Gumtree-Kowari User's Guide

Team DAV

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Chapter 1. Introduction

1.1. Who Should Read This Guide

This user guide is prepared for users of the neutron scattering instrument Kowari - Residual Stress Diffractometer at the Bragg Institute, ANSTO. It can also be used as a reference by the instrument scientists of Kowari.

1.2. System Requirements

· Hardware requirements

- Processor: 32-bit 1GHz or above CPU

- Memory: at least 1GB of free physical memory

- Storage: 1GB available space

- Video Card: support OpenGL V1.5

• Software requirements

- Windows XP or Vista

- Java SE JRE or JDK version 5 or above

1.3. Install and Run Gumtree-Kowari

1.3.1. Install and run Gumtree from NBI network.

If your computer is on the NBI network, you can run Gumtree from a the file server. To do so you need to open the Explorer window, and map your X: drive with the remote folder: \filer\scratch\xenv.

Gumtree-Kowari application shortcut on your computer.

On your desktop, find the below icon and double click on it.

Figure 1.1. Gumtree-Kowari application icon



1.3.2. Install and run Gumtree from ANSTO network

If your computer is on the ANSTO network, you can run Gumtree from the file server. To do so you need to open the Explorer window, map your X: drive with the remote folder: \\FIANNA\Sections\Bragg\Data Analysis Team \Share\xevn.

Open the folder: X:\gumtree\releases\apps\kowari, double click the file install.bat. This will install the Gumtree-Kowari application shortcut on your computer.

On your desktop, find the icon shown in Figure 1.1, "Gumtree-Kowari application icon" and double click on it.

1.3.3. Install and run a standalone version

Please contact Kowari instrument scientists or the software support team in the Bragg Institute for a copy of standalone version of Gumtree application.

Once you get the zipped application package of Gumtree, unzip the package into your local drive. In the target folder, you will find an executable file *kowari.exe* with an icon shown in Figure 1.1, "Gumtree-Kowari application icon". Double click on it to run Gumtree.

1.3.4. Login to SICS

If you are running remotely in NBI network, a window will pop up to ask you to login to SICS - the Instrument Control Sever, as shown in Figure 1.2, "SICS Login Window". Please ask for the login information from the instrument scientists. If you do not want to login to SICS, simply tick the checkbox Do not ask to login again, and click on Cancel button.

Figure 1.2. SICS Login Window



1.3.5. Open / switch to Analysis Window and Scan Experiment Window

If you are running on the NBI network, both the analysis window and the experiment window will be automatically opened. You can identify these windows by the titles. The title is located at the top left corner of the window. For example, Figure 1.3, "Title of Analysis Window" and Figure 1.4, "Title of Experiment Window".

Figure 1.3. Title of Analysis Window

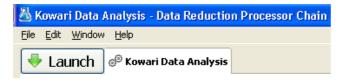


Figure 1.4. Title of Experiment Window



If you are running a standalone version of Gumtree, the above two windows will not automatically open at the

beginning. To launch both windows, click on the Launch button, and choose **Kowari Experiment** option.

To launch the data analysis window, click on the *Launch* button, choose *Perspective* option, then choose *Kowari Data Analysis* option.

To launch the experiment window, click on the *Launch* button, choose *Perspective* option, then choose *Kowari Experiment* option.

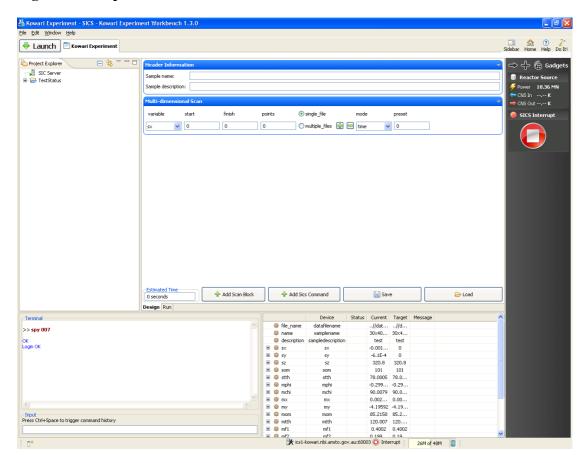
Chapter 2. Experiment Window

2.1. Introduction

The Kowari Experiment Window is a graphical user interface to do neutron scattering experiments on Kowari instrument. It consists of four window parts, the *Project Explorer*, the *Scan Design & Run*, the *Command Line Terminal*, and the *Instrument Status Table*. These applications can help user to do both instrument control and scan experiments.

To launch the Experiment Window, click on the *Launch* button. Choose *Perspective* option, then choose *Kowari Experiment* option. Figure 2.1, "Experiment Window" shows an snapshot of the Experiment Window.

Figure 2.1. Experiment Window



2.2. Getting Started with Scan Experiment

The *Gumtree Scan Experiment* application is a tool to simplify designing and carrying on neutron scattering experiment on Kowari instrument. To quickly getting started with this application interface, please follow the procedure described in this section.

2.2.1. Get the Instrument Ready

Before you want to do a scan experiment on Kowari, you need to make sure the hardwares required in your experiment are installed and the whole instrument is well aligned. These hardwares include the sample, the sample holder, and the sample environment facility. Your instrument scientist will help you with this. You need to work out how to configure the instrument to best suit your experiment requirements with the instrument scientist as well.

Once your experiment sample has been planted into the instrument, you need to measure the detail positions of the sample on the sample stage. Then you need to come up with a plan on how to perform the neutron scattering scan. Drawing the plan on a plot can help you to work it out.

2.3. Scan Design tab

Use the *Design* tab to create the scan tasks.

2.3.1. Header Information

Input the sample name and sample description in the *Header Information Block* in the Design tab, as shown in Figure 2.2, "Header Information". This information will be used to label your sample in the NeXus data file

Figure 2.2. Header Information



2.3.2. Add a Scan

To add more scans, click on the button **AMSGEREGE. A new scan widget will show up at the bottom of the Design tab. The new scan is by default the same type as the one above it.

2.3.3. Select Scan Type

To select the scan type, click on the drop down menu button A list of scan types will show up, as seen in Figure 2.3, "Scan Types". Simply choose the one you need, then the task block will change to the selected type. Please be careful of changing the type, because once you changed the type of a scan block, the editing previously done in this block will get lost. You will have a blank block in a newly selected type.

Figure 2.3. Scan Types



2.3.4. Scan Parameters

To use the Design tab to create a scan, you need to learn the meaning of the following arguments.

- *variable*: the scan variable. It is an instrument component, which can be a motor or an sample environment controller e.g., temperature controller.
- *start*: the start value for the scan variable.
- *finish*: the finish value for the scan variable.
- points: the total number of points in the scan.
- *mode*: the histogram memory mode. Available options are, *time* and *count*. If you set the mode to *time*, the histogram server will stop when the acquisition time reaches the number of seconds set with the *preset* argument.

If you set the mode to *count*, the histogram server will stop when the beam monitor counts reaches the number which is set by the *preset* argument.

• preset: the acquisition duration at each scan point, this is in seconds if the mode is time, or counts if the mode is count.

2.3.5. One-dimensional Scan

A one-dimensional scan means only one variable is changed in the scan. A graphical description of a one-dimensional scan is in Figure 2.4, "Icon of One-Dimensional Scan"

Figure 2.4. Icon of One-Dimensional Scan



Use the *Multi-dimensional Scan* block in the Design tab for this type of scan. For example in Figure 2.5, "One-Dimensional Scan", the scan will perform like this: drive *sx* motor to positions, 0, 1, 2 and 3. At each position, do a histogram memory acquisition for 120 seconds. The single_file choice helps to save all the data records into the same file. If you choose multiple_files option, each data record will be saved into a separate file.

