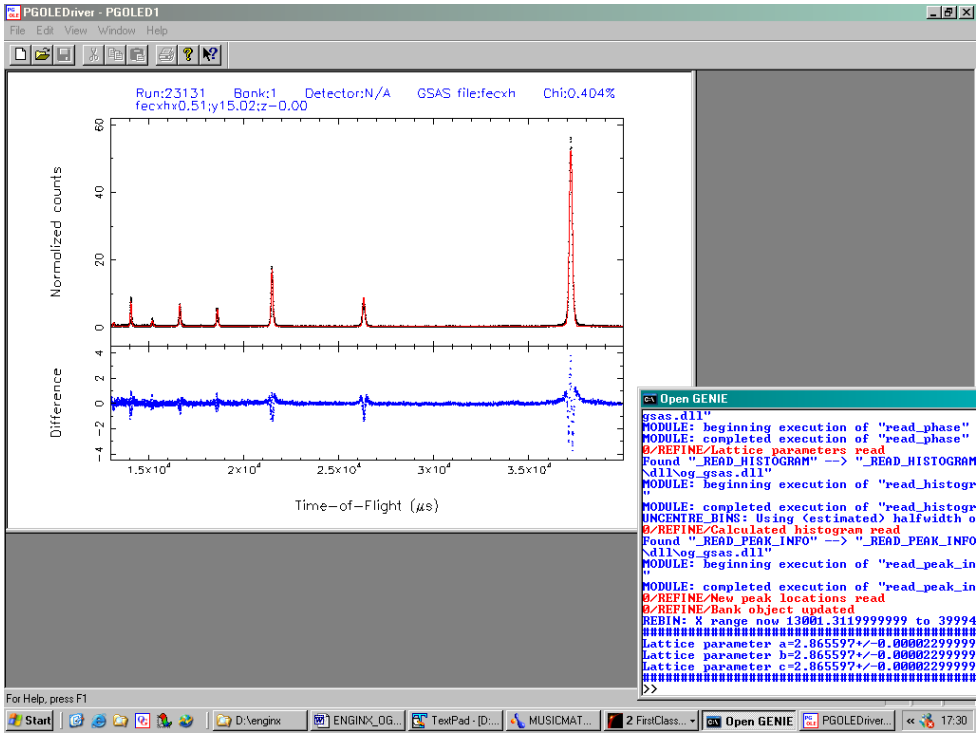

Figure 17: Fitted and experimental spectra, using the analyze command.

9.6.2 Exporting GSAS datafiles

If you would prefer to perform your own analysis using GSAS independently of EX-SBA, you can export a spectrum in GSAS .dat format by typing

```
gsas_file
```

This will prompt you for the run and bank numbers, and then tell you the location and filename of the file which is created. Ask the Instrument Scientist to provide you with

the correct instrument parameter file. To produce GSAS files for multiple runs, use the command

```
batch_gsas_file
```

and follow the prompts.

Caution: When exporting to GSAS format, peak intensities are scaled by a certain factor, which varies from run to run. If you want to compare peak intensities between runs, you will need to re-apply these scale factors after your GSAS analysis. Ask the Instrument Scientist how to access these scale factors.

9.6.3 Fitting a single peak

To find the exact position of a single peak, use the command

```
fit_peak
```

and then specify the run and bank numbers, and the TOF range to fit over. For instance:

```
>> fit_peak
Run number?: 23131
Bank number?: 1
Minimum TOF?: 25000
Maximum TOF?: 30000
```

which, after intermediate output, plots the fit on the graphics screen (Figure 18) and gives the fitted `peak` position in TOF:

```
0/FIT_PEAK/ Peak position :: 26280.693359375 +/- 0.864083230495452
microseconds
```

