Mantid 4 μ^+

Quick Start Guide for Muon Data Processing

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Introduction

The Mantid project provides a framework that supports high-performance computing and visualization of scientific data.

Mantid has been created to manipulate and analyze Neutron and Muon data, but could be applied to many other techniques. The framework is open source and supported on multiple target platforms (Windows, Linux, Mac).

Tailor made data reduction and analysis procedures can be formulated using Python scripting. However, this document focuses on the reduction and analysis of muon data collected from any of the ISIS muon spectrometers via a Graphical User Interface (GUI). This interface has been specifically designed to guide the Muon user through the data reduction and analysis procedure.

Mantid can be downloaded from,

http://download.mantidproject.org/

For reliability choose the 'Latest Stable Build'; however, as the interface is developing rapidly, the 'Nightly Development Build' may contain additional features and bug fixes that are useful for data analysis.

The accompanying Wiki,

http://www.mantidproject.org/Main_Page

contains a wealth of information and supplementary information regarding the Mantid project and its functionality.

It is assumed that the reader has a basic understanding of the muon technique and experimental setup.

This manual has been written using **Mantid Version 3.1.0**

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Getting Started

To launch the Muon Analysis GUI follow:

Interfaces > Muon > Muon Analysis

on the tool bar at the top of the main MantidPlot window.

The window shown in Fig. 1 should appear. A tab-driven approach guides the user through the standard data reduction and analysis procedure. The functionality contained within each tab (Home, Grouping Options, Settings, Data Analysis, Results Table) is discussed in turn.

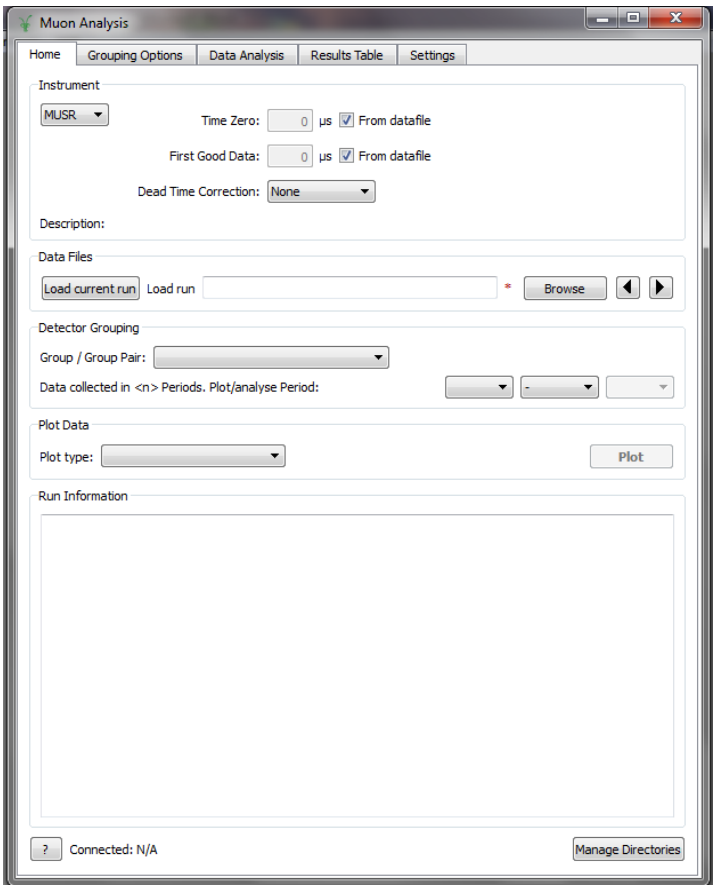

Fig. 1 The Muon Analysis GUI

You should ensure that Mantid is configured for your needs. In particular you should:

a) Select the default facility and instrument (this will be an option during installation)

b) Enable QtiPlot fitting to allow data sets to be analysed with Origin specific fitting tool. See Other Mantid Functions

c) Add paths to directories which contain your data. To do this, click on Manage Directories (see Fig. 1(a)). The following window (Fig. 1(b)) will appear. As an example, in the window below the directory \\britannic\MuonTrainingCourse\referencematerial\copper\Data has been added as a path by a) typing the directory name in the field below Data Search Directories and then b) clicking Add Directory. Once a path has been added, data stored in that location can be accessed simply by referencing the run number.

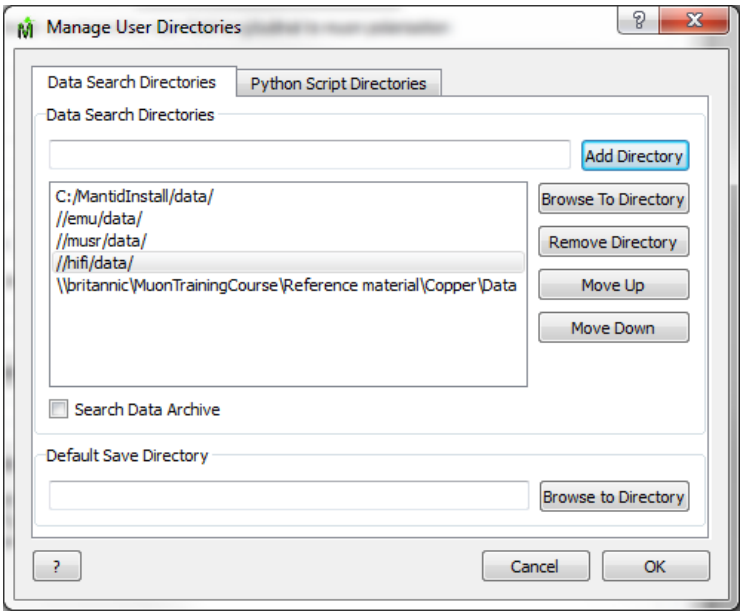

Fig. 1(b) The Manage User Directories GUI

The Tabs

I. Home

When launched, the Muon Analysis GUI defaults to the Home tab. This tab allows:

1. data files to be loaded
2. run information to be viewed
3. detector groupings to be selected
4. type of plot to be selected

To load a file either: Browse or Load Current Run or simply type a run number (assuming you have defined the directory(ies) in which your files are stored)

When typing a run number, or using the Load Current Run option, first select the desired instrument from the dropdown list. Regardless of the data input method, the Time Zero (μs) and First Good Data values are automatically updated. These values will have been determined by the instrument scientist during instrument calibration periods and are stored in the header block of the NeXus format raw data files that are saved once a measurement is finished. Once a data file has been successfully read, a new plot window will appear (e.g. Fig. 2)

NB: when browsing for files you can select multiple files or a string like "00015190-00015191". The counts (and number of frames) in the selected files will be added.

Plot options (such as symbol type, lines, binning etc) can be found under the Settings tab.

The default plot option is to display asymmetry i.e. the ratio of positron counts collected in the Forward (F) and Backward (B) detector arrays according to,

$$P_z(t) = A_o G_z(t) = \frac{F(t) - \alpha B(t)}{F(t) + \alpha B(t)} \qquad (1)$$

However, data collected only in the Forward, or Backward, detector banks can be viewed alone by adjusting the Group/Group Pair option. In addition, should data have been

collected using differed timing periods, as one would for example during an RF experiment, the data collected during each separate time period can also be viewed separately (again for either the Forward and Backward detector arrays) by adjusting the period number.

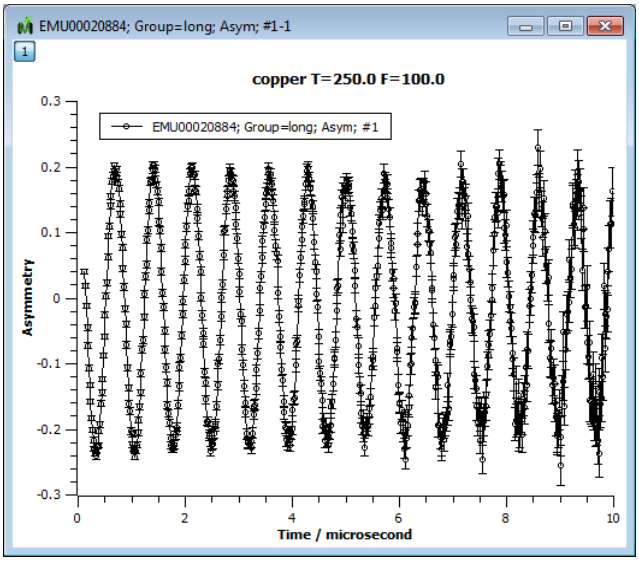

Fig. 2 The plot window. Launched when a data file is loaded

When plotting data according to (1) the default alpha (α) value is 1. An accurate alpha value can be determined using the Guess Alpha option found under the Grouping Options tab. Finally, the manner in which the raw data is presented can be adjusted using Plot Type. Asymmetry is the default option. However, both linear and log (y-axis) raw counts-per-microsecond plots can be generated.