Figure 2.5. One-Dimensional Scan



2.3.6. Simple Multi-Dimensional Scan

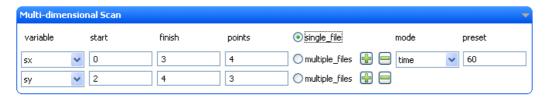
The multi-dimensional scan means more than one variable is changed in the scan. The way of these variables get changed is in a matrix way. A graphical description of such scan is shown in Figure 2.6, "Icon of Two-Dimensional Scan", which is a two-dimensional special case.

Figure 2.6. Icon of Two-Dimensional Scan



Use the *Multi-dimensional Scan* block in the Design tab to setup this scan. For example in Figure 2.7, "Multi-Dimensional Scan", it will drive *sx* and *sy* motors to the following coordinate positions, (0, 0.1), (0, 0.2), (0, 0.3), (1, 0.1) ..., (3, 0.3), totally 12 positions. At each position, do a histogram memory acquisition for 120 seconds. There are totally 12 data records will be generated. If you choose the single_file option, all data will be saved into the same file. If you choose the multiple_files option at the line for *sx*, there will be 4 files generated. Each file will contain 3 data records. If you choose the multiple_files option at the line for *sy*, there will be 12 records generated, with 1 data record in each file.

Figure 2.7. Multi-Dimensional Scan



2.3.7. Advanced Multi-Dimensional Scan

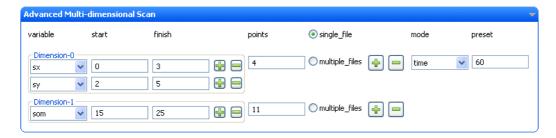
An advanced multi-dimensional scan is a scan that has one or more dimensions. And in each of the dimensions, you can change more than one variable. Use the *Advanced Multi-dimensional Scan* block in the Design tab to setup this scan. A graphical description of this scan is shown in Figure 2.8, "Icon of Advanced Multi_Dimensional Scan".

Figure 2.8. Icon of Advanced Multi Dimensional Scan



For example in Figure 2.9, "Advanced Multi-Dimensional Scan", the scan has two dimensions. In the first dimension, it moves motor *sx* and *sy* at the same time for each scan point. These coordinates are (0, 0.1), (1, 0.2), (2, 0.3) and (3, 0.4). For each coordinate of these positions, it will do a single dimensional scan on *som*. The total scan positions in this example is 44. If you choose the single_file option, all data will be saved into the same file. If you choose the multiple_files option at dimension 0, there will be 4 files generated. Each file will contain 11 data records. If you choose the multiple_files option at dimension 1, there will be 44 records generated, with 1 data record in each file.

Figure 2.9. Advanced Multi-Dimensional Scan



2.3.8. Arbitrary Scan

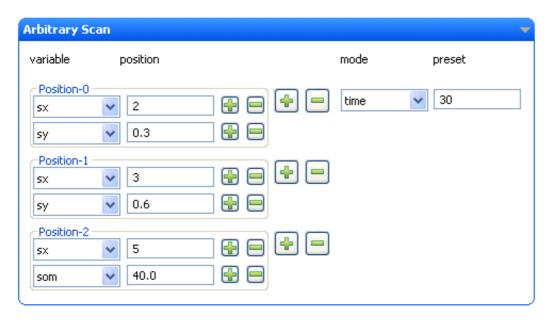
The Arbitrary Scan is a scan that you can change arbitrary variable in the instrument. A graphical description of such scan is shown in Figure 2.10, "Icon of Arbitrary Scan".

Figure 2.10. Icon of Arbitrary Scan



You need to define each position separately. For example, there are 3 scan positions. In each position, you change arbitrary parameters.

Figure 2.11. Arbitrary Scan



2.3.9. Run the Scan

To run the scan, change to the *Run* interface. To do so, click on the *Run* tab at the bottom of the Design tab, see Figure 2.12, "Switch to Run Interface". You will get Run interface. More information on this interface is provided later in this chapter. To run the script, simply click on the Run button.

Figure 2.12. Switch to Run Interface



2.3.10. Check the Scan Result

Once you click on the Run button, the status bar on top of the Run block will change colour and show RUNNING.

Meanwhile the timer at the top right will start, for example, when one line of the script gets processed, the colour of that line is changed to yellow. When the script processing is complete, the status label becomes READY and the timer stops.

To view scan data and data reduction result, please use the *Kowari Analysis Window*. If the analysis application window is open, it will pick up the newly generated NeXus data and load it into the *File Management*. To run the analysis algorithm, simply click on the file. The algorithm will start processing and the results will get shown in the plotting area. For more information about data analysis, please read Chapter 3, *Data Analysis Window*.

2.3.11. Add SICS Command Block

To add SICS command block, click on the button *** An empty SICS command block will appear. To add new commands in the block, click on the **** button. As shown in Figure 2.13, "SICS Command Block", there are two types of commands, the *Drivable* command and *Script* command.

- Use *Drivable* command to move a motor to certain position. Please select the motor name in the drop down list, and set the target position value.
- Use *Script* command to add SICS Tcl commands. You can add as many as possible lines of Tcl code to the text box.

Figure 2.13. SICS Command Block



Click on the - button, a drop down menu pops up, as show in Figure 2.14, "Command Drop-down Menu". You can use this menu to change the type of the command, delete it, or move it.

Figure 2.14. Command Drop-down Menu



2.4. Scan Design tab Advanced

In this section, we will introduce the advanced functions of the Design tab.

2.4.1. Move Scan

You can move a scan up or down. To move a scan up, click on the drop down menu button , select Move up. The scan will get switched with the scan above it. To move a scan down, select Move down in the drop down menu. The scan will get switched with the block blow it.

2.4.2. Remove Scan

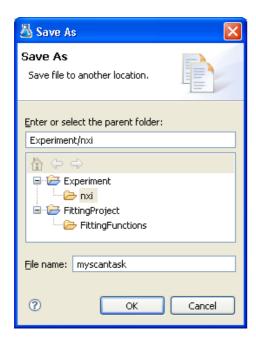
To remove a scan, click on the drop down menu button , select **Remove*. The scan will be removed.

2.4.3. Save and Load Scan

You can save the group of scans designed in the Design tab to a file in the Gumtree Project Folder and load it.

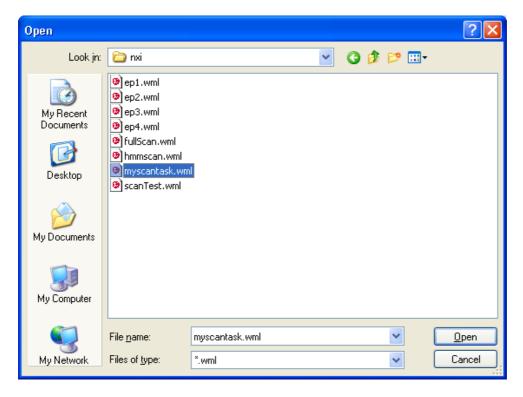
To save the group of scans, click on the source button. A Save As wizard window will pop up, as shown in Figure 2.15, "Save As' Wizard". You need to choose a project folder to store your file and provide a file name. Click OK button to confirm. By default, the extension name of the file is *.wml. After the file is saved, you can find it in the Project Explorer.