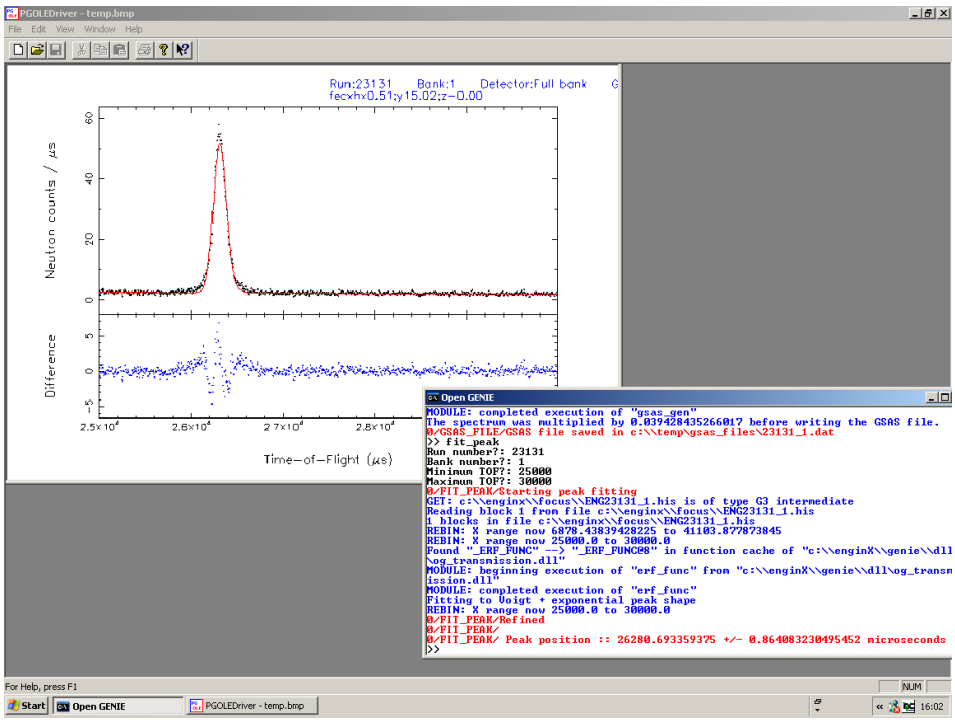

Figure 18: Fitting a single peak in EX-SBA.

To find the peak position in units of d-spacing, give the alternate command

```
fit_peak/d
```

9.7 Analyzing a scan

EX-SBA allows you to analyze a series of runs in one go. A series of runs is referred to as a scan. Scans may have different purposes – e.g. to study the strain variation within a specimen, or to find the location of a surface from the intergrated intensity. The main command for analyzing scans is (appropriately!) called `analyze_scan`. The best way to learn the various options available using this command is to try running it on some example spectra. For this purpose, focussed datafiles (.his files) for runs 23131 to 23148 are included in the EX-SBA installation. These runs correspond to a radial line scan of a cold expanded hole made of ferritic steel (Fe_alpha). This section takes you through an example exercise, but it is well worth trying out some other options on your own.

9.7.1 Strain scan – single peak fitting

To fit peak profiles to a number of peaks within a series of spectra, follow the procedure below.

```
>> analyze_scan
...
####################################################
######### Please, define your scan ################
####################################################
 (1) Sequential set of runs
 (2) Custom set of runs from file
 (3) Partial saves
 (0) Exit
####################################################
Please select your option: 1
```

Option 2 allows you to specify a non-sequential set of runs by reading them from an ascii file; option 3 allows you to use intermediate .s** (created using the **updatestore** command) from a single run – for example, to see how the lattice parameter error falls with counting time). For now, choose option 1, specify the run sequence 23131 to 23148, give the scan a name, and choose bank 1:

```
First run: 23131
LAST RUN: 23148
Name of scan, e.g:scan1 (to create output files names): tutorial1
Bank: 1
```

After intermediate output, you will be asked to select the independent variable to plot fitted values against:

```
####################################################
# Please, select independent variable of the scan ####
####################################################
 (1) X positioner
 (2) Y positioner
```

```
 (3) Z positioner
 (4) THETA positioner
 (5) Run number
 (6) External x-values (from file)
 (9) No plots
 (0) Exit
#####################################################
Please select your option: 5
```