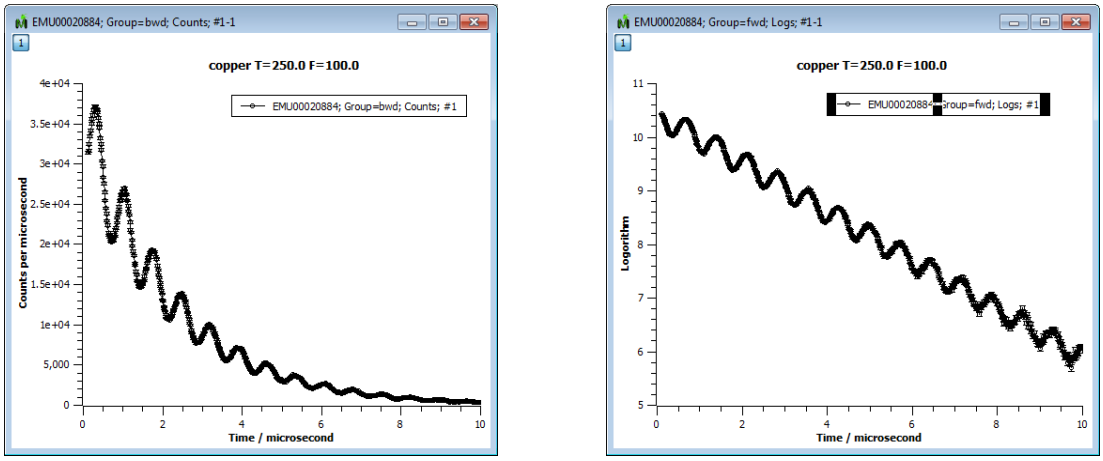

Fig. 3 Linear and log (y-axis) raw counts-per-microsecond plots

Summary

Input Field	*Description*
Instrument	Select the instrument on which the experiment is being / was run
Time Zero (μs)	Time Zero in units of micro-seconds (read from the NeXus data file)
First Good Data (μs)	First Good Data in units of micro-seconds (read from the NeXus data file)
Load current run	Load current run for the instrument specified in Instrument
Load run	Specify a run number or data file by typing a run number or use the Browse button to select
Arrow Buttons	Clicking these buttons will open the next (or previous) run in a series of runs
Group / Group Pair	Lists valid groups and group-pairs as defined in the Grouping Options tab
Periods	For single period data only the 1st Plot/Analyse Period drop down box is active. For multi period data all the drop boxes are enabled. Use these additional fields to plot the difference (or sum) between two timing periods
Plot type	Select the type of plot
Run Information	Information about the loaded measurement is printed to the screen
Manage Directories	Define location(s) of data files

II. Grouping Options

The Grouping Options tab allows:

- grouping files to be loaded, saved, modified or cleared
- regrouped data to be plotted
- alpha values to be determined from T20 measurements
- raw data plotting options to be selected

The Grouping Options options are shown below

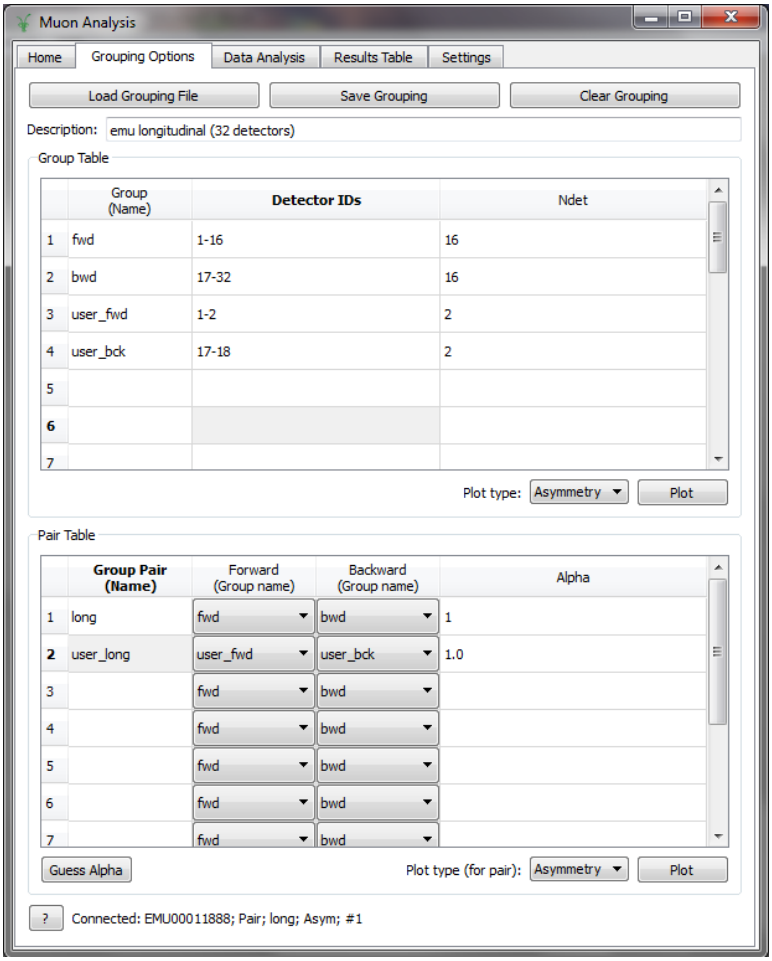

Fig. 4 The Grouping Options window

Standard detector groupings are usually loaded when a data file is opened. For example, for the EMu spectrometer detectors 1 – 48 and 49 - 96 are automatically assigned to the forward and backward detector arrays respectively and labelled fwd and bck. However, different detector grouping configurations can be entered manually in the Group Table input fields. To enter a new value click on the desired input field to activate. Such user specific configurations can be saved and/or re-loaded.

In Fig. 4 the user has also chosen a detector grouping which allows him/her to look at counts collected in Forward detectors 1-2 and Backward detectors 17-18 alone; as well as defining the standard EMu detector configuration. The user has assigned the names user_fwd and user_bck to these specific forward and backward detector groupings and coupled them using a Group Pair label user_long

Once defined, these new user grouping options propagate through the Muon Analysis tabs. For example, in the Home tab, the options under Group/Group Pair are automatically updated to include user defined detector configurations.

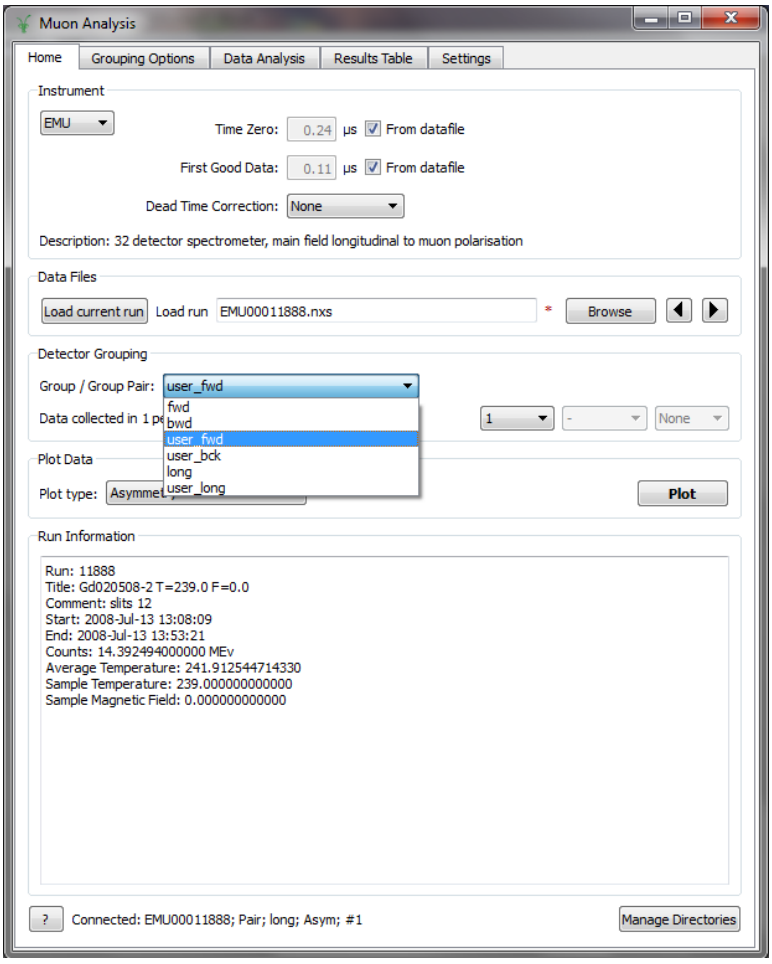

Fig. 5 The Home tab window with updated detector Grouping Options

Finally, alpha can be determined for any given detector pairing (via the analysis of transverse field data) by clicking on Guess Alpha. Click on a specific Group Pair name to select it. The alpha value column is automatically updated. The value in the column is applied to all subsequent data reduction when asymmetry plots are desired.