Figure 2.15. 'Save As' Wizard



• To load the saved group of scans, click on the Load button. A *File Selection* window will pop up, as shown in Figure 2.16, "File Selection Window". You can choose a file with an extension name of *.wml. The File Selection window allows you to locate any file in your file system.

Figure 2.16. File Selection Window



• Another way to load a saved scans is by drag and drop. In the *Project Explorer* block, locate the file you want to load. Simply drag and drop it into the Design tab. The file will be loaded. If the target file is not a scan file, an error message box will pop up.

2.4.4. Estimation of Total Run Time

The Design tab helps you to estimate how much time your group of scans is going to take. The text box that shows the estimation is located at the bottom left corner of the Design tab, as shown in Figure 2.17, "Run Time Estimation".

Figure 2.17. Run Time Estimation

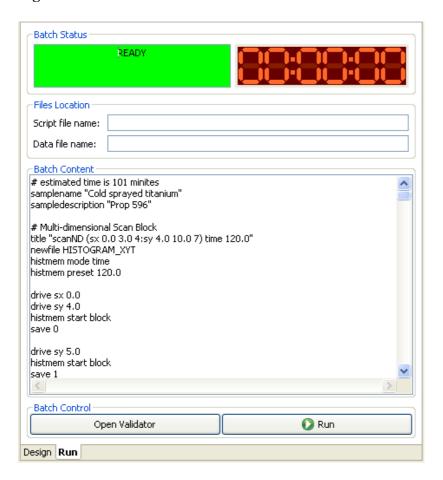


- If the scan modes of your tasks are *time*, the estimation will provide a value in time units. For example, *101 minutes* or *15 hours*.
- If the scan modes of your tasks are *count*, the estimation will provide a value in counts. For example, 20,000 *counts*. To achieve the same counts, it will take different amount of time in different experiments.
- If the scan mode of your tasks are a combination of *time* and *count*, the estimation will be time plus counts. For example, 3 hours and 10,000 counts.

2.5. Scan Run Tab

To run the scan, you need to change to the *Run* tab. To do so, click on the *Run* tab at the bottom of the Scan Design & Run. The Design tab disappears and is replaced with the Run tab, as seen in Figure 2.18, "Run tab". You can check the Tcl script that is going to be sent to SICS to run. Before you want to run the script, it is recommended to validate the script first. To validate the script, send the script to a validation server by clicking on the *Open Validator* button. To run the script, simply click on the

Figure 2.18. Run tab



2.5.1. Validate Tcl Script

The Tcl script generated by the Design tab will show up in the text area of the *Run* tab. Before you run the script, please visually check the script and validate it. Validation is done by sending the script to SICS running in simulation mode. To do the validation, click on the *Open Validator* button. A connection window will pop up to login in to SICS, as seen in Figure 2.19, "Validation Dialog". Simply input your SICS login name and password and click on *Validate*. The script should only take a few seconds to run. If there is a problem in the script code, the validation window will let you know. Otherwise it will tell you that the script validation has passed.

Figure 2.19. Validation Dialog



2.5.2. Run Scan Script

To run the Tcl Script, click on the Run button. Gumtree will send the Tcl script to SICS to run.

When SICS is running the scan script, the Run button changes to an Interrupt button. You can use this button to stop the script.

2.5.3. Interrupt the Scan

There are three Interrupt buttons available in the Gumtree application window.

- The most convenient way of stopping running of the script is to use the SICS Interrupt Button in the Sidebar. In every Gumtree window, there is a Sidebar located at the right side of the window. Single click on the button will stop SICS. To learn more about the Sidebar, please read Section 2.9.2, "SICS Interrupt".
- Once the script is running, the *Run* button in the *Run* tab will change to an Interrupt button. You can use this button to stop the script.
- There is an Interrupt button in the status bar at the bottom of the *Scan Experiment Window*, as shown in Figure 2.20, "Interrupt Button at the Foot Bar". You can use this button to stop the script.

Figure 2.20. Interrupt Button at the Foot Bar



2.5.4. Run Status

Once you click on the Run button, the status bar on top of the Run block will change colour and show RUNNING.

Meanwhile the timer at the top right will start, for example, when one line of the script gets processed, the colour of that line is changed to yellow. When the script processing is complete, the status label becomes READY and the timer stops.

Figure 2.21. Run Status



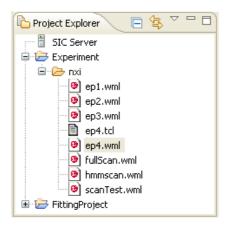
2.5.5. Drag and Drop Tcl Script File

You can drag and drop a *.tcl file from the Project Explorer block into the Scan Run tab. The *.tcl files must be Tcl script files. Once a script is loaded, you can either do a validation on the script or start running the script by clicking on the Run button.

2.6. Project Explorer

The Project Explorer is an application window for you to manage saved scan tasks. It is located at the top left of the Experiment Window. Figure 2.22, "Project Explorer Block" shows an example of the tree structure of the Project Explorer. You can copy and paste any type of file to the folders in the Project Explorer. However you can only load two types of files into the Experiment Window. One is *.wml files, which can be loaded into the Design tab. The other type is *.tcl files, which can be loaded into the Run tab.

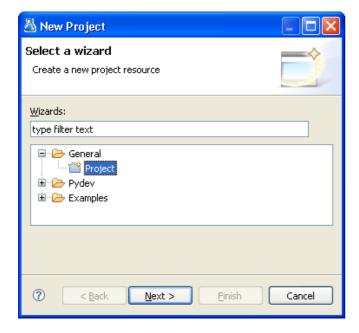
Figure 2.22. Project Explorer Block



2.6.1. Create Project

To create a new project, right click on the Project Explorer Block, an application menu will pop up. Choose *New - Project* option. A project creating wizard will pop up. Another way to show the wizard is to use the application window menu *File -> New -> Project*. In the wizard window, please choose the project type, *General -> Project*, as shown in Figure 2.23, "New Project Wizard". Then click on *Next*. In the next window, simply type in a name of the project, then click on *Finish*.

Figure 2.23. New Project Wizard



2.6.2. Add Folder

To add a new folder in a project, simply right click in the Project Explorer. In the pop up menu, choose *New -> Folder* option. A folder creation wizard window will pop up. Choose the project root or a parent folder where you want to put the new folder, and give a name to the new folder. Then click on *Finish*.

Figure 2.24. New Folder Wizard



2.6.3. Drag and Drop

- You can drag and drop a *.wml file into the Design tab. The *.wml files are saved by the Design tab at a previous time. Simply drag the file and drop it into the Design tab. The file will be loaded back by the Design tab. The Design tab will create the graphical scan commands accordingly.
- You can drag and drop a *.tcl file into the Tcl Runner Block. The *.tcl files are Tcl script files. Once a *.tcl file is loaded into the Script Runner, you can either do a validation on the script or start running the script by clicking on the Run button.

2.6.4. Other File Management Action

You can perform other file management actions on the Project Explorer Block. The supported actions are, *Copy and Paste*, *Move Files*, *Change Filename*, *Delete File*, and so on.

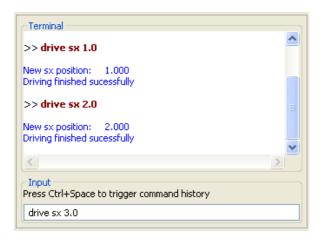
2.7. Command Line Terminal

To send a SICS command with the *Command Line Terminal*, simply type a SICS command into the Input text box. Then hit the *Enter* key. To read the command history, use the **CTRL** + **Space** key combination.