For now, choose to plot versus run number (option 5). You will then be asked to define the positions of peaks in the spectrum. You can do this graphically or by specifying them in an ascii file. However, if you know your material, you can simply specify the crystal structure:

```
#########################################################
## How do you want to define the peak intervals? #####
#########################################################
         (1) By selecting the material
         (2) By an external file
         (3) Graphically
         (0) Exit
#########################################################
Please select your option: 1

0/PREPARE/Please look at the plot and decide.

REBIN: X range now 6878.43839428225 to 41103.877873845
Minimum TOF to use in the refinements?: 13500
Maximum TOF to use in the refinements?: 40000
```

If you are going through this exercise having just completed the `analyze` exercise, you will already have defined a sample named fecxh, with a ferrite crystal structure (fe_alpha). In that case, continue as below (otherwise, you will need to give a sample name, choose the fe_alpha crystal structure, and specify a sample temperature).

```
0/PREPARE/
0/PREPARE/Current material is fecxh
0/PREPARE/
Do you want to define a new material (y/n)?: n
```

The routine will then perform peak fits on the first run. This allows you to check that you have defined the material correctly, in which case you can accept the settings:

```
...
#################################################
 The current sample is fecxh
 The shorter TOF to be used in the analysis is 13500.0
 The longer TOF to be used in the analysis is 40000.0
 There are 7 reflections within this range
 The lower reflection in this range is (1,1,0)  at  37200.0
 The higher reflection in this range is (3,2,1)  at  14060.0
 The peak with maximum intensity is (1,1,0)  at  37200.0
#################################################
Do you want to use these settings?: y
```

The program will then go ahead and fit profiles to all diffraction peaks in the TOF range, for all spectra, displaying the results graphically. Occasionally a fit may be unsuccessful, in which case the output will read:

```
0/W_MULTI_FIT/#########################################################
0/W_MULTI_FIT/Refinement not succesful!Please define the limits
manually!
0/W_MULTI_FIT/Press any key, then go to the plot.
```

```
O/W_MULTI_FIT/Click Right Button to define limits, press X to start
fitting!
O/W_MULTI_FIT/##########################################################
Go:
```

If so, press RETURN, and you will be prompted to click on the graph to define the x limits either side of the peak:

```
Click left to set x-bounds for region to fit, right to continue
```

Click on either side of the peak and press x (with the graphics window still selected) to continue fitting. Hopefully, the fit will then be performed successfully, in which case it will be shown graphically, and you will be prompted to accept it:

```
Are you happy with this fit (y/n): y
```

Eventually, all fitting will be finished, and plots of peak position, intensity and width will be shown for each peak (hkl indices shown at the top of the window), against the variable you selected (run number, in this case). To view the plots for each peak, select one of the PGOLED windows from the Window drop-down menu (see Figure 19).