Summary

Input Field	*Description*
Load Grouping File	Opens a file browser window. Use it to select a grouping file
Save Grouping	Opens a file browser window. Use it to save a grouping file
Clear Grouping	Clears group and pair tables
Group Table	Specifies a grouping. For a valid grouping a unique name must be provided and also a valid Detector ID string. Examples of valid detector ID strings includes: "1,2-5,7-9,11" which specify spectra 1,2,3,4,5,7,8,9 and 11
Plot (below Group Table)	Plots the group highlighted most recently in the group table. The type of plot can be selected
Pair Table	Specifies pairings of groups. A valid pair needs a unique pair name and associated alpha value
Plot (below Pair Table)	Plots the pair highlighted most recently in the pair table. The type of plot can be selected
Guess Alpha	Guess a new value for alpha for Group Pair highlighted / selected

III. Settings

The Settings tab allows the user to:

- modify plot styles (lines, symbols etc)
- change the time (x-axis properties) and y-axis scales
- re-bin the data for clarity
- adjust whether new plots are created or old plots are overwritten

The Settings options are shown below

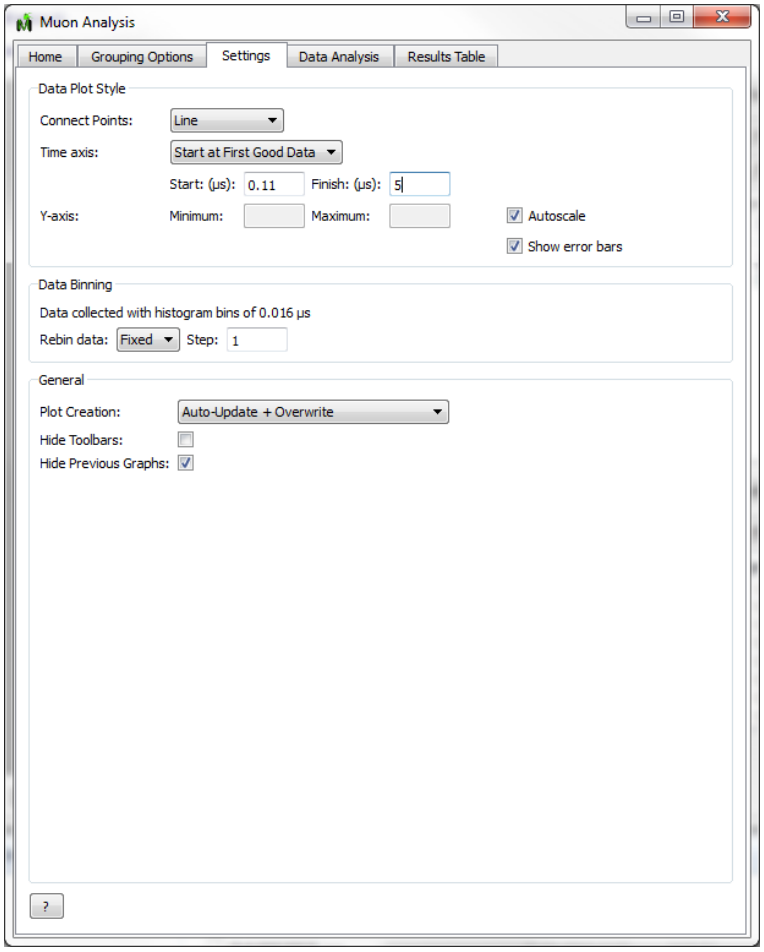

Fig. 6 The Settings tab window

General plotting styles can be modified using the Data Plot Style options. Plot options include Line plots, Symbol plots or both. Data can also be re-binned and the time and y-axis adjusted.

NB: when values are entered manually (for example the upper time limit in the Time Axis option) the entry needs to be followed by a carriage return for the value to be accepted.

It is suggested that the user selects Auto-Update + Overwrite when performing data reduction and analysis. This option stops MantidPlot creating a new plot window every time a modification is made to the plot style. Should a new data file be loaded, however, the existing window will not be overwritten. Instead, a new plot window will be opened.

NB: if a new data file is loaded then subsequent changes to the Settings options will apply to the newly created plot window.

There is also an option to Hide Previous Graphs that ensures only the graph for the current data file is displayed

MantidPlot toolbar options (which are mostly redundant when using the Muon Analysis GUI) can be hidden by selecting Hide Toolbars

As an example, raw data and re-binned data is shown below.

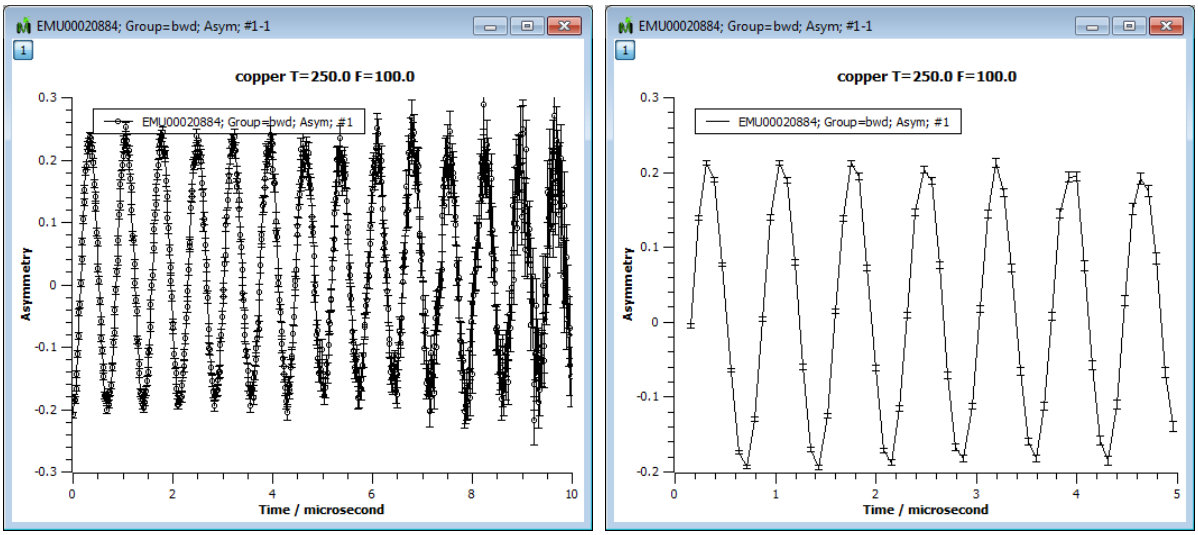

Fig. 7 Raw and re-binned data set

Summary

Input Field	*Description*
Connect Points	Dropbox with the options; line, line & symbol and scatter. These will change how the data looks once plotted
Time axis	Plots the data from t = 0 or from the first good bin
Start (µs)	Plots the data from this user defined start value. This box is greyed out if the time axis is set to "Start at Time Zero"
Finish (µs)	Plots the data until this user defined end value
Y-axis (Autoscale)	Uncheck Auto-scale to specify y-axis min and max limits
Minimum	Defines the lower plot limit on the y-axis. Greyed out if Auto scale is checked
Maximum	Defines the upper plot limit on the y-axis. Greyed out if Auto scale is checked
Show Error Bars	Show error bars on the plot if the tick-box is selected
Rebin Data	Default is None. If Fixed is selected then the Rebin Data step size input field is activated. The step size defines how many time bins the data is rebinned over
Plot Creation	Dropbox with the options; overwrite, auto-update, overwrite + auto-update & none
Hide Toolbars	Hides the MantidPlot toolbars. Useful on small screens
Hide Previous Graphs	Ensures only the graph for the current data file is displayed

IV. Data Analysis

The Data Analysis tab allows the user to:

- select functions to fit to the data
- change fit ranges and parameters
- fit data