Warning

Be very careful! You can put the instrument out of alignment or disrupt your experiment using this terminal.

Figure 2.25. Command Line Terminal



2.8. Instrument Status Table

The Instrument Status Table is located at bottom right of the Experiment Window. You can use this table to monitor certain parameters of the instrument. You can also change the parameter values by using this table.

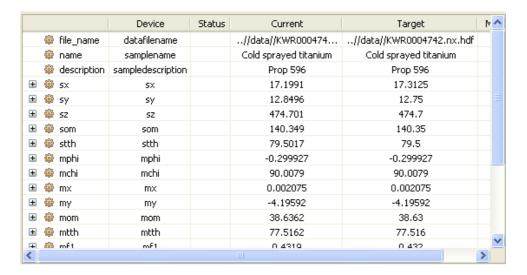
Warning

Be very careful! You can put the instrument out of alignment, or disrupt your experiment using this table.

The columns of the Instrument Status Table are:

- Device column: the sics name of the parameter.
- *Status* column: the status of the device. It can be *running*, or empty. Once you choose to drive the device, the status will change to *running*. It will change back to empty once the drive is done.
- Current column: the current position or value of the device.
- *Target* column: the target position or value of the device. You can use this column to drive the device or change the value. To do this, click on the *Target* column of the device. Type in the new value, then hit **ENTER** key.

Figure 2.26. Instrument Status Table



2.9. Gadgets Sidebar

In every Gumtree application window, there is a Sidebar. There are convenient Gadgets available in the Sidebar. Figure 2.27, "Gadgets Block" shows the Reactor Information gadget and Sics Interrupt gadget.

Figure 2.27. Gadgets Block



2.9.1. Show or Hide Sidebar

You have two ways of showing or hiding Gadgets Sidebar.

- Use the arrow button to fold the Sidebar.
- Use the *Sidebar* icon in the Gumtree quick launch menu bar to hid the Sidebar, as seen in Figure 2.28, "Sidebar Control".

Figure 2.28. Sidebar Control



2.9.2. SICS Interrupt

To quickly locate the SICS interrupt widget, find the button as shown in Figure 2.29, "SICS Interrupt Gadget" in the Gadgets block. Click on this SICS Interrupt button will send an interrupt signal and stop any action by the SICS server.

Warning

Hitting the interrupt will not immediately stop motion. A motor will go into its deceleration routine and come to rest as quickly as possible without damaging the instrument.

Figure 2.29. SICS Interrupt Gadget



Chapter 3. Data Analysis Window

The Kowari Data Analysis Window is a customised graphic user interface for reducing raw data acquired by Kowari. It consists of 4 parts, File Manager, Batch Data Processing and Export, Algorithm Control and Plot. The data is in binary *NeXus* format and contains raw data acquired in a Scan done using the Experiment Window.

To launch the analysis window, click on the *Launch* button, choose *Perspective* option, then choose *Kowari Data Analysis* option.

☐ ⚠ ⑦ ♪ Sidebar Home Help Do It! Launch & Kowari Data Analysis - P 🥬 🗶 🖏 🔞 🤊 0003115 D:\dra\kowaridata\KWR0003115.nx.hd 0003220 D:\dra\kowaridata\KWR0003220.nx.hd 0003221 D:\dra\kowaridata\KWR0003221.nx.hd 0003222 D:\dra\kowaridata\KWR0003221.nx.hd 0 20 x_pixel_offset () Raw Data & Fit Result; 7,000 6,000 | X min | 82.4577107 | X max | 97.5475 5,000 4.000 품 3,000 Export All #2,000 O0 Choose Source Dat use corrected data amplitude twoTheta (degrees) 0 Intensity Integration; enable efficiency 500,000 450.000 region of interests Mask 6 [-47.0, -137.0, > ephi (dearees) ✓ Apply

Relaunch

Report

Report

Figure 3.1. Analysis Window

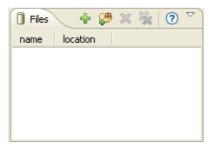
3.1. Getting Started with Data Analysis

A standard Kowari Data Analysis procedure includes the following steps: efficiency correction, geometry correction, 2θ integration and curve fitting. Please contact your instrument scientist for detail information about this procedure.

3.1.1. File Manager

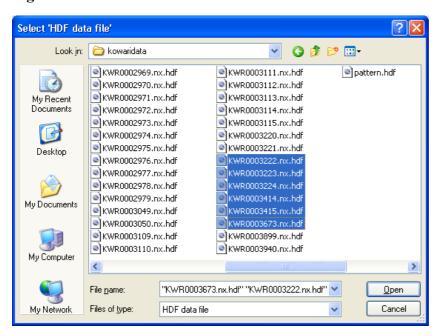
On the top left part of the window, there is the File Manager, as shown in Figure 3.2, "File Manager".

Figure 3.2. File Manager



Use button + to pop up the file selection window. You can get the same window popped up by clicking on the drop down menu and choose + Add File(s) option.

Figure 3.3. File Browser



By default, the File Browser will use a filter to show all the files that have an extension name of '*.hdf'. You can also set the filter to show all files by setting the *Files of type* option to '*.*'. You can use the file browser window to select multiple files at the same time. Then click the *Open* button to confirm your selections. Once one or more files have been selected, the analysis application will pick the last file in the selections and run the analysis algorithm on it. The results of the analysis algorithm will be plotted in the Plot area of the Analysis Window.

3.1.2. Algorithm Control

Algorithm Control is located in the bottom left of the Analysis Window. Please read the following items to tune the algorithms. If you need detail information about the algorithm parameters, please read Section 3.4, "Algorithm Control".

3.1.2.1. Frame

A *frame* is defined as a single detector histogram which is a 2-dimensional array of neutron count data and has been taken at a single point in a multi-point scan. The number of frames equals the number of scan points.

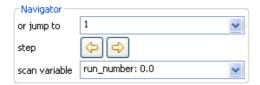
3.1.2.2. Navigation Control

By default when you first run the algorithm on a NeXus data file, it will pick the first *Section 3.1.2.1*, "Frame" frame of data to process. The correction result will show up in the uppermost Plot. It is a two-dimensional

plot of the detector reading after efficiency correction and geometry correction, if you have enabled these corrections. If there is more than one frame in the data file, you need to use the widgets in Figure 3.4, "Navigation Control" to navigate through the frames.

More detail can be found in Section 3.4.3, "Navigation Control"

Figure 3.4. Navigation Control



- The jump to drop down list shows all the frame IDs. You can select to analyse on a frame by selecting an ID.
- The step navigation buttons will help you to move forwards or backwards in the frame sequence.
- The *scan variable* drop down list shows all the scan variable positions where each frame of data is taken. You can analyse on a frame by selecting its scan variable position.

3.1.2.3. Efficiency Correction Control

The instrument scientist will prepare the efficiency map of the detector ahead of time. Please ask your instrument scientist for the location of this file. Once you know where to find this file, you can use the widgets in Figure 3.5, "Efficiency Correction Control" to load the efficiency file. Enable efficiency correction by selecting the checkbox.

Figure 3.5. Efficiency Correction Control



For more information on efficiency correction, please read Section 3.4.4, "Efficiency Correction Control".