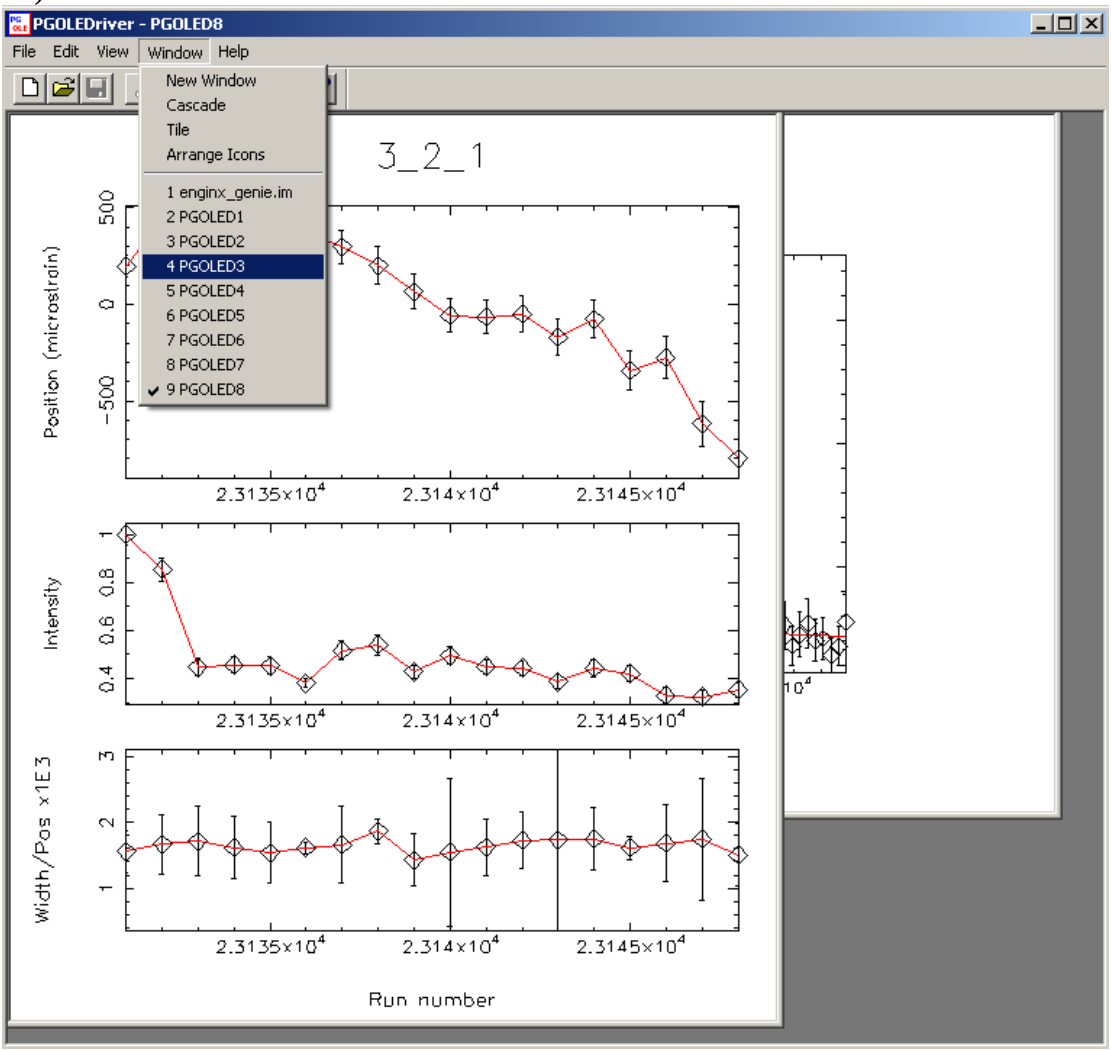

Figure 19:Plots generated for the 321 diffraction peak, using the analyze_scan command.

Answer yes to the following question:

```
Do you want to define the average peak strain (y/n)?: y
```

This will calculate the average strain over all diffraction peaks. Keep pressing RETURN until you get the Open Genie prompt once more.

You can use the plots generated by `analyze_scan`, but you may well wish to use the data to create your own plots. For this purpose, the routine writes ascii files with all the fitted data. The files are stored in the in_out_files sub-directory of your working directory. If you scroll up the output on the console window, you will see messages telling you the name and location of each file, such as

```
Peak positions for peak 3_2_1 have been written to:
        c:\\temp\in_out_files\tutorial1_bank_1_pos_3_2_1.OUT
```

The files contain tabulated data, with clear headings, such as “run number”, “d_space” and “error”.

9.7.2 Strain scan – Rietveld refinement

Instead of single peak fitting, you can use `analyze_scan` to perform a full-spectrum Rietveld refinement using GSAS by issuing the command

```
analyze_scan/gsas
```

Again, you can try this with run numbers 23131 to 23148, specifying single phase ferrite (Fe_alpha) as the material. The routine will take you through similar options as the single peak fitting version (e.g. defining the sample material, setting TOF limits, etc.). Do not be put off by some rather strange intermediate plots!

At the end of the routine, the refined lattice parameters will be written to an ascii file with filename of the form *_GSAS.OUT (e.g. tutorial1_bank_1_GSAS.OUT). Again, the file will be written to the in_out_files sub-directory, and an output message will confirm the name and location.