The Data Analysis tab options are shown below

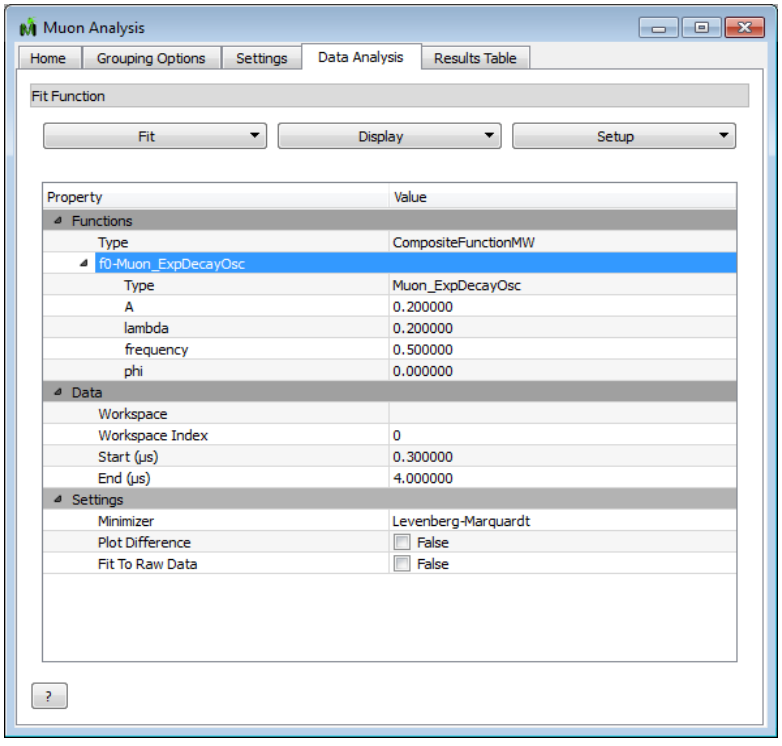

Fig. 8 The Data Analysis tab window

MantidPlot comes with a number of pre-complied fitting functions. Further functions may be compiled and installed or, alternatively, user specific functions can be defined within the fitter. A number of fit functions have been programmed which are specific to the analysis of muon spectra.

The muon specific functions are:

ExpDecOsc	$f(t) = A\exp(-\lambda t)\cos(\omega t + \phi)$
GauOsc	$f(t) = A\exp(-(\sigma t)^2/2)\cos(\omega t + \phi)$
Abragam	$f(t) = A\exp(-(\sigma\tau_c)^2(\exp(-t/\tau_c) - 1 + t/\tau_c))\cos(\omega t + \phi)$
StaticKuboToyabe	$f(t) = A(\exp(-(\sigma t)^2/2)((1-(\sigma t)^2)(2/3) + 1/3)$
StrexpExpo	$f(t) = A\exp(-(\lambda t)^\beta)$
GausDec	$f(t) = A\exp(-(\sigma t)^2)$
ExpDecMuon	$f(t) = A\exp(-\lambda t)$
MuonFInteraction	Implements equation (3) in reference *Brewer et al, Physical Review B 33(11) 7813-7816* to model the muon response under the formation of the FμF species
DynamicKuboToyabe	Fitting for the parameters A, σ and ν (the initial asymmetry, relaxation rate and hop rate, respectively) using numerical integration techniques

For the functions above:

λ and σ are in μs^{-1}

ϕ is in radians

ω is in MHz (note $\gamma_\mu = 0.013$ MHz/Gauss)

τ is in μs

Δ is in MHz

β is unit-less

To select a function right click on Functions (in the Property column) and select Add Function. Select Muon in list of function types that appear and the following options will appear

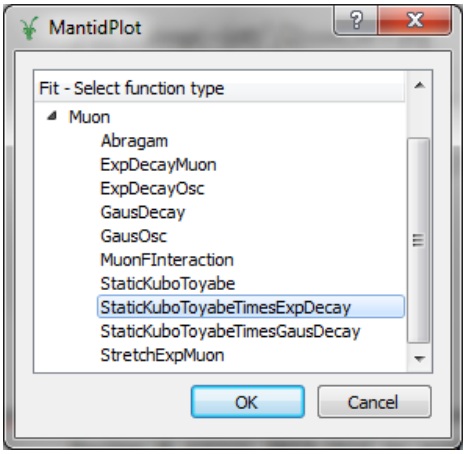

Fig. 9 Specific muon fit functions

To remove the function, right click on the function name and select Remove

Once the function has been selected it will appear in the Property column below Type. To examine a function's fit parameters, click on the small arrow beside the function name to expand the entry.

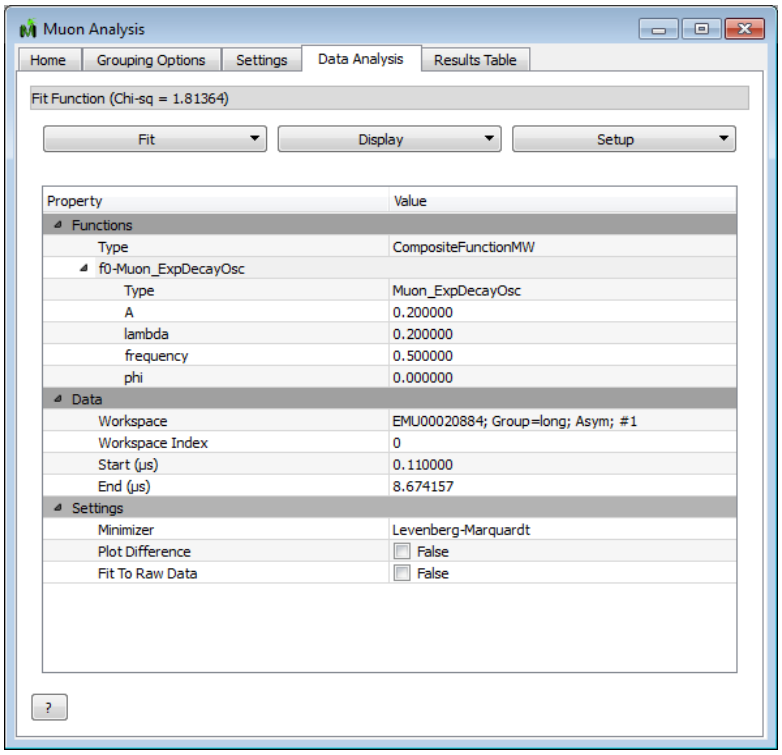

Fig. 10 Fit function parameters

Each fit function parameter can be adjusted manually. Click on the value shown to activate the input field and adjust

Once a fit function has been selected the plot window is modified, as shown below in Fig. 11. Default x-axis (time) limits for the fit are shown by two vertical blue lines. The user can adjust these limits by either i) clicking on the limit values shown in the Data Analysis window (under Data) and entering new values manually or ii) by using the mouse to independently slide each blue line to the required start and end position. Moving these fit limit lines automatically changes the limit values written beside Start (us) and End (us).

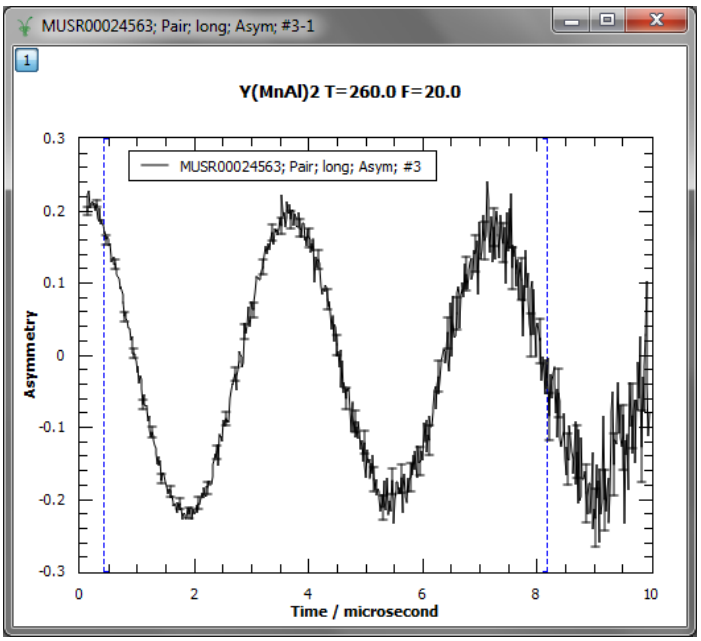

Fig. 11 Fit limit markers (blue)

Once the user is happy with the initial fit parameters, clicking Fit > Fit will fit the chosen function to the data. The fit parameters will be updated. If several data sets have been loaded, the user can choose which one to fit by clicking on the filename beside Workspace (under Data) and scroll through a drop down list of available datasets (Fig. 13). More information about workspaces can be found in the section Other Mantid Functions