3.1.3. Plot

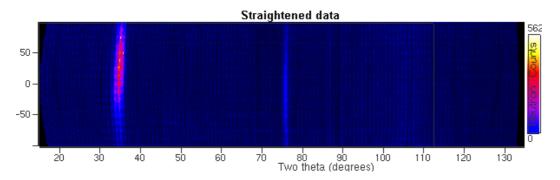
The Plot area is the right part of the window. There are three plots that show the results of the data reduction and analysis.

To read more information about how to control Plot, for example zoom see Section 3.7, "2D Plot Controls".

3.1.3.1. Corrected Data

The first Plot is a two-dimensional intensity plot that shows the corrected detector counts. If you have chosen to enable efficiency correction and geometry correction, it will plot the intensity data after these corrections. In the example of Figure 3.6, "Corrected Data", both the vertical and horizontal axes are the physical dimensions of the detector. The colour of each pixel in the plot represents the neutron count reading in that location of the detector.

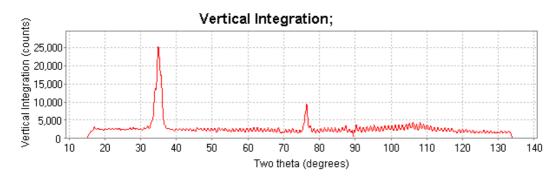
Figure 3.6. Corrected Data



3.1.3.2. Integrated Counts

The second Plot consists of two plots. The vertically integrated detector counts are shown as points, and a fit to these points is shown as a curve. If you have applied a *Region of Interests* (ROI) in the intensity plot above, the algorithm will do the integration only in the masked area.

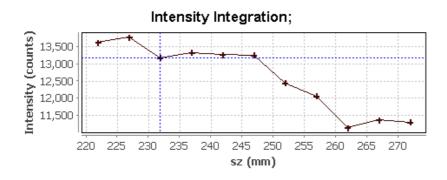
Figure 3.7. Integrated Counts



3.1.3.3. Scan Data

The third Plot shows the aggregated scan data. By default it shows the *intensity integration of the whole detector* vs scan variable plot. If you need more details about the result plots, please read Section 3.5, "Plot".

Figure 3.8. Scan Data



3.2. File Manager

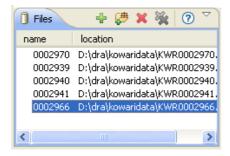
As shown in Figure 3.2, "File Manager", users can manage the data source files in this *File Manager*. This section details how to use the file manager to select files for analysis.

3.2.1. Add Files

You can use the button or drop down menu Add File(s) to open a *file selection window* as shown in Figure 3.3, "File Browser". Once one or more files has been selected, they will be imported into the *File Manager*. The names and locations of these files will be shown. By default, the analysis algorithm will use the last file in the selection as the input file and automatically Analysed and Plotted.

You can use this button to add one or many data files to the *File Manager*. However, only one file gets processed at a time and its result is plotted. The file that is processed gets highlighted, as shown in Figure 3.9, "File Manager".

Figure 3.9. File Manager



3.2.2. Add Folder

Use the button or drop down menu Add Directory to open a folder selection window as shown in Figure 3.10, "Folder Selection Window". Once a folder has been selected, click on the *OK* button to confirm your selection. This will import all NeXus files in that folder to the *File Manager*. The last file in the selected folder will be automatically Analysed and Plotted.

Figure 3.10. Folder Selection Window



3.2.3. Select an Input File

To Analyse a file, select that file by a single click. The selected file is highlighted and Analysis starts. You can only select one file at a time, hence only one file is Analysed and Plotted. You can use the *Arrow Up* or *Arrow Down* keys on your keyboard to navigate through the files in the *File Manager*.

3.2.4. Remove a File

To remove a file from the File Manager, you need to select the file. Please read Section 3.2.3, "Select an Input File" on the detail. Use button or drop down menu Remove File to remove the selected file. After removal,

the file located immediately below it in the File Manager will be highlighted and Analysed and Plotted. If there is no file below, the file above will be selected, Analysed and Plotted. If after removal, there is no file in the File Manager, Plot will be empty. Since it does not support multi-selection, you cannot remove multiple files unless you choose to Remove All Files.

3.2.5. Remove All Files

Use the button or drop down menu Remove All to remove all files in the *File Manager*. A confirmation window will pop up. If confirmed, all files are removed. Plot will be emptied.

3.2.6. Monitor Live Histogram Data

If Gumtree-Kowari is connected to SICS it will monitor any new NeXus file created or modified by the SICS server. To learn about how to connect to SICS server, please read Section 1.3, "Install and Run Gumtree-Kowari". When a new NeXus file is created, the File Manager will automatically read the file in. By default the files in the File Manager are sorted in a descending sequence. The new file usually has a larger numeric ID, so that it will be put on top of the file list in the File Manager. To Analyse and Plot the new file, simple click on it to select it.

If the selected file is modified by SICS, Gumtree-Kowari will detect this and read the modified file. If the frame entry in the file gets changed, Gumtree will re-run Analysis and Plot on the new result. If there is a new frame entry appended to the file, Gumtree will pick up the entry and Analyse and Plot it.

3.3. Batch Data Processing and Export

The Export All (batch data processing and save) button and a progress bar are located in the center left of the window, as shown in Figure 3.11, "Export and Progress Bar".

Figure 3.11. Export and Progress Bar

3.3.1. Batch Processing

You can reduce and export all files loaded into the File Manager. Using Export All, the NeXus data files are read sequentially and processed with the reduction algorithm. The one-dimensional vertically integrated result curves are saved into *XYSigma* ASCII files. For each NeXus file, there is one *XYSigma* file created. There is several lines of header information in the file to show the metadata. Each curve also follows a couple of header lines to tell the scan variable information.

To do batch processing, click on the button. A *Folder Selection Window* will pop up. After you confirm your selection, Gumtree will begin the process. The name of the exported files are the same as the NeXus files e.g. KWR1234567 but with an appended suffix and file extension. If efficiency correction is enabled in the *Algorithm Control*, it will append '_e' to the export file name. If geometry correction is enabled, it will append '_g' to the export file name. If there is a mask region applied, it will append the vertical boundary information of the region to the file name, e.g. '_-137.0_125.0' means vertical region from -137.0 mm to 125.0 mm. The extension will be *.xyd. An example of the file name is: KWR0003415_eg_-137.0_125.0.xyd, with efficiency correction, geometry correction and mask enabled. Data can also be saved one file at a time. See Section 3.5.4, "Save Scan Data"

3.3.2. Progress Bar

The progress bar represents the processing progress in two different modes.

1. File process mode. The Progress Bar shows the progress of processing all frames in a single NeXus file, when you choose to run the algorithm for a single file.

2. File export mode. The Progress bar shows the progress of exporting all files in the File Manager.

3.4. Algorithm Control

In this section, you will find information about how to tune the analysis algorithms. Figure 3.12, "Algorithm Control" shows an overview of the *Algorithm Control*.

Figure 3.12. Algorithm Control

-Navigator -					
or jump to	1				
step	♦				
scan variable	run_number: 0.0				
Efficiency Co	orrection				
folder path	file:/D:/dra/wombatdata/Effic >				
file name	eff_map.hdf				
enable	V				
Geometry Correction enable 🗹					
Apply Region of Interest and Mask					
ROI and mask <no mask=""></no>					
♣ Efficiency					

3.4.1. How to Change a Parameter

There are limited types of graphical widgets in *Algorithm Control*. They are checkbox, drop down list, file selection widget, navigation button and mask manager. Except for the navigation buttons, all changes to the above widgets

need a confirmation click on the button. After the file is Analysed and Plotted, the *Apply* button is greyed out. Once a change is made to the control widgets, the *Apply* button is highlighted. A single clicking on this button will apply all the changes made and start Analysis and Plot. Navigation buttons are exceptions, they do not need confirmation.