9.7.3 Exporting GSAS files

`analyze_scan/gsas` only performs a simple refinement (for example, it assumes untextured material). You may therefore wish to export GSAS .dat files. As explained in section 9.6.2, using the command `batch_gsas_file` to produce these files. Also, pay attention to the note of caution shown in section 9.6.2!

9.7.4 Analyzing integrated intensities

Sometimes you will not be interested in peak positions, but only in the integrated intensity of each spectrum. For example, this will be the case if are scanning through the surface of a sample to find its location. In this case, use the command

```
integrate_scan
```

and follow the prompts. You can try to improve the contrast of the scan by specifying the material and only integrating intensity over the TOF regions where you expect

peaks to occur – or you can define a TOF region of interest over which to integrate – or you can integrate over the whole spectrum.

After plotting the intensities, the routine will offer you two analysis options. The first option – "Find location of surfaces" – should only be used for a scan that has traversed two surfaces, in so-called "transmission mode". Such a scan will produce a symmetric intensity plot, since the path length is the same for all runs. The second option – "Find pin position" should be used when a "pin scan" is performed, i.e. when a thin wire is scanned through the beam in order to find the location of the neutron gauge volume. This is usually done when there is a suspicion that the system maybe misaligned (as a result of hitting the incident slit, for instance). "Find pin position" fits a Gaussian through the intensity profile, to find at which position the pin is centred in the gauge volume.

9.8 Building your own program

You can build your own measurement or analysis program with Open Genie by writing all the steps you want to do into an ASCII file. See the Open Genie User Manual (http://www.isis.rl.ac.uk/OpenGENIE/manuals.htm) to learn the syntax.

9.9 Installing EX-SBA

It is worth installing EX-SBA on your own computer, to learn how to use it as well as to be able to do data analysis when you have left ISIS. To install, follow the instructions in this section.

System Requirements: Windows 2000, XP, or NT 4.0 with Administrator powers and 100MB of hard drive

EX-SBA can be installed from a CD that it is available during your visit to ENGINX, or can be downloaded as a zipped file from
http://www.isis.rl.ac.uk/engineering/download/EX-SBA.zip .

From the CD:
1) Logon as Administrator.
2) Insert the CD, and follow instructions. Use the default options.
3) If CD doesn't start automatically, run setup_enginX.bat from the root directory of the CD.
4) Follow the instructions on the screen. Use default values for Open Genie installation.
5) Reboot the computer.
6) Run the program by double-clicking on c:\ENGINX\enginx.bat (or my_drive:\ENGINX\enginx.bat).

From the web:
1) Logon as Administrator.
2) Unzip enginx_CD.zip into an empty directory.

3) Run setup_enginX.bat from the unzipped files.
4) Follow the instructions on the screen. Use default values for the Open Genie installation.
5) Reboot the computer.
6) Run the program by double-clicking on c:\ENGINX\enginx.bat (or my_drive:\ENGINX\enginx.bat).

After the system is installed there should be a directory called C:\enginx (or D:\enginx, etc, depending on the drive you selected) with the following folders in it: FOCUS, GENIE, PAR, RAW_DATA, TEMPLATES.

9.9.1 Installation Troubleshooting

If the EX-SBA program does not run properly, it is likely to be because the installation program could not update the path and system variables. So, check the following:

a) Go to "Start→Settings→Control Panel→System→Advanced→Environment Variables"

b) Edit the PATH variable in the "System variables" box, and add the following at the end if not present:
;C:\GSAS\EXE;C:\enginx\genie\batch
(**Note:** replace "C:" for "my_drive:", i.e. the drive you selected during installation)

c) If not already defined, define a new variable in the "System variables" box:
Variable Name: GSAS
Variable Value=C:\GSAS
(**Note:** replace "C:" for "my_drive:", i.e. the drive you selected during installation)

d) If not already defined, define another new variable in the "System variables" box:
Variable Name: PGPLOT_FONT
Variable Value=C:\GSAS\PGL\GRFONT.DAT
(Note: replace "C:" for "my_drive:", i.e., the drive you have selected during installation)

If you still have problems, ask the Instrument Scientist.