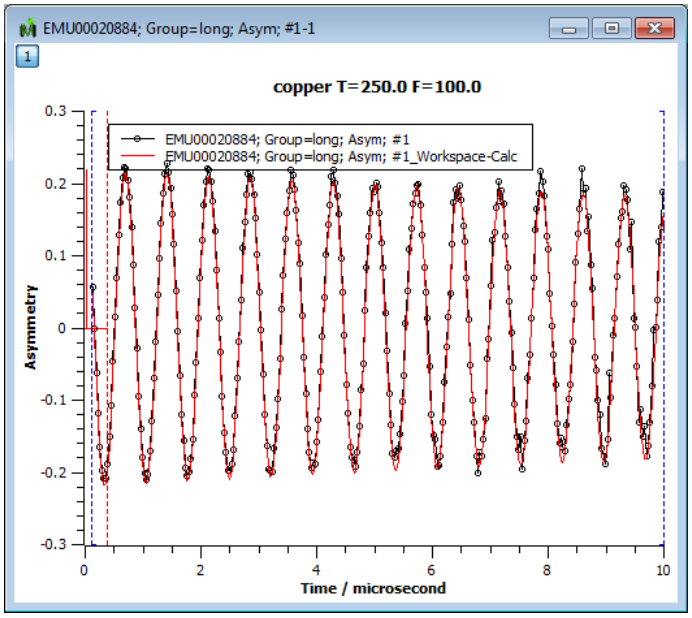

Fig. 12 The result of fitting function 'Muon_ExpDecayOsc' to EMU0020884

NB: when scrolling through a list of data sets to fit, select the entry with same name as that shown at the top of the data plot window. For example, to fit the data shown in Fig.12 one would select 'EMU00020884; Group=long; Asym; #1'

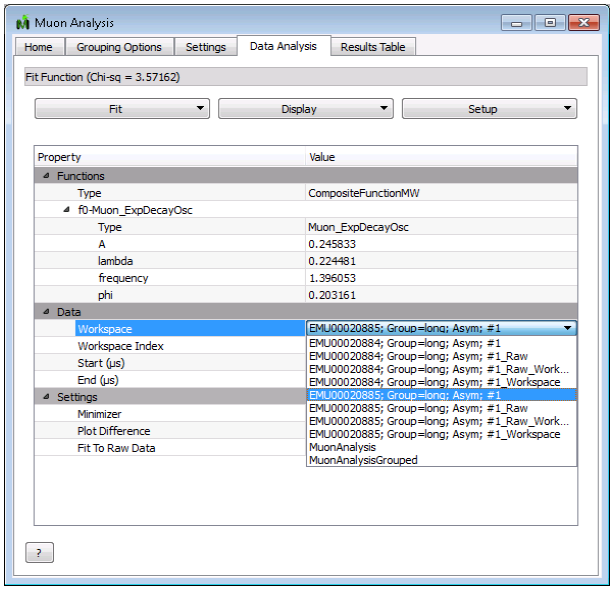

Fig. 13 The list of available data sets for analysis

Each fit parameter can be bound by certain fit limits (+/- 10% of its starting value, +/- 50% or a custom value), fixed at a specific user determined value or parameters can be tied together using some functional form.

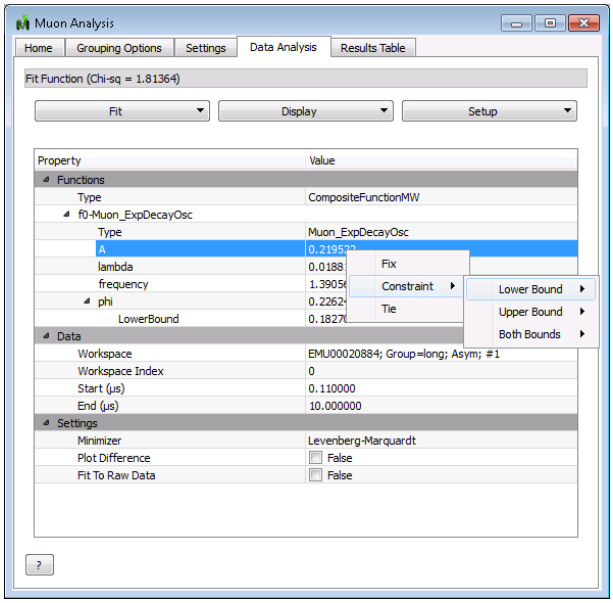

Fig. 14 Constraining fit parameters

To apply constrains, right click on the parameter of interest. The options shown in Fig. 14 will appear.

Functions with multiple components can be defined. These components can be combined through addition or multiplication

Addition

To create a fit function in which the various components are added i.e. $Gz(t) = A_1\exp(-\lambda_1 t) + A_2\exp(-\lambda_2 t)$ simply add additional components as described above. For example, Fig 15 shows the result of fitting a static Kubo-Toyabe function plus a simple exponential to the data.

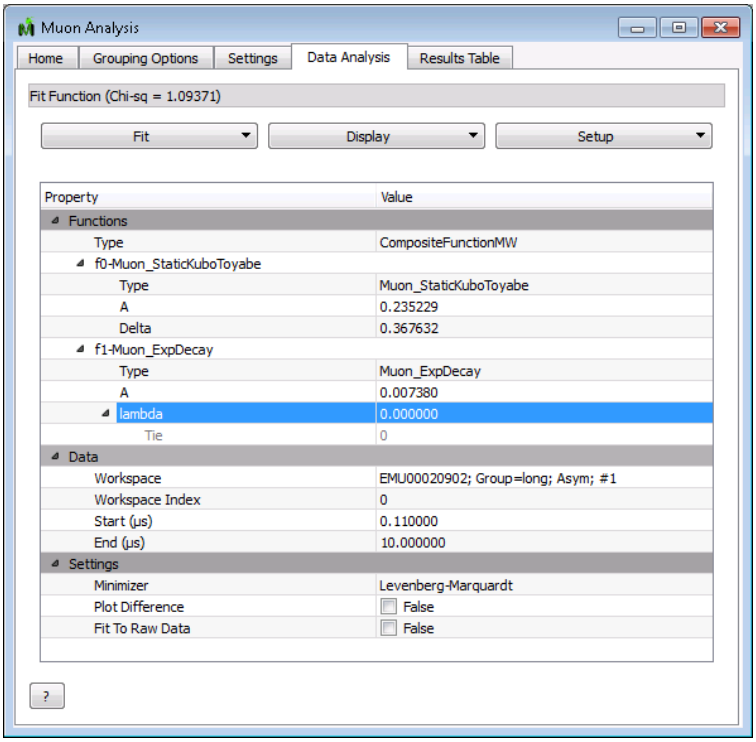

Fig. 15(a) Adding functions. The result of fitting a static Kubo-Toyabe function plus a simple exponential

Multiplication

To create a fit function in which the various components are multiplied i.e. $Gz(t) = A_1\exp(-\lambda_1 t) \times A_2\exp(-\lambda_2 t)$ first right click on Functions > Add Function and select ExpDecMuon. Expand the function so that all parameters are visible and click on ExpDecMuon in the Value column alongside Type (as shown below). From the dropdown list select ProductFunction

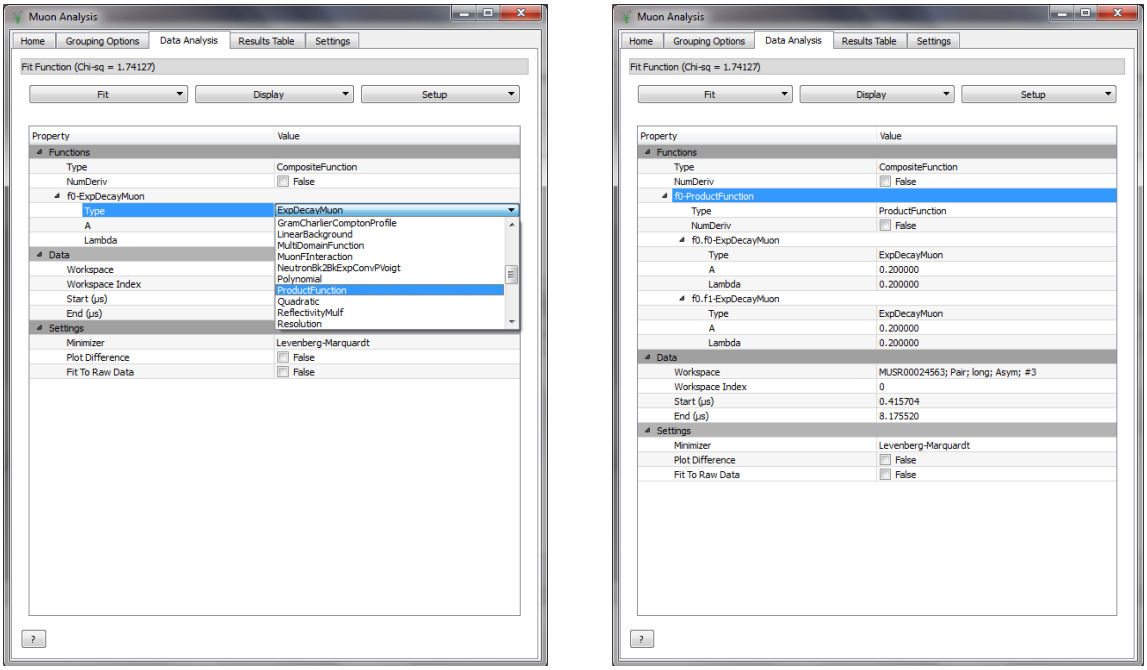

Fig. 15(b,c) Selecting ProductFunction option for multiplication and building a function