3.4.2. Use Corrected Data

In the NeXus file, the detector count data are accompanied with corrected data, which is corrected for count binning artefacts generated by the detector and its electronics. The corrected data is produced by the histogram server which uses dithering to balance counts in adjacent wires on the detector. By default, uncorrected data is Analysed and Plotted. Consult with your instrument scientist if you need to use the corrected data.

To use the wire corrected data, click to select the checkbox use corrected data ...

3.4.3. Navigation Control

There are three ways of navigating through the Section 3.1.2.1, "Frame" frame sequence in the NeXus file.

· Use frame index

The index of each frame will show up in the drop down list in Figure 3.13, "Frame Index". Choose the index of a frame that you want to show by a single click in the drop down list.

Figure 3.13. Frame Index

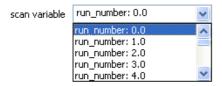




- Use navigation buttons . You can navigate backwards or forwards along the frame sequence with these buttons.
- Use scan variable position

The value of the scan variable for each frame will show up in the drop down list in Figure 3.14, "Scan Variable Values". You can choose to show a frame by selecting the scan variable value of that frame.

Figure 3.14. Scan Variable Values



3.4.4. Efficiency Correction Control

Usually the instrument scientist will prepare the efficiency map of the detector before you arrive and put it in your proposal directory. Please consult with your instrument scientist for the details of this file. To use the efficiency map file, you can use the widgets shown in Figure 3.15, "Efficiency Correction Control" to load it. Click on the

file selection button , to pop up a file selection window. Once the efficiency map file is selected, its path gets inputted into the text box. You can type the path of the file in the text box as well.

Figure 3.15. Efficiency Correction Control



You can enable or disable efficiency correction by changing selection of the checkbox. Click on the button to apply the change.



3.4.5. Geometry Correction Control

The geometry correction algorithm used in the analysis is to project a flat detector histogram onto a spherical surface. Please consult with your instrument scientist if you need to apply the geometry correction algorithm. To enable geometry correction, simply click to select the checkbox in Figure 3.16, "Geometry Correction Control".

Then click on Apply button to apply the change.

Figure 3.16. Geometry Correction Control



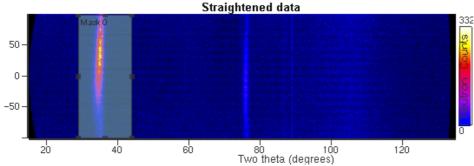
3.4.6. Region of Interest and Masking Control

In the analysis algorithm, you can put a series of mask as a single parameter to control selection of the detector histogram data. There are two types of masks, inclusive and exclusive. Inclusive masks are also called a *Region of Interest*, or ROI. If an ROI has been applied to the histogram data, only pixels included in the ROI will be considered in the analysis algorithm. Exclusive masks are called masks. If a mask has been applied to the histogram data, the pixels in the mask region will not be considered in the analysis algorithm.

There are two ways of inputting ROI or masks into the algorithm. One is to draw regions on the two-dimensional intensity plot in the plotting area. The other is to use the *Masking Properties Window* to define regions.

• To draw an ROI on the two-dimensional intensity plot, use **ALT + Left Mouse Button** combination to draw a rectilinear region on the plot. As shown in Figure 3.17, "ROI on 2D Plot", the colour of the ROI is green. To resize the ROI, move your mouse to the boarder of the region. The cursor becomes drag-able. You can drag the boarder to change the width or the height. To remove, move your mouse onto the ROI until the region gets focus. Push the **DELETE** key on your keyboard to remove.

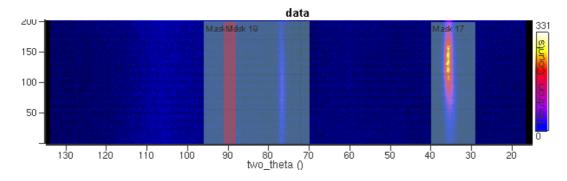
Figure 3.17. ROI on 2D Plot



• To draw a mask on the two-dimensional intensity plot, use **SHIFT** + **ALT** + **Left Mouse Button** combination. The colour of the mask region is red. Other properties of the mask are the same as the ROI.

You can draw as many ROI and masks on the intensity plot as you like. Figure 3.18, "Multiple ROI and Masks" shows an example of drawing one ROI and two masks on the intensity plot.

Figure 3.18. Multiple ROI and Masks



The other way of apply region selections is to define ROI and mask regions in the Masking Properties Window.

To open this window, click on the button in the algorithm control widget shown in Figure 3.19, "ROI and Mask Control".

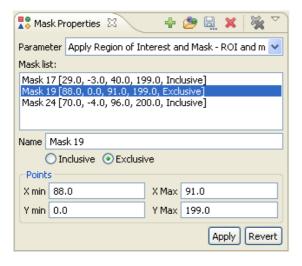
Figure 3.19. ROI and Mask Control



Figure 3.20, "Mask Properties Window" shows an example of masking properties window.

- To add a new mask, click on the button, a new mask item will show up in the *Mask list*. You can edit the position and size of the region by changing the coordinates of the mask in the *Points* widget. You can define as ROI or mask by switching between *Inclusive* and *Exclusive* options widget. You need to click on the *Apply* button to confirm any change.
- To change the name of the region, simply type in the *Name* text box.
- To remove a mask, click on the mask item. Then click on the * button.
- To remove all masks, click on the substant.
- To save all the masks to a file, click on the ... button. Pick a path and filename, then click on *SAVE*. All the masks drawn on the plot will be saved into the file in XML format.
- To load saved masks, click on the button. Choose a file saved previously, then click *OPEN*.

Figure 3.20. Mask Properties Window



The following logic describes how the regions define the selections of the histogram data.

- 1. If there is no ROI or mask region, all pixels in the detector histogram will be used.
- 2. If only masks exist, all pixels but the masked ones will be used.
- 3. If only ROI exist, only pixels in the ROI regions will be used.
- 4. If both ROI and masks exist, pixels in the ROI regions but not in the mask will be used.

3.5. Plot

There are three types of results for the Gumtree-Kowari data analysis, Corrected, Reduced and Analysed. In this section, we talk about these results.

3.5.1. Corrected Data

The first Plot shows the Corrected result. It is a two-dimensional detector histogram data plot. If you have chosen to enable efficiency correction and geometry correction, it will plot the intensity data after these corrections.

Figure 3.21, "Corrected Data" shows this Plot. The vertical and horizontal axes are the physical dimensions of the detector. Units of the axes are *mm*.

The colour of each pixel in the plot is coded by the number of neutron counts. The colour scale is located to the right of the plot. Readings from low to high coded by colors from dark to light.

Data View Fitting Mask Export Straightened data ør 50 -50· 80 90 Two theta (degrees) 30 z'n 40 50 60 70 100 110 120 130 X:32.48 Y:160.33 Value:28.097 | Zoom 100% | Status: Done

Figure 3.21. Corrected Data

To learn more information about the plot control, please read Section 3.7, "2D Plot Controls".