10 SSCANSS

Documentation for SSCANSS is in the process of being produced. Watch this space!

11 Monitoring your experiment

For many experiments, it is not necessary for someone to be in attendance at the beamline 24 hours a day. Nevertheless, mistakes and mishaps are all too common, and it is very worthwhile to keep a regular check on your experiment even when you are not present. There are a few simple ways you can do this:

- **Check the dashboard via the web**. The dashboard can be viewed on the web at http://www.isis.rl.ac.uk/DataWeb/Dashboards (select ENGINX from the drop down menu).
- **Check the webcams.** There are two webcams which view the sample position**.** The web addresses are: http://130.246.54.90/view/view.shtml (webcam 1) and http://130.246.54.87/view/view.shtml (webcam 2). These can only be viewed on the RAL site.
- **Check the present and averaged beam current.** The present beam current can be viewed via the dashboard (although note that it will read 0.0uA if the instrument is in SETUP mode). The averaged current (over the last hour and day) can be viewed at http://www.isis.rl.ac.uk/status/index.htm .

12 Further information

12.1 Networking your laptop in the ENGIN-X cabin

Network cables and ethernet connection points are available in the cabin. Plug in, and set your laptop to obtain an IPaddress automatically.

12.2 Archiving of data

You should try to ensure that by the time you leave ENGIN-X, you have focussed your data (i.e. produced .his files), and take these away with you. You will then be able to work with them on your own installation of EX-SBA. It is unlikely you will need the raw data again, but if you do, ask your local contact to retrieve it from the data archive. The data is archived on the ISIS network at the network share \\isisid\inst$\NDXENGINX\Instrument\Data in directories named according to cycle (you will need a password to access this). Log files are stored in the same directories. The stress rig datafiles are stored in the directory logs\Stress Rig.

13 Pitfalls (READ THIS SECTION!)

Bear in mind the short checklist below, to avoid making simple mistakes which might lead to accidents, poor quality data, or long periods of lost beamtime!

1. Have you moved Jaws 3 as close as possible to your sample?
2. Have you put the positioner into remote control?
3. Have you opened the shutter?
4. If you have performed a wall scan, have you subsequently issued **wallscan/off** to reduce the width of the DAE time bins?
5. Are all variables in your script of the correct type? E.g: **waitfor seconds=15** (integer); **motor/x 0.** (floating point); **waitfor uamps=40** (floating point).

14 Troubleshooting

Listed below are a range of problems and possible solutions, grouped into categories. It will be appreciated if you try to find the solution in this list yourself, before contacting your local contact at 3am!

14.1 Data acquisition

- **Runs are ending as soon as they begin (e.g. after 0.2 uamps)**

Check the script: Is there a **waitfor seconds=15** line after "BEGIN"? Without this, subsequent commands (e.g. **waitfor uamps=xxx**) may be ignored.

- **Open Genie on the control computer doesn't obey your commands!**

Have you re-started Ray of Light? After doing this you must always start a new Open Genie window (Start > Open Genie). The old window will not listen to you. In any case, try opening a new window and see if it will accept your commands.

- **Open GENIE complains at script**

Have you declared all variables?
Make sure scripts end with a new line.

- **Script runs directly after issuing loadscript command**

Is there a minus sign in the script title? Open Genie won't like it!

14.2 Data analysis

- **Binning of spectra looks wrong (too few points)**

Have you performed a wall scan using wallscan/on? Make sure "wallscan/off" has been issued afterwards - otherwise the TOF resolution will be wrong.

- **Spikes in spectra**

You can limit the maximum intensity in the spectra using the command:
xfocus/spikes run bank ymax
Example: **xfocus/spikes 33456 2 1000**

This creates a new .his file with the spikes chopped.

- **Spectrum appears empty**

This may be because the spectrum is plotted on the wrong y-scale due to a large spike in intensity. Try the tip above for removing spikes in the spectra.

- **Information lost from titles**

Maximum length of titles is 24 characters - anything else will be lost, even though it is seen on the dashboard.