Now build the required product function by selecting the individual function components to be multiplied. As shown in Fig 15(c), to add components right click on f0-ProductFunction and select Add Function to build the required model. *NB: FIt functions with both additive and multiplicative components can be created. For example in Fig. 15(b), $G_z(t)$ = (GausOsc x ExpDecay) + Lorentzian*

Finally, sequential fitting of one function to many runs can be performed by selecting Fit > Sequential Fit. The following GUI appears:

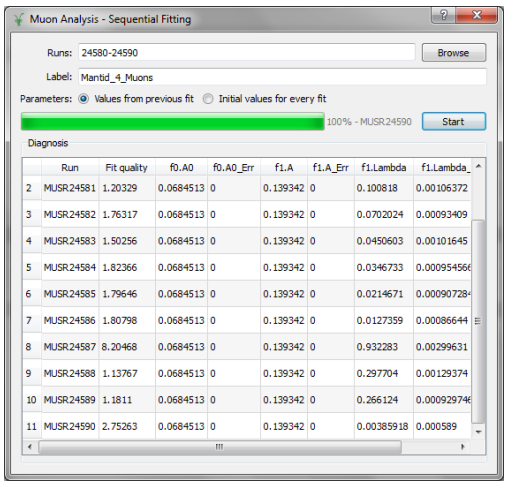

Fig. 16 The Sequential Fit GUI

Either browse for the run numbers to fit or type the sequence into the Runs field i.e. 25480-25490. In the Label field enter the name of the workspace to be written out into the Workspace pane and that contains all the fitting data. Click Start - the green bar indicates progress

Summary

Input Field	*Description*
Fit	Allows the user to Fit the data or undo a fit
Display	Allows the user to plot a guess based on the function(s) loaded. This option can also be used to clear fit curves
Setup	Complex fit descriptions can be saved and restored. Alternitively, all function information can be cleared. An option to search for peak is also available if appropriate
Functions	Lets the user select the function(s) with which to fit the active data set. Parameters can be adjusted or constrained as described. Complex functions can be saved or re-loaded
Data	Allows fit limits to be set. Allows the user to choose which data set to fit
Settings	Allows the user to choose which minimisation algorithm the fitting process uses. The default minimiser is the Levenberg–Marquardt algorithm. Difference plots can be requested (i.e. data minus fit) and the fit can be applied to the raw data rather than any re-binned data shown in the plot window

V. Results Table

The Results Table tab allows the user to:

- create a result(s) table from either individual files or sequential fit data
- select which instrument log values (temp, field etc) to write out alongside the fit parameters
- choose to write out fit information from one or several data files

The Results Table tab options are shown below:

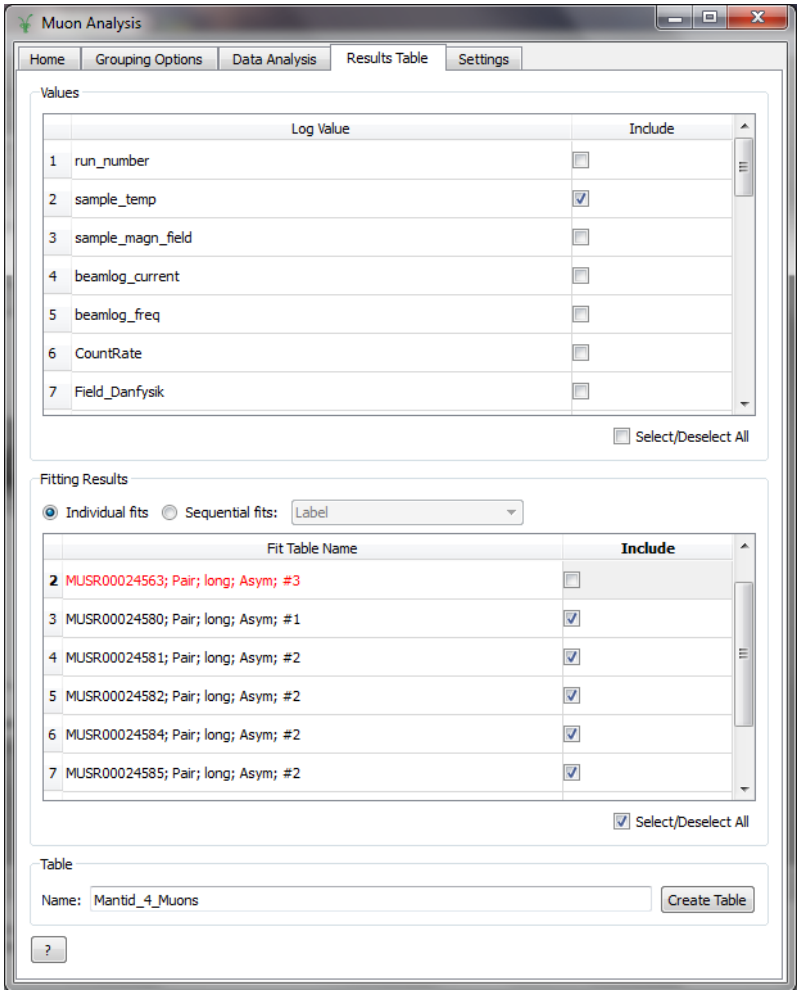

Fig. 17 The Results Table tab options

In Fig. 17 the user has chosen to create a results table which contains i) the parameters generated after fitting data files 24580 to 24585 INDIVIDUALLY and ii) the sample temperature associated with each of these data sets. The user has decided to call this particular result table 'Mantid_4_Muons' and created it by clicking Create Table.

The different coloured 'text' delineates between runs that have different fit parameters. For example, in Fig 17 all the workspaces represented by black text were fitted using an exponential decay function and a flat background. The entry in red was fitted using an oscillating exponential decay function.

The resulting results table, 'Mantid_4_Muons', appears in the list of Workspaces.

The results from sequential fitting can be exported in a similar fashion. Select Sequential Fits, check all the fit files that are to be written out, as well as the required experiment parameter(s). Enter a name for the resulting Results Table workspace and click on Create Table

The data contained in any Results Table workspace can be viewed by right-clicking on the workspace name, i.e. 'Mantid_4_Muons' and selecting Show Data.

The different columns contained in a results table can be plotted by first:

i) selecting the x,y (and maybe error) columns of interest (hold down Ctrl and click on the columns required)

ii) Once all the columns have been selected, right click and select 'Plot'. A new plot window will appear

Results table data may be analyzed using the QtiPlot fitting interface included in Mantid (see Other Mantid Functions)

Summary

Input Field	*Description*
Log Values Table	Allows the user to select which instrument log values to include in the results table
Select/Deselect All	If checked then all the log values are included in the results table. If unchecked then no log values are written but, instead, specific log values can be selected by the user
Fitting Results Table	A group listing all the runs / data files for which fit parameters exist
Select/Deselect All	If checked then the fit results from all the runs listed are selected and written to the results table
Name	A user defined name for the results table
Create Table	Creates a results table which contains fit results and log values from all the ‘checked’ options

Other Mantid Functions

This section explains:

- the concept of workspaces
- how to use QtiPlot fitting
- how to export data
- how to overlay data

I. Workspaces

Workspaces hold the data in Mantid. They come in several forms, but the most common is the Matrix Workspace which represents XYE data for one or more spectra. In MantidPlot the data contained in a workspace can viewed as a matrix or a table, and graphed in many ways including Line graphs, contour plots and 3D graphs.