3.5.2. Integrated Counts

The one-dimensional reduction result is located in the second plot. It is the integration of the corrected histogram data in vertical direction. The horizontal axis of the curve has been converted into 20 values. Figure 3.22, "Integrated Counts" shows the integration result with a fitting curve. The integration result is plotted in Diamond markers and the fitting result is in a curved line. You can choose different marker shape for the plot. Please refer to Section 3.6, "1D Plot Controls".

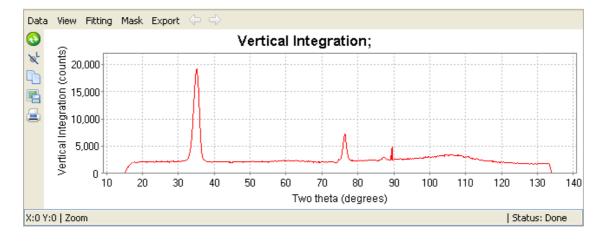
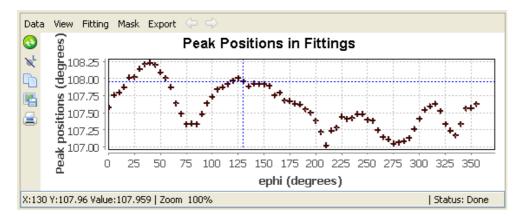


Figure 3.22. Integrated Counts

3.5.3. Scan Data

The analysis result of the algorithm will show up in the third plot in the plotting area. The horizontal axis of the plot is always the scan variables. For example, Figure 3.23, "Scan Data" shows the peak positions of the fitting of the frames vs the scan variable values.

Figure 3.23. Scan Data



All features in the 1D curve plot are supported by this Plot. However there are additional features for this plot.

· Jump to a frame

Double click on a point to pick the histogram frame that has a scan variable value as your selection. The algorithm will pick the frame as input and start processing. As a result, in the first plot of the plotting area, it will show the correction result of that frame. In the second plot, it will show the reduction result of that frame.

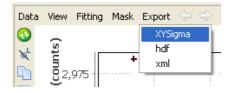
3.5.4. Save Scan Data

You can save different analysis results in multiple formats. The supported file formats are *binary (HDF5), ASCII(3 columns)*, and *XML*. There are different advantages in saving into different formats.

- HDF (Binary HDF5) format is a popular format in neutron scattering science. The NeXus data files created in Kowari experiments are also in HDF5 binary format. The data saved in HDF5 format are compressed, which helps to save storage space. Such file that contains analysis result can be easily read back by Gumtree applications.
- XYSigma (ASCII, with 3 columns table) format is more human-readable. This format is only supported for exporting one-dimensional curve data. The 3 columns are the AXIS, the VALUE, and the ERROR respectively.
- XML format is available for both the two-dimensional result and one-dimensional curve result. The advantage of using this format is that it easily holds the metadata and it is human readable.

To choose to save the result in your local drive, click on the *Export* item in the plot menu, as shown in Figure 3.24, "Export Result Menu". Then choose the file format you want to save. A file selection window will show up. Choose the folder and give a name to the file, then click *Save*.

Figure 3.24. Export Result Menu



3.6. 1D Plot Controls

The following features are about features supported by a one-dimensional curve plot, for example the reduction result plot or the analysis result plot. To learn about the meaning of the 1D results, please read Section 3.5.2, "Integrated Counts" and Section 3.5.3, "Scan Data".

3.6.1. Plot Window Control

3.6.1.1. Zoom

To zoom in certain region of the 1D plot, simply *push down the left mouse button and draw a rectilinear box from top left to bottom right* on that region. You can use this action to zoom in up to possible zooming levels.

To zoom out to the original level, *push down the left mouse button and move it up or left*. Another way to zoom out is to click on the 3 button at the top left corner of the plot.

3.6.1.2. Pick a point in the curve

Single click on a point in the curve, it will provide a crossing at the point in blue colour. The crossing clearly tells the positions of the point. The detail values of the position will also show up in the status bar at the bottom of the plot.

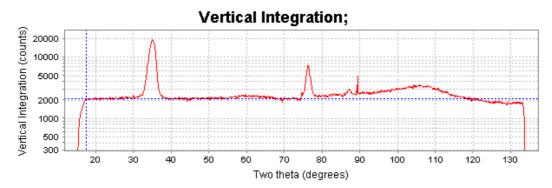
Figure 3.25. Point Properties

X:95.58 Y:50.19

3.6.1.3. Switch between logarithmic and linear axis

Click on the button to switch the vertical coordinate axis between logarithm axis and common axis. Figure 3.26, "Logarithm Axis" shows an example with logarithm vertical axis in the plot.

Figure 3.26. Logarithm Axis



3.6.1.4. Copy to clipboard

Click on the button to copy the current plot image into system clipboard. You can paste the image into common Windows imaging application such as *MSPaint* and *MSOffice* applications.

3.6.1.5. Save to image file

Click on the button to save the current plot to an image file in your file system. A *Save As* window will pop up for you to pick the folder and file name for the image file. It supports three image file formats: *BMP*, *JPEG* and *PNG*.

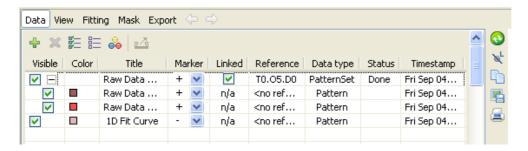
3.6.1.6. Print the plot

Click on the button to print the current plot image. Two windows will pop up for you to setup the layout properties and to choose a printer.

3.6.2. Data

Click on the *Data* item in the plot menu bar, a Data Control Block will show up in the left side of the plot. For example, Figure 3.27, "Data Control" shows the block of the integration result plot.

Figure 3.27. Data Control



The following features are supported in the Data Control Block.

3.6.2.1. Visible

The first column of the data control area is visibility control. Select or deselect the check box in that column to show or hide the data.

The one-dimensional curve data is called *Pattern* in Gumtree plotting space. Some time, the data fed to the plot can be a group of such one-dimensional data, which we call *PatternSet*. By default, all *Patterns* under the *PatternSet* will show up in the Visibility Control Area. Click on the button \Box to fold the *PatternSet* so that it hides the *Patterns* within it. Click it again to unfold it. Deselect the visibility checkbox of the *PatternSet* will set all *Patterns* in it invisible.

3.6.2.2. Color

Use the *Colour* column to change the colour of the curve shows in the plot. By default, the colors of the curve data are selected automatically from a rainbow colour series to be different from each other. You can change the colour of a single curve by clicking on the colour label in the *Colour* column. A *Colour Selection Panel* window will show up as in Figure 3.28, "Colour Selection Panel". You can either choose a basic colour or click on the *Define Custom Colors* to generate a customised color. Click on OK to confirm the change.

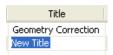
Figure 3.28. Colour Selection Panel



3.6.2.3. Title

By default, the title in the 1D plot uses the title of the data that put into the plot widget. So that you can control the title of the plot by changing the title of the data. To change the title, simply click on the current title of the data in the *Title* column, then type in a new text.

Figure 3.29. Change Title



3.6.2.4. Marker

You can change the marker shape of each curve in the plot. To change the marker shape, simply click on the drop down list in the *Marker* column and select one from the available marker shapes. Table 3.1, "Available Marker Shapes" shows the available marker shapes and their names.