- **.dat files created using batch_gsas_file don't have full TOF range**

Before issuing **batch_gsas_file**, set the TOF range to greater than required, e.g
enginx.bank[1].t_min=1000
enginx.bank[1].t_max=99000

(for bank 1, similarly for bank 2).

14.3 Positioner

- **Positioner has crashed**

Go into the tunnel. The positioner controller is the large beige cabinet directly to your right. Twist the large red power switch (labelled Danger 240V), wait for a few seconds, then twist back on. Wait for the display on the operator panel to prompt you to press the green "Control On" button, and then do so. Home theta and follow instructions on paper stuck on the operator panel (set datum at -0.16º). If you have entered the tunnel you will need to hit the search button inside it when closing up the hutch.

- **Positioner tries to go to ridiculous position (e.g. very large x or y)**

Have you defined a scan about the present position, but forgotten to read it in? HIT STOP if you are unsure!

- **Positioner is not moving to the positions specified (no error message)**

Make sure the positioner is in remote control (not local) - the remote control button on the control GUI should be showing bright green. WARNING - this is a common error which has resulted in useless data acquisition for long periods of time!!

14.4 Stress rig and furnace

- **Communication lost between stress rig and control computer (flashing red error message: Stress Rig: Error Generated: "GPIB**

Write in Read values from Instron.vi -> Stress Rig.vi. Possible reasons: LabVIEW: Cannot add Resource. or NI-488: GPIB bus error.

The most guaranteed way of restoring communication is to turn off the ENGIN-X control computer, stress rig controller (on/off switch on back), and the National Instruments GPIB interface box (small box on floor near stress rig controller). Then re-boot the computer and turn the stress rig controller back on. When both are running, turn on the GPIB box. Finally, re-start the stress rig VI (click the arrow on the top left-hand corner).

Don't forget to start logging your variables again after re-starting the VI.

- **Optical furnace fails to light up**

Check the cooling water flow (meter attached to supply pipe). Sometimes even when there is flow, the meter reports no flow - as indicated by unlit LED. Tapping the meter may be sufficient to rectify the problem - if so the red LED will light up.

Check that the maximum power output is not set too low in the VI.

Check communication between the computer and furnace controller - e.g. if you change the setpoint temperature on the VI, is it updated on the controller display?

- **Stress rig does not respond after issuing stressrig/setpoint … command**

Is the stress rig in the correct control mode? E.g. if you issue **stresssrig/setpoint stress xxx**, then the stress rig will only respond if it is already in load control mode. To change the control mode, issue **stressrig/control channel** (e.g. **stressrig/control stress**).

15 Appendix A – Chopper and DAE Settings

Listed below are some commonly used chopper settings time-of-flight window settings.

C6=6.2m chopper; C9=9.4m chopper.

Material	Frequency (Hz)	Opening Times (μs)		TOF window (μs)		Max d (Å)
		C6	C9	Min	Max	
Al	25	1367	2050	10000	49999	2.4
α-Ti	25	1733	2600	14000	53999	2.55
bcc/fcc Fe, Ni	25	1067	1600	6000	45999	2.1
Calcite	17	1133	1700	6000	65999	3.1
Ni γ/γ′	17	2133	3200	15000	74999	3.6
FePd	25	1200	1800	8000	47999	2.25
Zr	25	2333	3500	19000	58999	2.7
V-Nb	12.5	1000	1500	5000	84999	

16 Appendix B – ENGIN-X commands

This appendix lists Open Genie and EX-SBA commands commonly used at ENGIN-X, but is not an exhaustive list. Follow the hyperlinks for examples of the use of the commands.

Open Genie instrument control commands

begin
cha title
end
file_scan
loadscript
motor
pause
resume
updatestore
stressrig
waitfor
wallscan

EX-SBA / Open Genie data analysis commands

add
analyze
analyze_scan
analyze_scan/gsas
batch_focus
batch_gsas_file
display
find_pin
fit_peak
gsas_file
integrate_scan
rfocus
set/ext
units
xfocus
xfocus/spikes