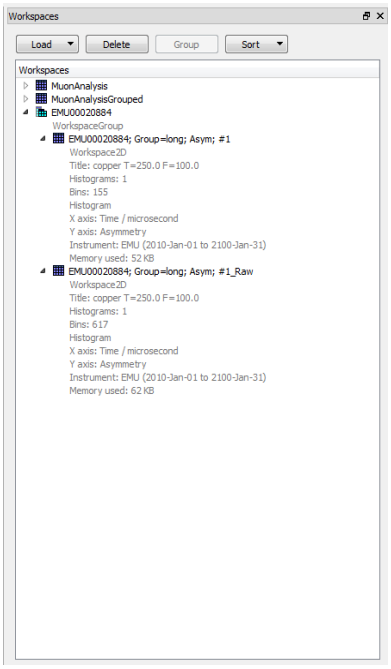

Fig. 18 The workspace list window

Interaction with workspaces is typically through an interface. Matrix Workspaces are typically created by executing one of Mantid's 'Load' algorithms or are the output of algorithms which take a Matrix Workspace as input.

In addition to data, workspaces hold a workspace history, which details the algorithms which have been run on this workspace.

When a muon data set is loaded, the three Matrix Workspaces listed in Fig. 18 (in this case for EMU data file 20884) are created automatically. The workspace list pane is found on the right-hand side of the main MantidPlot window.

Workspace: MuonAnalysis

The workspace, MuonAnalysis, holds within it raw positron counts / μs for each individual detector. To examine the data collected in a single detector, right click on workspace MuonAnalysis and select Plot Spectrum. The following input fields appear.

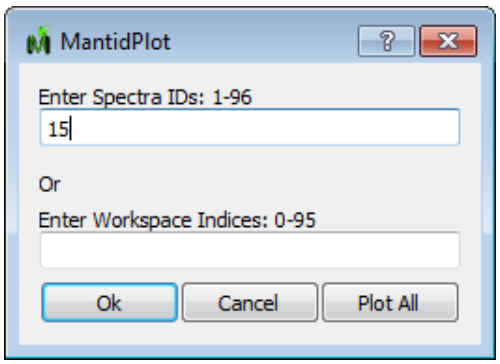

Fig. 19 Raw data plotting options

On EMU there are 96 detectors hence ID numbers: 1-96. Enter a detector (ID) number and click OK to plot the associated raw data. The raw counts / μs for detector 15 is shown below.

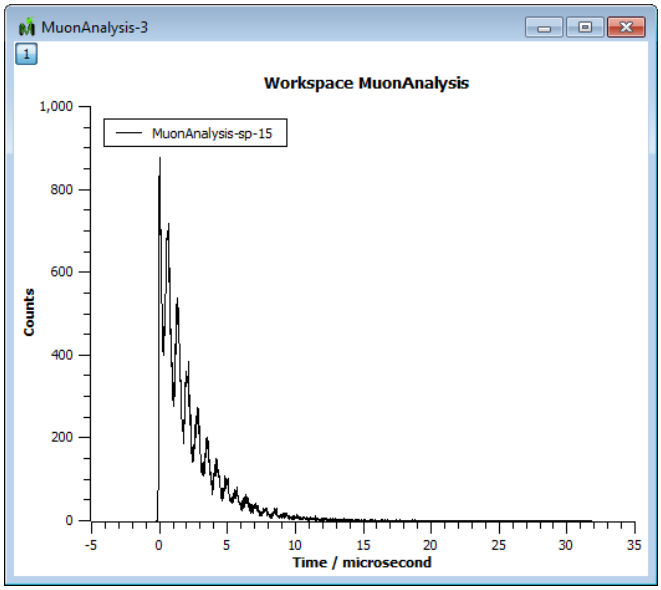

Fig. 20 Raw data (counts / μs) collected in EMU detector 15

NB: Clicking on the small arrows beside the workspace name expands the entry and allows the user to see specific workspace information.

Workspace: MuonAnalysisGrouped

Unlike MuonAnalysis, MuonAnalysisGrouped contains data in raw counts / μs but collated as specified under the Grouping Options tab. For the example given above, we find that workspace MuonAnalysisGrouped contains only 2 spectra. This is because Mantid has been instructed to process the raw data such that all the counts in Forward detectors (1-48) are summed. Similarly, all the raw data collected in each of the Backward detectors (49-96) has been added.

Workspace: INST_Run_Number

This work space contains two sub workspaces with the naming convention,

INST_Run_Number; Group = Name; Asym; #1_RAW and INST_Run_Number; Group = Name; Asym; #1

where INST is the instrument name, Run_Number is the run number, Group is the name of the Forward and Backward detector grouping label as defined under the Grouping Options tab. Workspaces with an extension _RAW contain RAW (i.e. non-binned) data.

For example, in Fig. 18 we see that workspace EMU00020884 contains EMU00020884; Group=long; Asym; #1 (155 bins) and EMU00020884; Group=long; Asym; #1_RAW (617 bins). The difference in bin numbers is a result of the User re-binning the data as defined under the Setting tab.

In general the muon analysis GUI hides workspaces from the user; however, an understanding of their functionality is sometimes useful to take advantage of some of the more advanced features of MantidPlot. In particular, for those seeking to develop a specialist analysis method, the GUI can be used for the initial data reduction with user coded Python or C++ algorithms acting on workspaces to process the final result. This type of hybrid workflow demonstrates the versatility of the MantidPlot interface.

Other types of object, such as Tables, Matrices and Notes, may be created through the MantidPlot interface. As these are not workspaces the Algorithms can't directly be applied. However, Tables may be converted the either a Table or Matrix workspace through an option on the analysis menu for subsequent data processing. For instance, converting the Results Table to a matrix workspace enables MantidPlot fitting the be carried out (however, see section III below for an alternative method of analysing results using the QtiPlot fitting).

II. Exporting Data

To export the data contained within any listed workspace click on the Algorithms tab at the bottom of the workspace list pane. The options shown in Fig. 21(a) should appear. Select SaveAscii from the dropdown menu (beside Execute) and click Execute.

The SaveAscii Input Dialog box should appear (Fig. 21(b)). Select a directory (for the written data file) and specify a file name. The workspace to be exported can be selected from the dropdown list next to InputWorkspace. The user can also, for example, define which workspace Indices (Min and Max) to export, choose the type of data separator used in the file, add comments and decide whether to WriteXError.

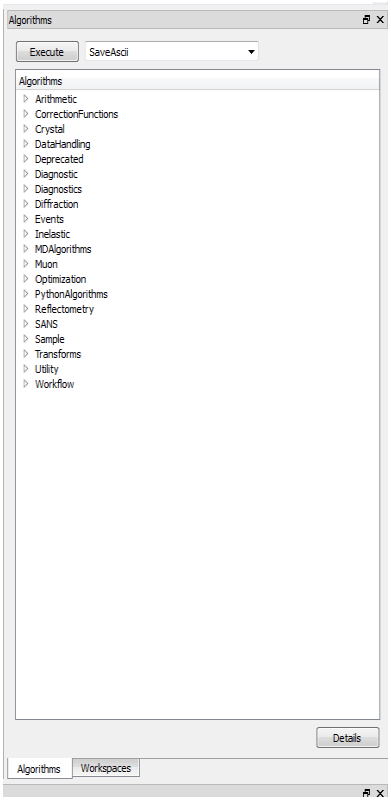

Fig. 21(a) The Algorithms options

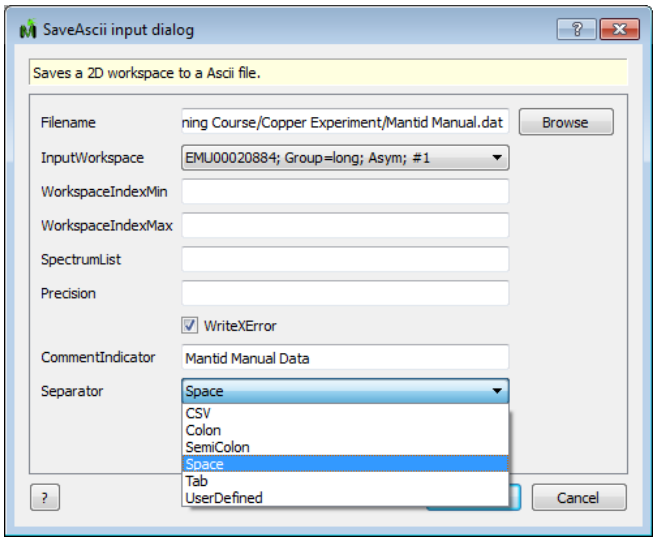

Fig. 21(b) The SaveAscii dialog box

III. QtiPlot

Enabling QtiPlot allows data sets and workspaces to be analysed using a suite of inbuilt Origin fitting algorithms. To enable QtiPlot follow View > Preferences > Fitting. The following window should appear. Select Enable QtiPlot Fitting