Table 3.1. Available Marker Shapes

Name	Icon	Style
Line Only	-	
Diamond	*	* * * * *
Diagonal Cross	x	* * * * * * *
Regular Cross	+	+ + + + + +
Up Triangle	٨	* * * * * * *
Down Triangle	v	* * * * * *
Line Diamond	_*	* * * * *
Line Diagonal Cross	-x	* * * * * * *
Line Regular Cross	-+	+++++
Line Up Triangle	_^	+ + + + + +
Line Down Triangle	-v	+ + + + + +

3.6.2.5. Linked

To link the data with the algorithm means when the algorithm is processed again, new result data will overwrite the current data. This makes the plot updates automatically to the most recent result. By default this feature is enabled. To disable it, simply deselect the checkbox in the *Linked* column.

3.6.2.6. Metadata columns

The metadata columns show the plot data information.

- Reference column shows the ID of the algorithm that generates this plot.
- Data type column shows the type of the data, such as Pattern or PatternSet.

- Status column shows the status of the algorithm that generates this plot, for example, InProgress, Done or Error.
- *Timestamps* column shows the time stamp of this plot data generation.

3.7. 2D Plot Controls

The following features are about two-dimensional plots, e.g. Corrected Data plots (see Section 3.5.1, "Corrected Data")

3.7.1. Plot Window Control

The following features are supported by the two-dimensional window

3.7.1.1. Zoom

To zoom in certain region of the 2D plot, simply *push down the left mouse button and draw a rectilinear box* on that region.

To zoom out use the key combination, CTRL + Z to zoom out to the next zoom level.

To zoom out to the original level, use key combination, CTRL + SHIFT + Z or click on the button at the top left corner of the plot.

3.7.1.2. Pan

Pan is available if the plot has been zoomed. Push down the CTRL key, then drag the image to pan in any direction.

3.7.1.3. Show pixel properties

Moving your mouse cursor to a pixel on the plot will get the pixel properties shown in the status bar. It tells you the horizontal axis value, the vertical axis value and the intensity reading on that pixel. It also tells you the zoom level.

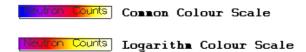
Figure 3.30. Pixel Properties

X:-35.45 Y:-55.03 Value:0 | Zoom X:150.36% Y:151.12%

3.7.1.4. Switch between linear and logarithmic colour scale

Using logarithm colour scale can help to reveal lower intensity pixels in the plot. By default, the plot will use the common colour scale. Click on the button to switch between common and logarithm colour scale. See Figure 3.31, "Linear and Logarithm Colour Scales" for the difference between common colour scale and logarithm colour scale.

Figure 3.31. Linear and Logarithm Colour Scales



3.7.1.5. Copy to clipboard

Click on the button to copy the current plot image into system clipboard. You can paste the image into common Windows imaging application such as *MSPaint* and *MSOffice* applications.

3.7.1.6. Save to image file

Click on the button to save the current plot to an image file in your file system. A *Save As* window will pop up for you to pick the folder and file name for the image file. It supports three image file formats: *BMP*, *JPEG* and *PNG*.

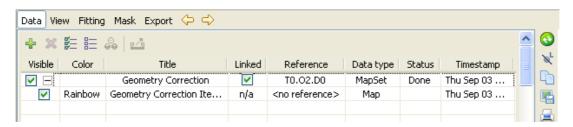
3.7.1.7. Print the plot

Click on the button to print the current plot. Two windows will pop up for you to setup the layout properties and to choose a printer.

3.7.2. Data

Click on the *Data* item in the plot menu bar, a *Data Control* will show up in the left side of the plot. For example, Figure 3.32, "Data Control" shows the block of the integration result plot.

Figure 3.32. Data Control



The following features are supported in the Data Control Block.

3.7.2.1. Visible

The first column of the *Data Control Block* is visibility control. Select or deselect the check box in that column to view or hide the data.

A two-dimensional data is called Map in Gumtree plotting space. Some time, the data fed to the plot can be a group of such two-dimensional data, which we call MapSet. By default, all Maps under the MapSet will show up in the visibility control area. Click on the button \Box to fold the MapSet so that it hides the Maps within it. Click it again to unfold it. Deselect the visibility checkbox of the MapSet will hide all Maps in it.

3.7.2.2. Color

Use the *Color* column to change the colour scale of the two-dimensional plot. By default, the colour scale picked is Rainbow colour scale. All the supported colour scales are shown in Figure 3.33, "Colour Scales".

Figure 3.33. Colour Scales



To change the colour scale, simply click on the current colour scale name in the *Color* column. A drop down list will show up as shown in Figure 3.34, "Select Colour Scale". Choose your selection to change the colour scale.

Figure 3.34. Select Colour Scale



3.7.2.3. Title

By default, the title in the 2D plot uses the title of the data that put into the plot widget. So that you can control the title of the plot by changing the title of the data. To change the title, simply click on the current title of the data in the *Title* column, then type in a new text.

Figure 3.35. Change Title



3.7.2.4. Linked

To link the data with the algorithm means when the algorithm is processed again, the new result data will overwrite the current data. This makes the plot update automatically to the most recent result. By default this feature is enabled. To disable it, simply deselect the checkbox in the *Linked* column.

3.7.2.5. Meta data columns

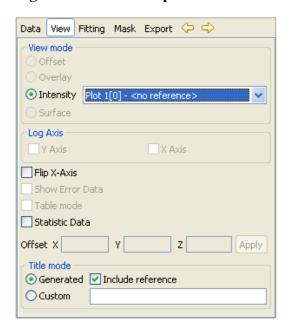
The metadata columns in the data control area shows the plot data information.

- Reference column shows the ID of the algorithm that generates this plot.
- Data type column shows the type of the data, such as Map or MapSet.
- Status column shows the status of the algorithm that generates this plot, for example, InProgress, Done or Error.
- *Timestamps* column shows the time stamp of this plot data gets generated.

3.7.3. View

Click on the *View* item in the plot menu bar will show up the View Properties Control, as shown in Figure 3.36, "View Properties Control".

Figure 3.36. View Properties Control



· View mode - Intensity

Use this to choose the Plot data. It is supported to put multiple plot data into the 2D plot widget. They can be in single *Map* data, or enclosed in *MapSet* data (for more information, please see Section 3.7.2, "Data"). All available 2D Maps are available in the Intensity drop down list as shown in the above figure. Click on the drop down list to choose a Map data to plot.

• Flip X-Axis

Use the checkbox of Flip X-Axis to flip the plot and axis horizontally.

· Statistic Data

Click on the *Statistic Data* checkbox to show statistic properties of the plot data. The statistic properties will show up in the right part of the plot in table mode.

• Title mode - Generated

By default it will use the title of the plot data as the plot title. You can choose the *Custom* radio button to overwrite the title. Simply type new text in the text box will change the title of the plot.

3.7.4. Fitting

Under construction

3.7.5. Mask

To enable of disable the Mask feature, use the *Mask Control*. Click on the *Mask* item in the plot menu bar. The Mask Control will show up as shown in Figure 3.37, "Mask Control".

Figure 3.37. Mask Control



By default the Mask feature is enabled. To disable this feature, click on the Mask enabled checkbox. If disabled, the Plot will not show any mask or ROI. The drop down list in the Mask Control provides options of which algorithm parameter will take the mask. To learn more information about how to use masks in an algorithm, please read Section 3.4.6, "Region of Interest and Masking Control".

3.7.6. Export

Use this menu to save data. See Section 3.5.4, "Save Scan Data"

3.7.7. Navigation Bar

If there are more than one dataset in the Plot, you can use the navigation buttons in the Plot menu bar to jump forwards or backwards in the sequence. If there is only one dataset, this feature is disabled.