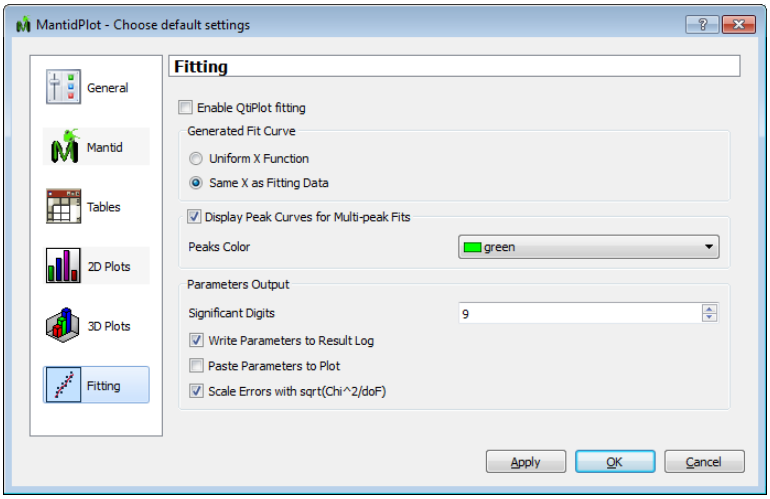

Fig. 22 The Choose Default Settings window

When QtiPlot fitting has been enabled, and a data file has been loaded, Analysis appears in the list of options above the main MantidPlot window toolbar.

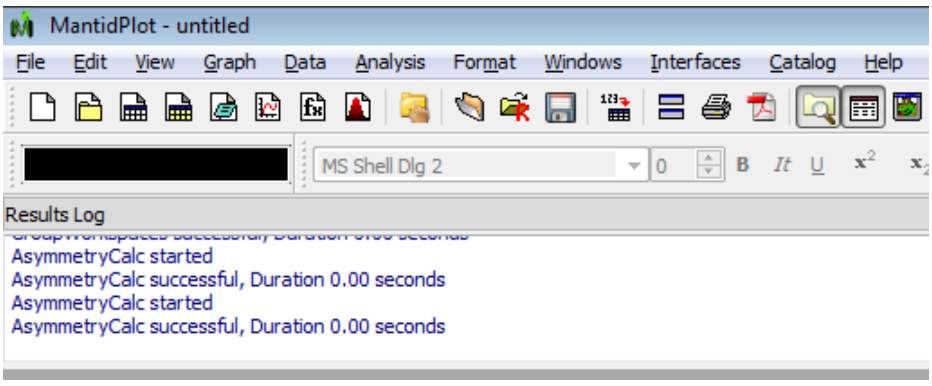

Fig. 23 Tool bar options at the top of MantidPlot. Analysis appears when QtiPlot is enabled

The fitting options found under Analysis are shown below

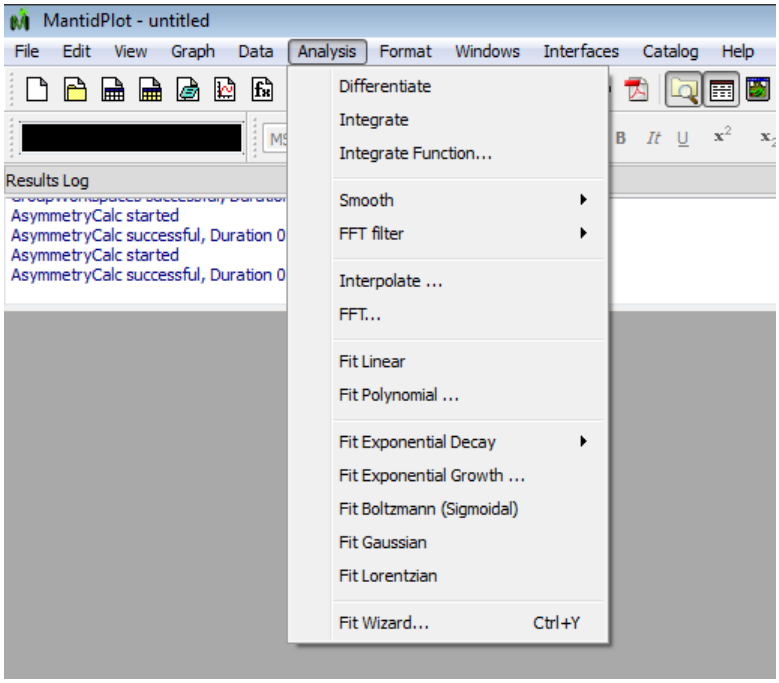

Fig. 24 The QtiPlot analysis options

IV Overlaying Data

To overlay data, select the plot window in which you wish to compare data. Right click on the plot window and select Add/Remove Curve. A list of available data sets will appear. As an example, in Fig. 25 we have the option of adding the data contained in the workspace EMU00020886; Group=long; Asym; #1 to the plot window of EMU00020897; Group=long; Asym; #1. To do so, first select EMU00020886; Group=long; Asym; #1 in the left hand pane and then click the 'right' pointing arrow. Reversing this process removes data from a plot window.

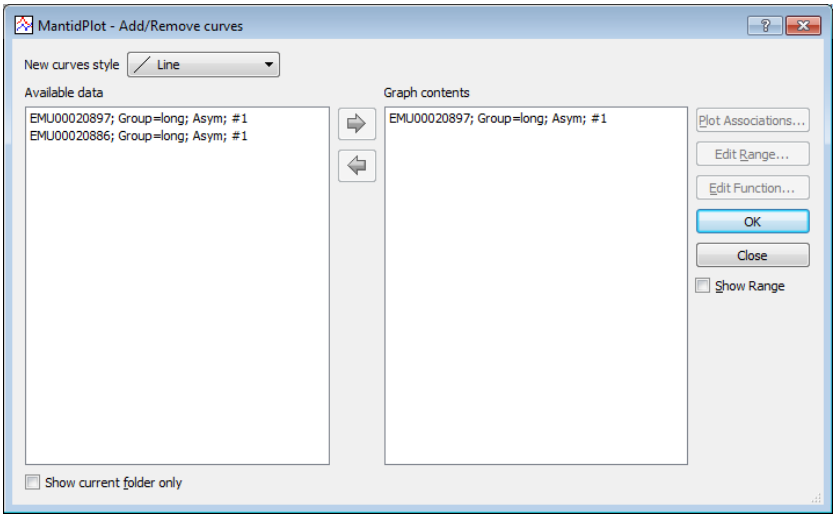

Fig. 25 Add / Remove Curves options window

The result is shown below (Fig. 26). The plot style (line, scatter, line+scatter etc) of the added data set can be selected using the New Curves Style drop down menu at the top of the Add/Remove Curve window (Fig. 25).

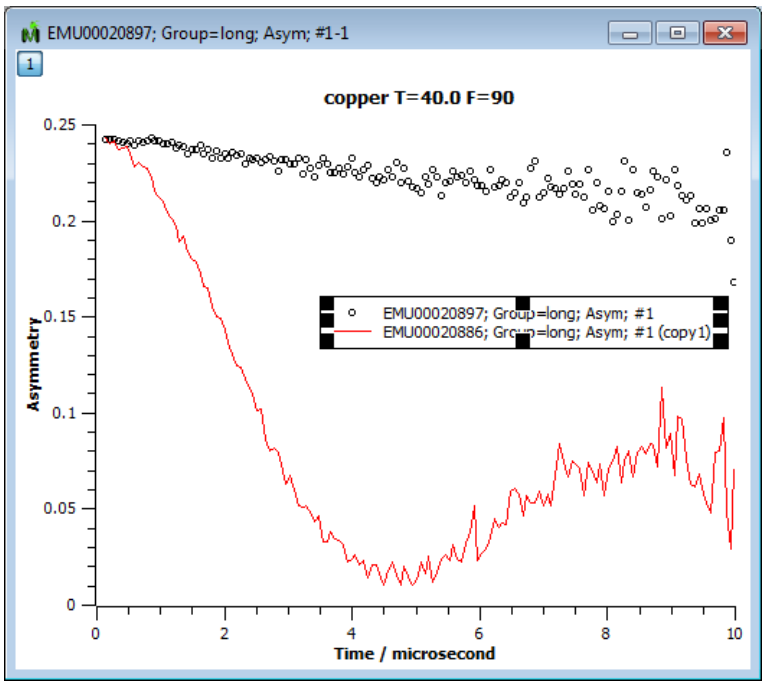

Fig. 26 The result of adding EMU00020886; Group=long; Asym; #1 to the plot window of EMU00020897; Group=long; Asym; #1

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